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# THE CRYSTAL BALL INSTRUCTION MANUAL

## VOLUME TWO:
## FOUNDATIONS FOR DATA SCIENCE

version 1.1

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# The Crystal Ball Instruction Manual

Volume Two: Foundations for Data Science

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The LaTeXsource for this book is available from: https://github.com/rockladyeagles/crystal-ball-2.

# Contents

# Chapter 1

# Intermission and review

Welcome to Volume Two of the Crystal Ball series: *Foundations for Data Science*! I titled the first volume "*Introduction to Data Science*" because it led you through a dip-your-toes-in-the-water experience. You took a brief tour through the various elements in this diverse field and got a feel for what it was all about.

Since you're still reading, this means you're still interested, and ready to explore the next level. In *Foundations*, we'll solidify your growing knowledge so that you have a firm base on which to build everything else. Future volumes in this series will cover applications, advanced techniques, and some special data types that require special treatment. But it all ultimately rests on the skill set you'll have built in Volumes One and Two of this series.

We're going to dive right in. But first, let me make a list of some of the things I'm counting on you being pretty solid on:

- Atomic and aggregate variables
  - `int`s, `float`s, `string`s
  - NumPy `array`s, Pandas `Series`es, `DataFrame`s
  - What all these look like in memory
- Scales of measure (especially categorical vs. numeric)
- Assocation vs. causality
  - Causal diagrams
  - Dependent and independent variables
  - Observational studies vs. controlled experiments
  - Confounding factors

- Statistical significance
- Exploratory Data Analysis
  - Bar charts
  - Histograms
  - Contingency tables
  - Scatterplots
  - Boxplots
  - Quantiles
  - Outliers
- Python stuff
  - Creating and performing calculations on atomic data
  - Creating and accessing NumPy arrays
  - `for` loops
  - `if` statements (and `if`/`elif`/`else`)
  - Functions and methods
    - Calling a function/method vs. writing a function
    - Passing arguments (both atomic and aggregate)
    - Return values
    - Function that modify in-place vs. returning a copy
  - Pandas `Series` & `DataFrames`
    - Reading from a `.csv` file
    - The "index"
    - `.value_counts()`
    - `.groupby()`
    - Using `.iloc[]` vs. `.loc[]` vs. `[]`
    - Single ints/labels vs. slices vs. lists
    - Queries
    - Recoding / transforming columns
- ML concepts
  - Classification vs. regression
  - Features and target attribute
  - Training data, test data, and new data
  - Random sampling
  - The "prior" vs. "posterior"
  - Evaluating a classifier

All these topics were covered in *Crystal Ball* Volume One. If any of them are iffy, you might take an hour or two to flip back through them and brush up!

# Chapter 2

# Navigating the Spyder's web

We'll be using Spyder this semester: a Python-based data analysis environment written especially for Data Science and scientific programming.

It comes with the Anaconda distribution, as does pretty much everything else we'll use this semester (scikit-learn, NumPy, SciPy, Pandas, Matplotlib, *etc.*) Download it from here: `https://www.anaconda.com/download`.

**Note:** make sure to get Python **3.something**, not **2.something***!! (They are *not* mutually compatible.) The number(s) after the dot don't matter so much. But before the dot *must* be a **"3"**.

And don't worry: all the stuff you learned last semester using Python Jupyter Notebooks still applies! The only difference is that using an IDE (Integrated Development Environment) like Spyder is not Web-based: it's entirely offline, responsive, and more feature-rich. Instead of a Notebook in a browser, you'll be creating your own Python source code files (each of which has a `.py` extension) and executing them directly.

As with a Notebook, a Python source code file (`.py`) can have English text as well as Python code. However, the English text must be "commented" by prefixing each non-code line with a hashtag

("#"). This tells Spyder that the line in question is not intended to be parsed and executed when the program is run.

## 2.1 The Spyder tutorial

First, download the latest version of Anaconda for your platform from `https://www.anaconda.com/download`. This will take a while, after which you should be able to start the Spyder IDE (details depend on your operating system).

Spyder comes with a nice tutorial, so it would be duplicative for me to reiterate those instructions here. As of this writing, you can access it by choosing "Spyder Tutorial" from the "Help" menu once you start Spyder. Make sure to click on each little green arrow to expand it as you go. (Btw, I don't recommend clicking on links in this tutorial, since it brings you to the linked section but then gives you no obvious way to get back where you were. Perhaps I'm missing how.)

Go through the entire tutorial now. You can *skip over* the following sections, however:

- "Strive for PEP 8 Compliance"
- "Automatic Symbolic Python"
- "Other observations"
- "Documentation string formatting"

We won't be using any of those features in this course or this book.

There are a few concepts you'll encounter in this tutorial which were not covered in the previous book. They include:

- The concept of the "IPython console," the pane in the lower-right of the Spyder screen with which you can interact and see output. This is somewhat different (but better) than the way Jupyter Notebooks acts with its cells and printed-output-of-each-cell. Get very comfortable with using the console.
- The concept of a "docstring," which is text enclosed in triple-double-quotes (`"""`) immediately after a function `def`inition,

and which then shows up in the console if you type `help(`*function_name*`)`. This is mildly useful.

- The concept of an interactive debugger, which can be a very useful IDE feature.

## 2.2 Configuration

Finally, a couple of settings you should change before we crack our knuckles. These are on the "Preferences" page, which you can get to these via "Tools > Preferences" in Linux or Windows, or via "Python/Spyder > Preferences" on MacOS:

1. Under "Editor," find the "Source Code" tab, and make sure that the "Indentation characters" is set to "4 spaces."
2. Under "IPython console," find the "Graphics" tab, and set the "Graphics backend" to "Inline." Make sure that after doing this, you can type a graphics command like this into the console:

```
import pandas as pd
silly = pd.Series([4,9,8],index=['bill','kevin','jane'])
print(silly)
silly.plot(kind='bar')
```

and see the resulting plot on the "Plots" pane of the upper-right window. (You may have to click on the word "Plots" to show this.)

## 2.3 A note about folders/directories

One common gotcha I'll mention that plagues many new Spyderers has to do with where files are stored on your computer. You probably know that your computer stores its information in a cascading hierarchy of **files** and **folders** (folders are also called **directories**). A file is a single unit of information, which can be opened by an application; it might contain text, a song, an image, or even video.

A folder/directory, on the other hand, is a *container* of files (and often, other directories).

Perhaps you're the kind of person who likes to arrange their information in a sensible way, using directories as an expressive organizational mechanism. Or perhaps you're the kind who just plops everything down wherever, knowing you can search for it later. Either way, what's important to know is that Python, when it tries to read a file (say, with `pd.read_csv()`) is going to *look* in a certain folder/directory in order to find it. If it doesn't find it there, it throws up its hands.

This is frustrating for students who download data (maybe a `.csv` file) from a website, but don't really understand *where* their browser put this file on their hard drive. They then write a Python program – undoubtedly saving that `.py` file to a different folder than the one the `.csv` file is in – which attempts to open it and comes up empty.

The solution is actually really simple: *store your data files in the same folder as your Python files.*

Right now, you should create a folder to hold all your code and data for this course. Name it something sensible, and remember how to navigate to it. Then:

- Whenever you create a new Python program, "Save as..." the `.py` file into this folder.
- Whenever you download a data file, store it in this folder.[1]

Onward!

[1] If your browser automatically stores downloads in a "Downloads" folder of some kind, either reconfigure your browser to prompt you for a location when it downloads, or else manually copy the files that you download into your new folder.

# Chapter 3

# EDA: review and extensions

In this chapter, we'll review the **EDA** (**Exploratory Data Analysis**) material you learned in Volume One, and also present a few additional techniques.

Remember, when you're first exploring some data, the first and most basic questions to ask are:

1. Is the data **univariate** or **bivariate** (or **multivariate**)?[1]
2. Is it **categorical** or **numerical**?[2]

The answers to these questions determines what kind of **statistic** is relevant, and what kind of **plot** is appropriate.

[1] "Univariate" data means that you're looking at only one variable, even if there are many observations of that variable. A bunch of people's SAT scores comprises a univariate data set, as does a bunch of political affiliations, salaries, or declared majors. "Bivariate" data contains *two* pieces of information for *each* observation: if I have data about both the SAT score and the college GPA for each of a bunch of students, that's a bivariate data set. Another example: a data set with both the gender and the salary for each of a bunch of adults.

[2] Recall that a "categorical" variable is qualitative, typically chosen from a set of possible values. Gender, political affiliation, and declared major are all examples. "Numerical" variables are (duh) numbers: salary, GPA, SAT score. Numerical variables can further be refined by their scale of measure (ordinal, interval, ratio), although that often doesn't affect the appropriate type of exploratory statistics and plots too much.

Example: let's say we're exploring a data set of great works of literature:

```
books.iloc[0:5,:]
```

```
                    gender  year     lang   words  chaps
name
Jane Eyre                F  1847  English  183858     38
Brothers Karamazov       M  1879  Russian  364153     92
Anna Karenina            M  1877  Russian  349736    219
The Inferno              M  1320  Italian   45750     34
Huck Finn                M  1884  English  109571     43
```

For each book, we have the `gender` of the author, the `year` and `language` in which it was written, and the total number of `words` and `chap`ters it contains. Clearly `gender` and `lang` are categorical variables, while `year`, `words`, and `chaps` are numeric.

## 3.1 Case 1 – univariate data: categorical

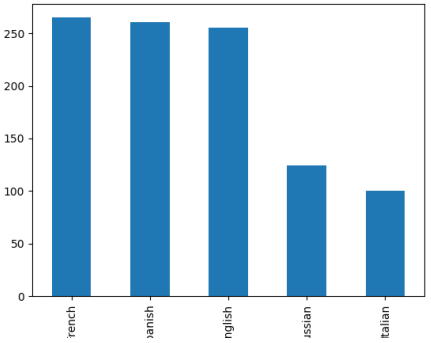
When looking at just one variable, which is categorical in nature, the appropriate analysis is the **one-dimensional contingency table**, which shows the counts of the various values. Let's create a contingency table for the book languages, using the `.value_counts()` function from Pandas:

```
books['lang'].value_counts()
```

```
French     299
English    247
Spanish    217
Russian    150
Italian     92
Name: lang, dtype: int64
```

The most appropriate plot is a **bar chart** of these counts, which you can create by simply tacking `.plot(kind="bar")` at the end:

```
books['lang'].value_counts().plot(kind="bar")
```




## 3.2 Case 2 – univariate data: numeric

When your single variable of interest is numeric, as is the `words` column, the appropriate statistics are **mean**, **standard deviation**, and the various **quantile** statistics (**minimum**, **.25 quantile**, **median**, **.75 quantile**, and **maximum**):

```
books['words'].mean()
books['words'].std()
books['words'].quantile([0,.25,.5,.75,1])
```

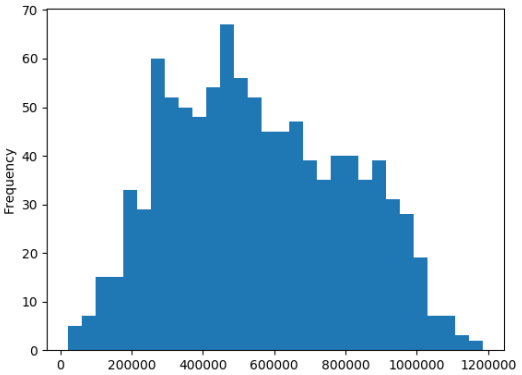
```
436739.737
232384.719
0.00      5443.0
0.25    241492.0
0.50    462552.0
0.75    637765.0
1.00    805341.0
```

Translation: on average, the books in our data set each have about 436,739 words, and if distributed normally (which we haven't checked yet) about $\frac{2}{3}$rds of them are in the range 436,739 ± 232,384 (or between 204355 and 669123 words). The shortest book has 5443 words, the longest a whopping 805,341, and half the books in the data set have 462,552 or less. A quarter of the books have fewer than 241,492 words, and three quarters have fewer than 637,765.

The best plot in this case is the **histogram**:

```
books['words'].plot(kind="hist",bins=30)
```

which shows the entire "lay of the land" of the distribution of values. Remember to experiment with the number of `bins`, since you can get very different pictures of how the data is distributed depending on your bin size (more on that in Chapter 4).




## 3.3 Case 3 – bivariate data: cat–cat

If you want to explore the relationship between two different variables, both of which are categorical, you need a **two-dimensional contingency table**. One way to get this is to use `.value_counts()` again, this time in conjunction with `.groupby()`:

```
books.groupby('gender')['lang'].value_counts()
```

```
gender  lang
F       French      79
        English     52
        Spanish     34
        Italian     29
        Russian     11
M       French     209
        English    196
        Spanish    193
        Russian    115
        Italian     87
Name: lang, dtype: int64
```

which shows, for each `gender`, how many books in each `lang` are in the data set. I personally think the `pd.crosstab()` function is a bit easier on the eyes for this, though:

```
gender_lang = pd.crosstab(books['lang'], books['gender'])
print(gender_lang)
```

```
gender    F    M
lang
English  52  196
French   79  209
Italian  29   87
Russian  11  115
Spanish  34  193
```

### Margins: raw counts

The `pd.crosstab()` function is also useful for computing **margins**, or row/column aggregate information. The easy part is to include "`margins=True`" as an argument to `pd.crosstab()`. The tricky part is understanding the different ways of presenting the margins, since they're each subtly different and often confused. So heads up.

Our first use of margins will be to simply compute **raw counts**:

```
gender_lang_m = pd.crosstab(books['lang'], books['gender'],
    margins=True)
print(gender_lang_m)
```

```
gender      F    M   All
lang
English    52  196   248
French     79  209   288
Italian    29   87   116
Russian    11  115   126
Spanish    34  193   227
All       205  800  1005
```

The word "margins" refers to the "`All`" row and the "`All`" column. In this table, they contain *the total counts for each row, and for each column.* Inspect the table and verify this is so: for each row (say, `English`) the sum of the `F` entry (52) and `M` entry (196) is equal to the total in the `All` entry (248). Similarly, the sum of the entire first column (the `F`'s for all languages, which are 52, 79, 29, 11, and 34) is equal to the `All` element of that column (205). And of course, the sum of the `All` rows – or `All` columns, same diff – is the grand total of 1005.

### Margins: overall percentages

Now suppose we *divide every value of this table* by the grand total. (We could literally divide by the number 1005, or divide by `gender_lang.loc['All']['All']`, since that's how to programmatically obtain the value of the bottom-right-hand entry.) This gives us **overall proportions**, and if we multiply by 100, **overall percentages**:

```
print(gender_lang_m / gender_lang_m.loc['All']['All'] * 100)
```

```
gender       F      M     All
lang
English   5.17  19.50   24.68
French    7.86  20.80   28.66
Italian   2.89   8.66   11.54
Russian   1.09  11.44   12.54
Spanish   3.38  19.20   22.59
All      20.40  79.60  100.00
```

Note carefully how to interpret this result: the sum total of all the table's entries (except for those in the `All` row/column) is equal to 100%. This tells us that over $\frac{1}{5}$th (20.8%) of all these books *were written in French by males*, only about 1% of the books *were written in Russian by females*, and so forth.

### Margins: percentages by column

By contrast, sometimes it's more helpful to have *each column* add up to 100%, rather than the entire table adding up to 100%. You can accomplish this like so:

```
print(gender_lang_m.div(gender_lang_m.loc['All'],axis=1) * 100)
```

```
gender        F       M     All
lang
English   25.37   24.50   24.68
French    38.54   26.12   28.66
Italian   14.15   10.88   11.54
Russian    5.37   14.37   12.54
Spanish   16.59   24.12   22.59
All      100.00  100.00  100.00
```

(For now, the "`.div()`" call, and the "`axis=1`" thing, are best to just follow verbatim rather than trying to understand what they mean.)

Notice that every `All` entry at the bottom is now equal to 100. (The `All` entries on the right side are *not*.) This view of things allows us

to see the language data *on a per-gender basis*. For instance, over 38% *of all the female authors* wrote in French, whereas only 26% *of all the males* were in French.

### Margins: percentages by row

We can do the corresponding process on a by-row basis by changing our syntax to this:

```
print(gender_lang_m.div(gender_lang_m['All'],axis=0) * 100)
```

```
gender       F      M    All
lang
English  20.97  79.03  100.0
French   27.43  72.57  100.0
Italian  25.00  75.00  100.0
Russian   8.73  91.27  100.0
Spanish  14.98  85.02  100.0
All      20.40  79.60  100.0
```

Important: there are *two* changes here from the previous example, only one of which jumps out at you. The obvious one is that we have "`axis=0`" instead of "`axis=1`". But the one that's easy to miss is that instead of "`gender_lang.loc['All']`" we now have "`gender_lang['All']`" (with *no* "`.loc`"). If you forget this part, you'll get nonsense.

If you do it correctly, each *row* (not column) will now sum to 100%, which gives us gender data *on a per-language basis*. For example, we can see that 91.27% *of the Russian books* were written by men, but only 75% *of the Italian ones* were.

### *Warning!*

Now you can stare at these numbers to get a feel for the them, and this is encouraged. Remember, though, the proper way to test whether there's a **statistically significant** relationship between

two categorical variables is to use a $\chi^2$ test. And that leads me to mention a very common pitfall.

Recall that when you call `scipy.stats.chi2_contingency()`, you pass it the contingency table. All well and good. But you must remember to pass it *the original contingency table* ***without*** *margins!* Once you've started to compute and display margins, it's all too easy to forget that adding margins *adds a row and a column to the table* (for the "`All`" information) and if you give `chi2_contingency()` this extraneous data it messes up the whole $\chi^2$ computation.

This is why in all the examples above, I deliberately changed my variable name for the "margined" table from `gender_lang` to `gender_lang_m` (`m` stands for "margins.") This is a nice visual reminder that I *don't* want to pass this table as an argument to `scipy.stats.chi2_contingency()`: instead, I want to pass the vanilla, margin-less table `gender_lang`. I suggest you do the same.

### Plotting multiple categorical variables

Finally, what about plots for multiple categorical variables? One choice that is (rarely) used for this is called a **mosaic plot**, but they're so difficult to interpret that I don't really recommend them. A more common choice is a **heat map**, which can be both beautiful and effective.

This brings us to our next `import` statement, this time of the Seaborn graphical visualization library:

```
import seaborn as sns
```

Seaborn is a terrific package that is widely used by Pythonistas in the Data Science community. It provides great support for several important kinds of plots that aren't implemented (or are implemented suckily) in base Python and the other libraries we've used. One such plot is the heat map, which you can create simply by passing the Seaborn function a contingency table:

```
sns.heatmap(gender_lang)
```

(Notice I passed `gender_lang`, not `gender_lang_m`. We don't want to plot the margins as though they were entries!) The result is shown in Figure 3.1 (p. 16). It's disorienting at first, but the key to grasping the message is to look at the color spectrum at the far right of the diagram. Here we see *a mapping of numbers to colors.* In this particular color scheme (there are many others to choose from), a light tan color indicates a high value up near 200, whereas a dark black color indicates a low color down below 40. In between, the colors go through shades of purple and red and orange, each indicating progressively higher values.[3]

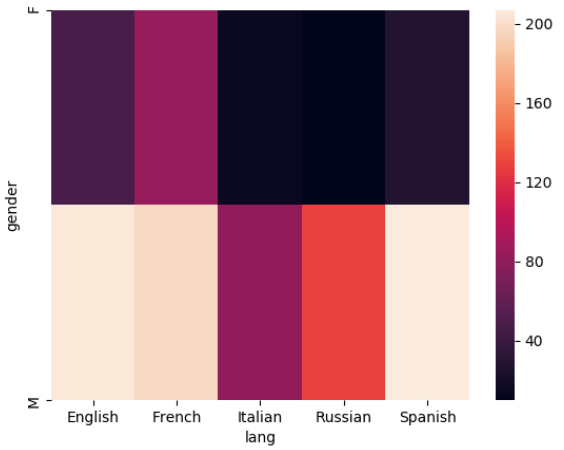



**Figure 3.1:** A heatmap of two categorical variables.

With that firmly in mind, look now at the main part of the image. You'll see there are two "axes," one for `gender` and one for `lang`,

[3]Btw, there are lots of other color schemes available; you can add a value for the "`cmap`" argument to your `heatmap()` call giving the color scheme's name. I personally like the "`seismic`" one since it makes it extremely clear which colors go with high vs. low values. You can get a list of the available ones by passing `cmap="list"` as the second argument to `heatmap()`.

just like in our `gender_lang` contingency table. And there are ten rectangles, one for each combination of values of those two categorical variables. In fact, you'll see that this heat map is really just a pictorial representation of this table:

```
print(gender_lang)
```

```
lang    English  French  Italian  Russian  Spanish
gender
F            48      84       15       10       28
M           205     197       82      129      207
```

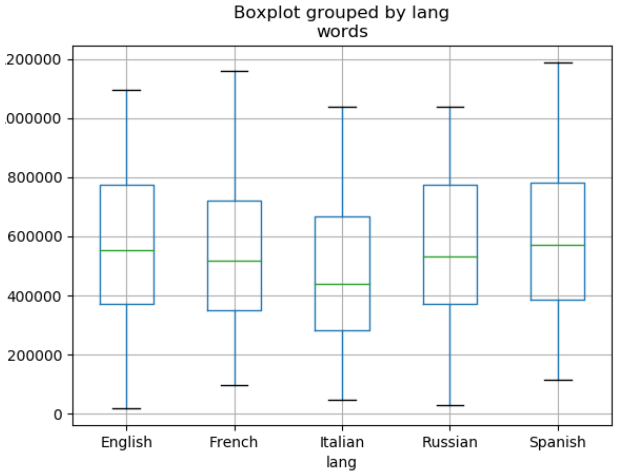
A heat map is like looking at a table "from above." Looking down on `gender_lang`, we see that the highest peaks are `English` and `Spanish` males, with `French` males close behind. `French` writers stand out among the females, who otherwise have lower quantities across the board. If you glance back and forth between the table and the heat map, you'll see that the heat map has brighter/more-light-tan rectangles in exactly the places where the table has a high value, and darker rectangles for lower values. Sanity check that just as the numbers 84 (`French` females) and 82 (`Italian` males) are almost identical in magnitude, so the two corresponding rectangles are almost exactly the same shade of purple.

## 3.4 Case 4 – bivariate data: cat–num

Suppose the two variables you're interested in are one categorical and one numerical. For instance, maybe you're wondering whether men or women have contributed more recent literary works, or which languages tend to have longer books.

The right plot here is the **box plot**, since it allows you to easily compare groups. For the language vs. length example:

```
books.boxplot(column='words', by='lang')
```

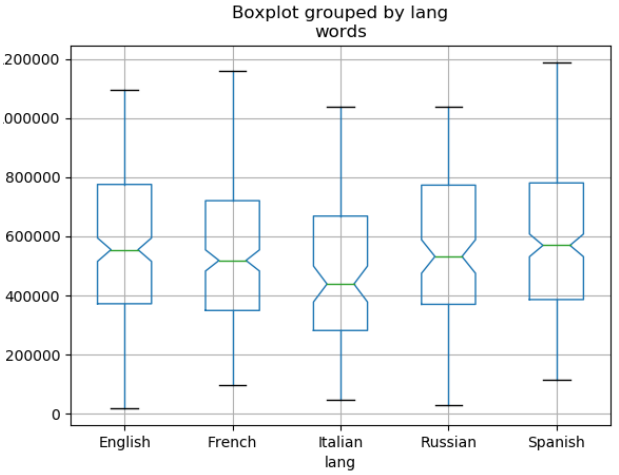



Apparently Italian works are a bit shorter than the other languages (especially French), but it's hard to tell whether there's any truly significant difference between the averages among the various groups. Recall that one way to find this out is a ***t*-test for the difference of means**, using `scipy.stats.ttest_ind()`.

Here's another way. You can use a ***notched* boxplot**:

```
books.boxplot(column='words', by='lang', notch=True)
```

As long as your group sizes are big enough, this visually indicates whether or not there is a stat sig diff between groups, based on *whether the notched areas overlap*. In the above case, the English and French notches overlap, which means we can conclude nothing reliable about English works being longer than French ones. However, the English and Italian notches do *not* overlap, which means we *should* feel confident about declaring that on average, English works are longer than Italian ones.




## 3.5 Case 5 – bivariate data: num–num

Finally, the case where our two variables of interest are both numerical. The obvious plot type here is the **scatter plot**, which shows one point for each observation, with its $x$ and $y$ position determined by its values for each variable.

```
books.plot.scatter(x='year', y='words')
```

The result is Figure 3.2. Clearly a big takeaway is that literary works have been getting steadily shorter over the years. You'll remember that the statistical reliability of this conclusion could be confirmed (or denied) by taking a look at the Pearson's correlation coefficient.

### Scatter plot matrices

So a single scatter plot is easy enough to generate. Sometimes, though, you have a data set with many variables, and it's nice to get a bird's-eye view of all the possible pairings. This is actually easy to do, by generating something called a **scatter plot matrix**.

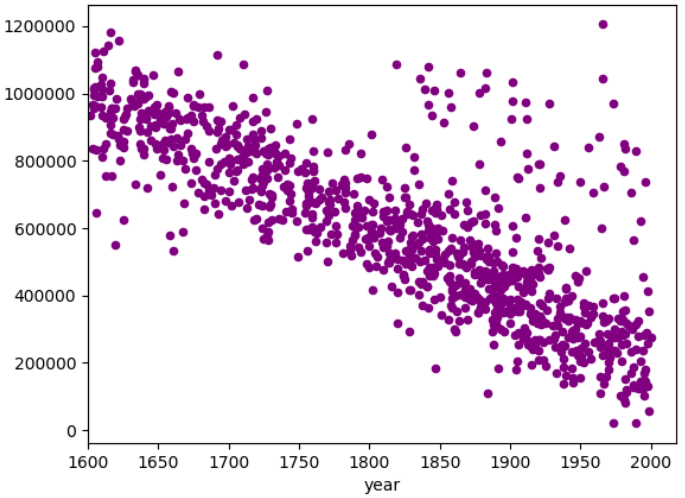



**Figure 3.2:** A scatter plot of two numerical variables.

Scatter plot matrices look pretty "busy," but that's because there's a lot of information there, so let's give them a go.

First, we're going to make sure that only do the analysis on the *numeric* columns. I'll create a new variable called `books_num` (for "books: numeric") to hold just the numeric variables:

```
books_num = books[['year','words','chaps']]
```

(Mind the double boxies!)

And now, the scatter plot matrix:

```
pd.plotting.scatter_matrix(books_num, alpha=1)
```

Don't worry about the `alpha` part for the moment. The result of this command is in Figure 3.6 (end of the chapter, p. 26). As I said,

it's busy: almost too much to look at. You'll understand it when we go through the components, though.

First, notice that the overall figure is a $3 \times 3$ grid of smaller figures, and remember that we passed `scatter_matrix()` a `DataFrame` with three columns. Each little figure in this grid depicts *two* of the `DataFrame` variables scatter-plotted against each other.

Take the left-middle grid square on the side for starters. This grid square is labeled "words" on the left and "year" on the bottom. It is therefore a scatter plot of `words` vs. `year` – *exactly* the same plot as in Figure 3.2 (take a moment to visually compare these). And the upper-middle grid square also involves the same two variables, although this time it's `year` vs. `words`; it contains the same information as the middle-left, but the axes are reversed.

If you look at the lower-left and upper-right corners of the grid, you'll see the result of a `chaps` vs. `year` (and `year` vs. `chaps`) scatter plot. And the bottom-middle/right-middle squares plot `words` vs. `chaps`. Every pairwise combination of variables is present here (twice).

What about the upper-left to lower-right diagonal? These are grid squares which should ostensibly have a scatter plot of "`year` vs. `year`", "`words` vs. `words`," *etc.* Obviously that doesn't make sense – a scatter plot of a variable against itself would be useless (think out why this is true). So Pandas does us a favor and at least shows us *something* in these squares that's useful. And the useful thing it shows is our favorite plot for univariate numeric data: the histogram. The upper-left corner is a histogram of the `year` variable by its lonesome, the middle square is a histogram of `words`, and the bottom-right is a histogram of `chaps`. This lets you see the distribution of each of your variables in isolation, right alongside their correlation with every other variable in the set. Neat.

Scatter plot matrices can be a powerful tool for EDA, so you can quickly identify what variable pairings might be of interest (*i.e.*, might have associations). They're not usually used for a final presentation of analysis results, since they really contain too much information to be effective for that.

The trick to using a scatter plot matrix for EDA is to run your eyeballs over the plots, looking for straight-ish lines (as opposed to amorphous clouds). In the `books` case, all three of our variables are pretty strongly correlated, but you can see from Figure 3.6 that the `words-year` association is the most pronounced. The `year` and `chaps` variables, although somewhat correlated with each other (you can see a downward trend in the bottom-left grid square) are more "noisy," meaning that the link between them isn't as precise and predictive.

### Transparency

The "`alpha`" parameter we skipped over earlier has to do with scatter plots that have too many points to see clearly. You've probably had experience with scatter plots that look like a big blue cloud: there are so many points plotting next to and on top of each other that you can get any sense of where they're most concentrated. One solution to this is to add the `marker="."` parameter to your call to `df.plot.scatter()`: this tells Python to use a tiny dot instead of a larger circle.

There are limitations to this, though, especially for a truly huge number of points. A better solution is to use **transparency**, which is what the `alpha` parameter – on a scale of 0.0 to 1.0 – controls. When `alpha` is set all the way to 1.0, dots are plotted the way you normally see them: all the way opaque. By reducing this number, each dot gets plotted in a partially transparent way, so that only if lots of dots are plotted in the same general area will they become fully dark and visible.

## 3.6 Case 6 – multivariate data

All of the previous examples involved either one or two variables. But what if you have more than that? How do you plot them?

It gets tricky when you try and make sense of too many different entangled variables at once. However, it can be done, in most circumstances, if you're on your game in terms of interpretation.

Let's talk about the three-variable case in particular. First off, it helps a lot if at least one of the variables is categorical. If all three are numeric, then you essentially need a three-dimensional plot (such as a 3-d scatter plot, contour plot, or a wireframe plot) which are difficult to interpret. (Humans just aren't very good, it turns out, at visualizing things in three dimensions. Most people, however, are quite good at two dimensions.)

### Grouped scatter plots

Suppose one of your variables is categorical and the other two numeric. In this case, sometimes a good option is to use a **grouped scatter plot** which depicts the categorical values via different styles of point: different colors are the most common, but different shapes can be used too.

The Seaborn library's `scatterplot()` function lets us do this:

```
sns.scatterplot(data=books, x="year", y="words", hue="lang")
```

The `data=books` parameter tells `scatterplot()` which `DataFrame` we want to use. The `x` and `y` parameters specify what we want on the x and y axis of our plot, and `hue="lang"` bit tells Seaborn which variable we want the color – or "hue" – to be based on.

The result is in Figure 3.3. From it, we can see that (in our fictitious data set) although books seem to have been getting shorter over time, this isn't true of the `Russian` books, which are staying more a constant size. This observation wasn't really possible without involving all three variables in the plot, which is why a grouped scatter plot was valuable here.

### Facets

More generally, a technique which is applicable to lots of different kinds of plots involves adding **facets**. With facets, you can partition a single plot into multiple plots, thereby effectively showing multivariate data with more than two variables.


**Figure 3.3:** A grouped scatter plot.

To illustrate facets, let's do the same kind of thing we did with a grouped scatter plot in Figure 3.3. First, we create a "`facet`" variable by calling Seaborn's `FacetGrid()`, passing it our `DataFrame` and which variable we want it to use to split into subplots:

```
facet = sns.FacetGrid(books, col='lang')
```

The "`col`" stands for column, not because `lang` is a `DataFrame` column (although it is), but because we want each subplot to be in its own column.

We then follow this up with a call to the `.map()` method of this `facet`:

```
facet.map(plt.scatter, 'year', 'words')
```

In plain language, this says "please map a scatter plot, of `words` vs. `year`, to each subplot." The result is as in Figure 3.4. Each of the five languages appears on its own separate subplot, which in each case is a plot of the `words` vs. the `years` for books in that language.

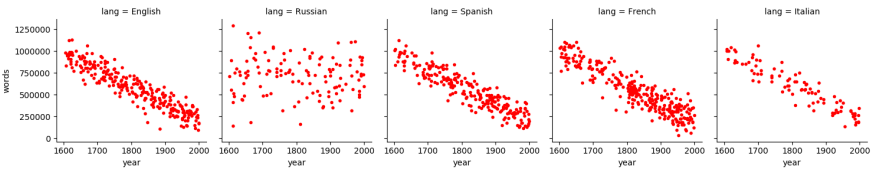



**Figure 3.4:** A faceted scatter plot.

The reason the `FacetGrid()` function has the word "grid" in the title is because you can go hog wild by specifying not only columns for the subplots, but rows:

```
facet = sns.FacetGrid(books, row='gender', col='lang')
facet.map(plt.scatter, 'year', 'words')
```

The resulting Figure 3.5 has *ten* different subplots, one for each combination of `gender` and `lang`. And all nicely labeled, too!

Notice that the Figure 3.5 infographic is analyzing *four* variables all acting in concert: two that determine the subplot (`gender` and `lang`) and two that are plotted against one another in each of the subplots.

Facets can also be used with box plots, heat maps, histograms, *etc.*, depending on how many variables you have and how many of them are categorical or numerical. In every case, one subplot is

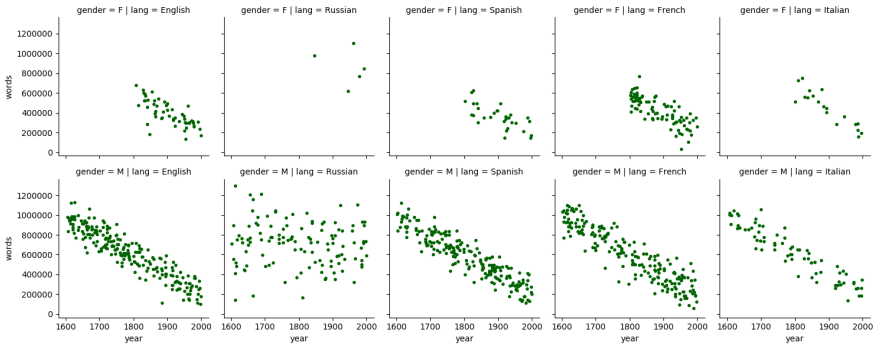



**Figure 3.5:** A faceted scatter plot with two faceted variables.

created for each subset of the data that has particular value(s) for the faceted variable(s).

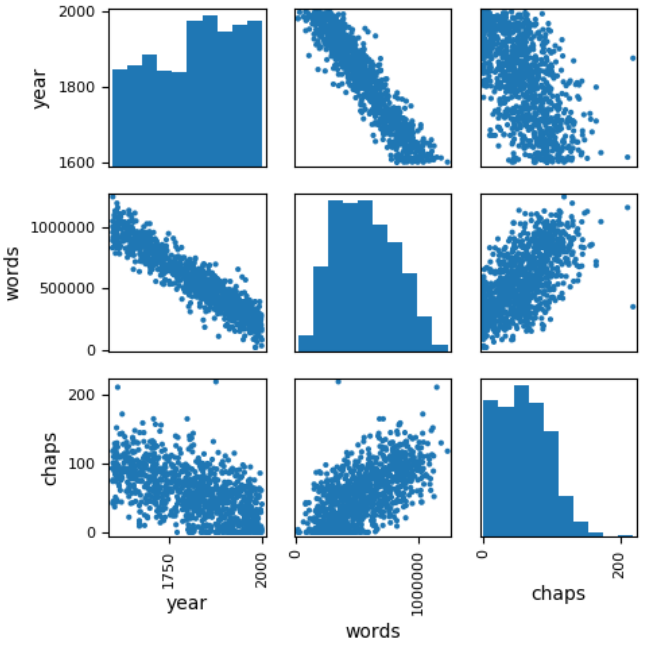



**Figure 3.6:** A scatter plot matrix of the `books DataFrame` (restricted to only numeric variables).

# Chapter 4

# KDEs and distributions

## 4.1 Limitations of histograms

Histograms are a great tool for seeing the distribution of a numerical, univariate sample. As we'll see in this chapter, though, they have some deficiencies. One problem is that a data set doesn't uniquely determine a histogram: instead, we must specify parameters such as the bin size and the "alignment" of the bins (*i.e.*, where exactly the breaks occur), and the resulting display is colored (no pun intended) by those choices.

Consider this simple data set[1]:

```
2.1, 2.3, 1.9, 1.8, 1.4, 2.6, 1.7, 2.2
```

Suppose we choose a bin width of 1. If we positioned the *left* edge of each bin at 0, 1, 2, 3, ..., we would get the histogram on the left side of Figure 4.1.

```
data = np.array([2.1, 2.3, 1.9, 1.8, 1.4, 2.6, 1.7, 2.2])
plt.hist(data, bins=[0,1,2,3,4])
```

[1] From Janert, P. K. (2010). *Data Analysis with Open Source Tools: A Hands-On Guide for Programmers and Data Scientists.* O'Reilly Media.

Our interpretation would probably be: "looks like the values occur pretty uniformly throughout the range 1-3."

But if we shifted our bin alignment to be on the "halves" (0.5, 1.5, 2.5, ...), we get this histogram on the *right* side of Figure 4.1.

```
plt.hist(data, bins=[-.5,0.5,1.5,2.5,3.5,4.5])
```

Now we may be liable to think: "it looks like a steeply-peaked distribution with most values right near the center value of 2."

Yet the data is the *same*! :-O

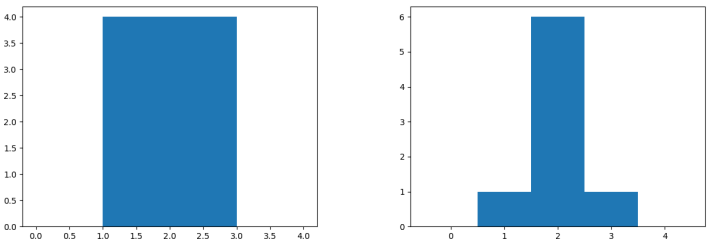



**Figure 4.1:** Two histograms of the *same* data set!

## Data vs. process

Now you might dismiss this idiosyncrasy as merely a one-off quirk that only shows up when the data is carefully arranged so as to trigger it. And there's some truth to that. But the real problem with histograms is bigger and more conceptual: it has to do with *what we're really trying to visualize in the first place.*

In Data Science, paradoxically, very often we don't actually care about the *data* so much as we care about the underlying *process* that generated the data. This "**data-generating process**" **(DGP)** – whether it's a geographic fault, a mystery author, a sports team, or an economy – leaves behind evidence of its behavior (seismic tremors, sentences, sports statistics, income levels) which we dutifully collect and then analyze. The purpose is (almost) always to

draw inferences about how that DGP works, not to learn about the individual bread crumbs themselves.

To our present point, when we look at a histogram of (say) GPAs of a sample of UMW students, we're not actually interested in what those sampled GPAs precisely are, strange as that may sound. We're instead interested in what they tell us about UMW student GPAs in general. We want to draw conclusions about the **population** by looking at the **sample**.[2]

Let's say we hung out at the fountain on campus walk, and asked unsuspecting volunteers to let us measure how tall they were. The histogram of the result might look like Figure 4.2.

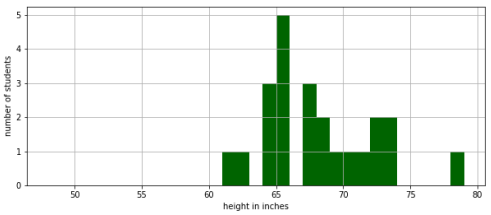



**Figure 4.2:** A histogram of a sample of UMW student heights.

The histogram is using "1 inch" as a bin size. By inspecting it, we can see that the shortest person in our sample was 62 inches tall (or 5-foot-2), the tallest was 78 inches (6-foot-6), and the most common height was 65 inches (5-foot-5), among other things.

But consider this. Our sample had five students who were 5-foot-5, three who were 5-foot-7, but *none* who were 5-foot-6. This is perfectly possible with samples, of course – you're only getting a random set of students, and there are bound to be little quirks like this. But on what basis do we label it a "quirk?"

[2]If you haven't encountered these words before, the "population" is the entire set of relevant objects of study that are out there in the world, most of which we'll never get a direct measurement for because they're just too numerous. The "sample" is the small subset of the population that we did get a measurement for. A classic example is political polling: we don't really care that much how the 2,000 people in our telephone poll are going to vote for President; what we care about is how the country as a whole will vote for President. So we assume that the sample is reflective of the population, and reason accordingly using statistical tests as our guide.

If you're like me, your inclination is to say, "yeah, okay, in this particular sample we happened to be missing any 5-foot-6 people, but it's not like we're going to draw any grand conclusions from that fact. We're not going to deduce that 'UMW students are almost never 5-foot-6 – they're almost always either a tad shorter or a tad taller than that.' Such a conclusion would be ludicrous!"

I sympathize and agree. But really, we only know this because we bring **background knowledge** to the problem. We've all seen lots of people of various heights, and we know something about how genetics and nutrition and other factors play into a person's height, and it just screams "wrong!" to think that there's some magic "missing height" out there, right in the middle of otherwise quite common heights, that for some reason is virtually unattainable.

Think about it, though: if we were studying an *unknown* phenomenon, about which we had no previous experience, it would be pretty audacious for us to infer the existence of lots of "66's" which we never actually observed, simply on the grounds that there were lots of 65's and 67's in our sample. My point is not to forsake your background knowledge: quite the opposite, you should make good use of it! My point is only to draw attention to the justification we're using to infer the existence of plenty of 66-inch-tall (5-foot-6) people in the population, even though we never actually observed any.

So my main point is this. Although we look at a histogram like this one in order to see "the lay of the land" – to see which values of the numeric variable are more frequent, and which are less frequent – if we're smart we can't help but recognize two different aspects to the figure. Some of the histogram's features are generalizable, and indicative of what the population probably looks like: we'd (correctly) gather that many or most UMW students were between 60 and 80 inches tall, with the majority in the 65-ish to 75-ish range. But some of its features we'd (correctly) characterize as mere artifacts of this particular sample, like the weird fact that we happen to have several 65-inchers and 67-inchers but no 66-inchers.

What we'd really like is a plot that obscures (or "smooths over") the second kind of thing, while still revealing the first kind of thing. In

other words, we'd like a plot that shows us the features of the data that are probably generalizable, while hiding the individual nooks and crannies. Such a plot is coming right up in Section 4.2, below.

Just to finish venting, I'll list yet another couple of problems with histograms:

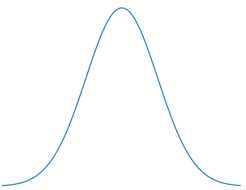
- They inherently lose information, since by definition data points with specific, precise values are munged into "the nearest bin."
- They don't handle outliers very well. A single outlier way outside the normal range forces us to either (a) include a lot of empty cells in the middle, or (b) choose an unreasonably wide bin width that doesn't work for the majority of points.

## 4.2 Kernel Density Estimates (KDEs)

One solution to these unfortunate histogram problems is a more advanced technique called a **Kernel Density Estimate**, or a **KDE**.

A "**density**" (or "**probability density**") is defined as a single, strongly-peaked function that has an area under its curve of exactly 1. It indicates how likely certain values of a numeric variable are to occur: values for which the density is high are more probable. Probability densities play a starring role in understanding the tendencies of both real and randomly-generated data.

When we talk about a "**kernel**," we just mean a density shape that we're going to make lots of copies of and add up together. Normally (no pun intended!) we will use a **Gaussian kernel**, which means "a bell curve a la the normal distribution":



(In math and stats, "Gaussian" and "normal" are synonyms.)

One thing we have to decide on is the *width* of this kernel — which in our case essentially means "the standard deviation of the normal distribution we're using." This is kind of like having to choose the bin width for histograms, but in practice the choice turns out not to be as critical. The width we choose is called the kernel's **bandwidth**.

Okay, now visualize this. In order to form a KDE, we place a *copy* of this kernel on the x-axis at each data point, and then add up all the kernel contributions to make a smooth curve. This has the effect of smoothing out all the jaggedy ups and downs of the actual histogram. The goal is to reflect the "true, underlying" shape of the data for the entire population.

There are several different ways to do this with Python packages. The Seaborn library has a good "`kdeplot()`" function. Using plain SciPy, we can call the `gaussian_kde()` function and pass it the bandwidth as a second argument. This returns a function that can be used to evaluate the KDE at any data point. (Read that sentence again: a function that returns a function? It can be confusing.) Then, we can plot it by creating a range of values to evaluate the KDE at, and plotting those values against the KDE's values.

It's easier than it sounds when you run the actual code:

```
import scipy.stats
kde = scipy.stats.gaussian_kde(data,bw_method=.5)
x_vals = np.arange(0,10,.1)
plt.plot(x_vals,kde(x_vals))
```

The "`data`" argument to `gaussian_kde()` is the array you're working with, and "`bw_method`" (a dumb name) gives the kernel's bandwidth. (`x_vals` is an array of the x coordinates you want to plot the KDE for, and should cover the range.)

Now stare at the four plots in Figure 4.3. These are all KDEs for the green Figure 4.2 histogram, but each one uses a different bandwidth. Choosing a larger kernel bandwidth effectively smooths out the KDE more, spreading the contribution of each point quite

a bit farther from its original position. Choosing a narrower kernel focuses each data point's contribution more precisely at its actual value, making the plot choppier.

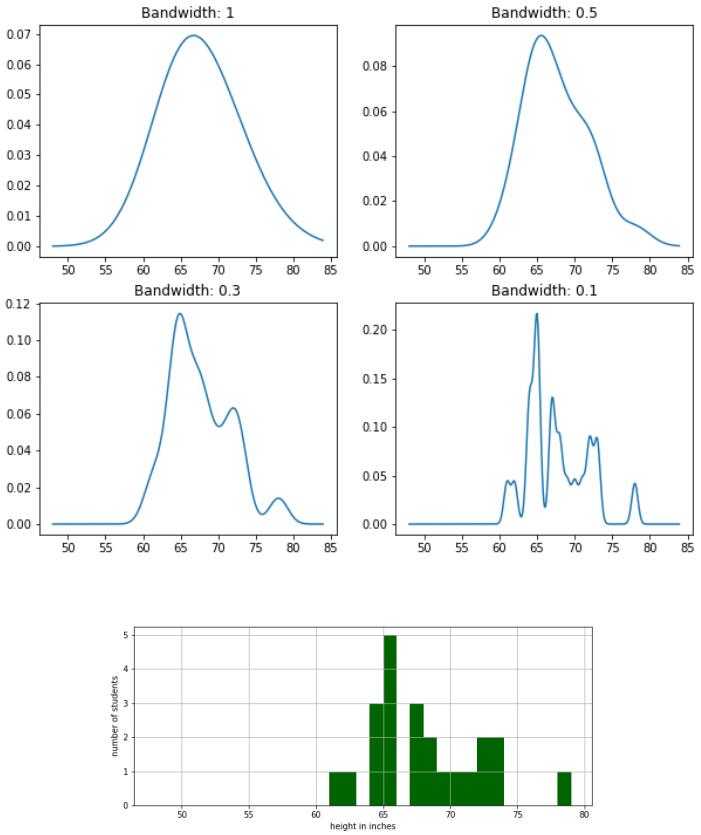



**Figure 4.3:** Gaussian KDEs with bandwidths of 1, .5, .3, and .1, respectively, for the data behind the green Figure 4.2 histogram (repeated here).

In practice, it's another parameter to play with. If the data follows a smooth distribution, you can use a wider bandwidth which will "blur" each data point more and give a more intuitive view of the general distribution characteristics. If the distribution is more wiggly, though, you need a narrower bandwidth to see all the relevant detail. Which of the Figure 4.3 bandwidths do you think best

captures the "true" distribution of the points in the histogram?

Like most things in Data Science (and in life), there's no one true hard-and-fast right answer. There is instead a range of points of view, many of which may be illuminating.

# Chapter 5

# Random value generation

One very useful skill is the ability to quickly create *synthetic* (artificial; generated by your own code and random-number generators) data sets that have certain properties. Sometimes we use such data to sanity check the results of our code with "idealistic" (simplified and known) inputs. Sometimes we use synthetic data as a baseline with which to compare real-world data sets that we suspect have similar characteristics. And sometimes we simply don't have access to relevant real-world data but we need inputs into some simulation process.

This chapter and the next will teach you the essentials of this process.

## 5.1 Setting the seed

Generating **random number**s (and other **random value**s) is an activity we perform surprisingly often in Data Science. "Random numbers," as it turns out, aren't truly random, because the programming language uses a bizarre – but deterministic and repeatable – algorithm to come up with them. This is nice, because we can guarantee that each time we run a program we'll get the same sequence of random numbers. We do this by setting the random number generator's **seed** to a particular value. It helps us in debugging our code, because otherwise, a shifting sequence of numbers

would be a frustrating moving target.

NumPy provides a really nice library for all this, all of which is in the namespace `np.random`. To set the random number generator's seed, all you do is call its `seed()` function and pass it your favorite number:

```
np.random.seed(13)
```

(I chose 13 because that was my little league baseball jersey number as a kid.) I recommend you put this line of code (with any positive integer you like) near the top of any `.py` file in which you do random value generation. If you want a different sequence of random values later, you can either change the integer to something different, or comment out the line altogether by prepending a "`#`" character.

## 5.2 Generating random numbers

To actually generate a random number value, you first have to figure out what **distribution** you want it to come from. Think of a distribution as a KDE from last chapter: it's a way of specifying which values are more common and which are less. The two standard distributions we'll use most are:

- **Normal/Gaussian**. As mentioned on p. 31, a "normal" distribution is a standard bell curve with a central **mean** and a **standard deviation** that determines how wide the curve is. The Gaussian distribution with mean 65 and standard deviation 4 (perhaps representing the speed of various cars on the highway) is shown on the top half of Figure 5.1.
- **Uniform**. A uniform distribution specifies that every value within a certain range (a **min** and a **max**) should be *equally likely*. An example for a min of 0 and a max of 60 (perhaps representing the minute past the hour that various babies in a maternity ward were born) is shown on the bottom of the same figure.

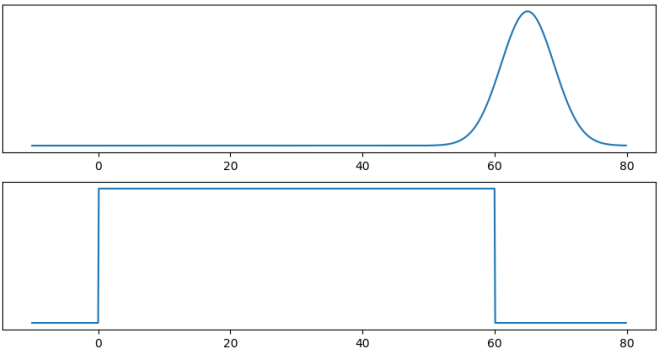



**Figure 5.1:** A normal, and uniform, distributions, shown as KDE-like curves.

If you're interpreting Figure 5.1 correctly, you can see that if we generate random numbers from the top distribution, the majority will be between 60-ish and 70-ish miles per hour, with many near 65 mph and almost never anything lower than 50 or greater than 80. If we generate them from the bottom distribution, however, the babies' birth minutes will all be between 0 and 60 but with no particular tendency towards any value in that range more than any other.

## Generating normal random numbers

Let's see if that works. The three arguments to `normal()` are (1) the mean of the distribution, (2) the standard deviation, and (3) how many random numbers you actually want. We'll just start with one at a time:

```
np.random.seed(13)
print(np.random.normal(65,4,1))
```

```
[62.15043735]
```

```
print(np.random.normal(65,4,1))
```

```
[68.01506551]
```

```
print(np.random.normal(65,4,1))
```

```
[64.82198769]
```

```
print(np.random.normal(65,4,1))
```

```
[66.80724935]
```

True to form. We keep getting numbers quite close to 65 mph, with a little bit of variation. Note that if we reset the seed to our original value, our next call to `normal()` gives an identical result to the first one, above:

```
np.random.seed(13)
print(np.random.normal(65,4,1))
```

```
[62.15043735]
```

And of course it's easy to generate many speeds at a time (say, eight):

```
print(np.random.normal(65,4,8))
```

```
[60.81849148 61.8440439  59.95357622 67.25138714 64.02669499
 68.65496282 66.26940369 65.50921312]
```

Notice that each time we call `normal()`, we get an array back (even if it has only a single value).

By the way, we should sure expect that if we generate many random speeds, and take their average, it should be pretty darn close to 65 mph:

```
print(np.random.normal(65,4,1000).mean())
```

```
65.01577962051226
```

Yep.

### Generating uniform random numbers

Uniform random values can be generated the same way, but with the `uniform()` function, which takes as its arguments (1) the min, (2) the max, and (3) the number of desired values:

```
np.random.seed(13)
print(np.random.uniform(0,60,1))
```

```
[46.66214463]
```

This synthetic baby was born at 46.6 minutes past the hour. What about the next one?

```
print(np.random.uniform(0,60,1))
```

```
[14.2524732]
```

And the next one?

```
print(np.random.uniform(0,60,1))
```

```
[49.45671196]
```

And the next eleven?

```
print(np.random.uniform(0,60,11))
```

```
[57.944951 58.356066 27.206954 36.542547 46.531591 38.496800
 43.321093  2.102191 17.906968  3.510749 51.423656]
```

Of course, resetting the seed gives us our original sequence back:

```
print(np.random.uniform(0,60,5))
```

```
[46.66214463 14.2524732  49.45671196 57.94495188 58.35606683]
```

(Check those numbers with the previous ones to convince yourself.)

And finally, let's sanity check the average:

```
print(np.random.uniform(0,60,1000).mean())
```

```
29.2049841447296
```

Yay. "On average," our thousand synthetic babies are born at about half past the hour, which is what we'd expect.

## 5.3 Generating categorical random values

NumPy also provides a way to generate *categorical* values with certain frequencies, through its `choice()` function. You give it an array of the possible values, and it chooses one:

```
np.random.seed(13)
np.random.choice(['Steelers','Patriots','Giants'])
```

```
'Giants'
```

```
np.random.choice(['Steelers','Patriots','Giants'])
```

```
'Steelers'
```

(As always, resetting the seed will restart the same sequence of random team choices from the beginning.)

Other useful arguments to `choice()` include:

- `size` – the number of elements you want in the resulting array.
- `replace` – if `False`, the elements will be drawn from your list *without replacement* (meaning once a value is chosen, it will not be chosen again). This is often useful.
- `p` – a list of *probabilities* (in the range 0 to 1) specifying how likely each element in the list is to be chosen. (Note these must sum to 1; and NumPy, stupidly, will not normalize it for you.)

To illustrate:

```
print(np.random.choice(['Steelers','Patriots','Giants'], size=14,
    p=[.3,.6,.1]))
```

```
['Steelers' 'Patriots' 'Patriots' 'Patriots' 'Giants'
 'Steelers' 'Steelers' 'Patriots' 'Patriots' 'Steelers'
 'Patriots' 'Giants'   'Steelers' 'Patriots']
```

We asked for 14 random teams, and we told it to give us `Steelers` 30% of the time, `Patriots` 60%, and `Giants` only 10%. I think you'll agree that the resulting array was pretty faithful to that. (Of course, you'll get a different random array each time.)

Finally, let's test a large random array and verify that the requested percentages are approximately correct:

```
pd.Series(np.random.choice(['Steelers','Patriots','Giants'],
    size=1000, p=[.3,.6,.1])).value_counts()
```

```
Patriots    584
Steelers    319
Giants       97
dtype: int64
```

Our friend the `.value_counts()` method confirms that it pretty much checks out.

# Chapter 6

# Synthetic data sets

Last chapter we learned the basic skills for generating arrays of random values – both numeric and categorical. Now let's apply these to creating **synthetic data set**s that contain more than one variable.

We'll concentrate here on the two-variable case, but the idea is easily extended to three or more. The important new question, now that we know how to generate single arrays in isolation, is: to what degree do we want our pair of synthetic variables to be correlated, and how do we make them so?

## 6.1 Two numeric variables

Let's start with the case of two numeric variables. As you know from Volume One, there can be an association, or not, between them. The Pearson's correlation coefficient measures this: if its $p$-value is less than our $\alpha$ setting (typically .05), then we deem there to be a meaningful association, and the $r$ value tells us whether the correlation is positive or negative.

### Uncorrelated numeric variables

On one extreme, let's say you wanted to create a data set with two completely *uncorrelated* numeric variables – like the heights

(in inches) and the SAT scores of a group of college applicants. Then you'd just generate two arrays, one at a time:

```
heights = np.random.normal(65, 8, 100)
sat_scores = np.random.normal(1000, 300, 100)
```

How did I choose those particular means and standard deviations? I made them up. And I played with them until they looked reasonable.

Scatter plotting these (see left side of Figure 6.1, p. 45), and running a Pearson correlation, should reveal they are independent of each other:

```
plt.scatter(heights, sat_scores)
plt.xlabel("height (in)")
plt.ylabel("SAT score")
print(scipy.stats.pearsonr(heights,sat_scores))
```

```
(-0.025053425275878834, 0.8045806864145338)
```

A $p$-value of .8046 says "nope, not significantly correlated." And of course there's no reason why they should be: we just generated two different random arrays, for different ranges.

Incidentally, you might be troubled by the fact that a few of our SAT scores are outside the legal range:

```
print("min: {}, max: {}".format(sat_scores.min(),
    sat_scores.max()))
```

```
min: 304.29, max: 1618.35
```

Real SAT scores are supposed to range between 400 and 1600, the Internet tells me. We could fix this by using the NumPy `.clip()` method, which imposes a high and low cutoff as its arguments:

```
sat_scores = sat_scores.clip(400,1600)
print("min: {}, max: {}".format(sat_scores.min(),
    sat_scores.max()))
```

```
min: 400.0 max: 1600.0
```

The revised scatter plot is shown on the right side of Figure 6.1.

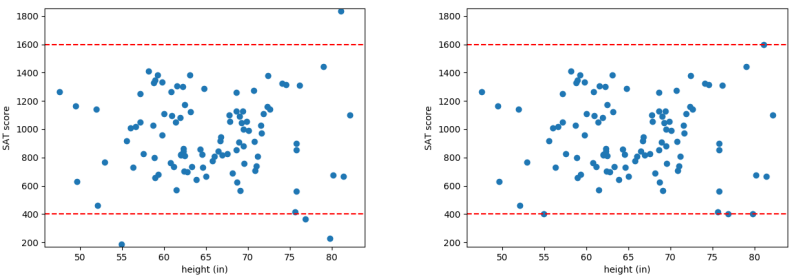



**Figure 6.1:** Uncorrelated numeric random variables. The right-hand plot has SAT scores "clipped" to stay above 400 and below 1600.

## Totally correlated numeric variables

On the other extreme, if two variables are *completely* correlated, then one is simply a direct (linear) function of the other. That's easy to accomplish by creating only *one* randomly, and then using it to compute the other:

```
weights_lbs = np.random.normal(150, 30, 100)
weights_kg = weights_lbs / 2.2
```

Clearly a person's weight in pounds completely determines their weight in kilograms: all you do is divide by a constant factor to convert between units.

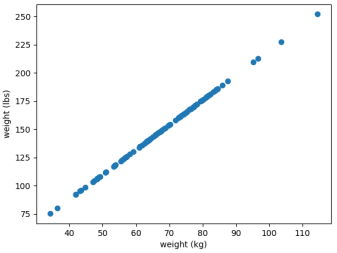



**Figure 6.2:** Two *completely* correlated numeric variables.

Scatter plotting these gives a perfectly straight line (see Figure 6.2), and Pearson tells us they're totally correlated (the $p$-value is rock bottom 0.0, and $r$=1):

```
print(scipy.stats.pearsonr(weights_lbs,weight_kg))
```

```
(1.0, 0.0)
```

## Somewhat correlated numeric variables

Now let's take the most common and interesting case: a data set in which our two numeric variables are *partially*, but not completely, correlated. (By "partially correlated" I just mean that there *is* an association between the variables, but it's not a rigidly perfect one, like the one between weight-in-pounds and weight-in-kg.)

What we'll do is first generate one of the variables independently and randomly, and then compute the second as a function of the first *with added* ***noise***. "Noise" is a strange (and somewhat misleading) term that's used in a variety of statistical situations. Here it means "random other factors that influence a numeric variable's value up or down."

As an example, let's create a synthetic data set with two variables about high school seniors: her SAT score, and her high school GPA. A moment's thought will tell you that this indeed falls under our third, "somewhat correlated" case: students with better SAT scores also on average tend to have higher GPAs, but this is an imperfect relationships that doesn't always hold completely.

Our strategy is as follows. First, randomly create an array of synthetic SAT scores. Then, calculate each student's GPA as a function of her SAT score, plus a random "nudge" either up or down to account for other random factors.

For our noise factor (the "nudge") we'll take the most common approach: a normally-distributed random variable with a mean of zero. This is called "**white noise**," for various semi-interesting reasons. We use a mean of 0 for this because on average, we don't want the random "nudges" to be biased in either the up direction or the down direction. On average, we want the net nudge to be zero.

Okay. Now see if you can understand the two lines of code we use to implement this strategy:

```
sat_scores = np.random.normal(1000, 300, 100)
gpas = sat_scores * (2.5 / 1400) + np.random.normal(0, 1, 100)
```

The `sat_scores` line is the same one we had before. We're then modeling the high school GPA of a student as *somewhat* correlated with his SAT score. The "$\frac{2.5}{1400}$" multiplier is an attempt to quantify the relationship between the two variables, which of course are measured on completely different scales. We're guestimating that a 1400 on the SAT would kinda sorta equate to about a 2.5 GPA. Notice that the second component of `gpas` is a normally distributed noise component *with zero mean.* (Why a standard deviation of 1? Just a guess. We can tweak it later if we don't like the results.)

Now this is a good first attempt. Notice two assumptions/limitations, though:

1. We're assuming that the relationship between the two variables is *linear* — namely, that "the first value times a constant" is a good estimate for the second value. In reality, of course, the relationship is often more complex: it might be better modeled as the *square* of the first value, for instance, or "$e$ to the" first value, or the cube root of the first value, *etc.*

2. We're assuming that the "zero point" for the two variables coincide: in other words, a zero for one value would on average roughly correspond to a zero for the other. In the above case, we're assuming that a person who got a 0 on the SAT would have, on average, a 0 GPA. If this isn't appropriate, we should add an **intercept term** (a constant) to our generative formula. This takes our generated second variable and just shifts it, wholesale, to a new region of the number range.

We'll stick with the first assumption (linearity) for the moment, but be more flexible about the second. If we include an intercept term, our formula for generating the dependent variable boils down to:

$$\texttt{dep\_variable} = m \cdot \texttt{indep\_variable} + b + \texttt{np.random.normal(0, } \sigma\texttt{, } n\texttt{)}$$

which is the familiar equation for a line ($y = mx + b$) with a noise term added in (with $\sigma$ standard deviation). Now we have to estimate decent values for $m$, $b$, and $\sigma$. How should we do this?

My preferred approach is to identify a "high-ish" value of the first variable, and estimate a (roughly, on average) corresponding value of the second variable. Then do the same for a "low-ish" value. Then, plug those into the $y = mx + b$ formula and solve for the slope and intercept.

Example: let's generate a synthetic data set of two variables: the number of hours a person has practiced playing the Dance Dance Revolution (DDR) videogame in their lifetime, and the score they achieved in a DDR contest (on the song *Kakumei*). Clearly, there

should be some (positive) relationship between the two quantities: when `num_hrs` is high, you'd expect `score` to also be high. If you're familiar with the game, though, you know that the zero points for these variables do *not* coincide: even if you've never ever played at all, you'll still manage to stumble through the song, learn how to play as you go, and get a positive score.

Based on my knowledge of the game (which I suck at, by the way), I estimate:

- A decent player who has practiced for 100 hours might get a score of around 60 million.
- A sucky-ish player who has practiced for only 10 hours might get a score of around 30 million.

Running the algebra[1], I get:

$$60 = m \cdot 100 + b$$
$$30 = m \cdot 10 + b$$
$$\ldots \textit{insert algebra here} \ldots$$
$$m = .333, b = 26.667$$

Thus we get back-of-the-envelope estimates of $m$ and $b$.

Now how to estimate $\sigma$, the standard deviation of the noise term? Play with it. The larger it is, the more your second variable will deviate from the perfectly straight line we would predict solely from

[1] Linear algebra fans can avoid doing all the mechanical steps by noting that our two equations form the following matrix equation:

$$\begin{bmatrix} 100 & 1 \\ 10 & 1 \end{bmatrix} \cdot \begin{bmatrix} m \\ b \end{bmatrix} = \begin{bmatrix} 60 \\ 30 \end{bmatrix}$$

NumPy can solve this for $m$ and $b$ like so:

```
X = np.array([[100,1],[10,1]])
Y = np.array([60,30])
print(np.linalg.solve(X,Y))
```

```
[ 0.33333333 26.66666667]
```

But only if you're feeling lazy.

the $y = mx + b$. Remember that with the normal distribution, two-thirds of your data points will fall within one standard deviation from the mean. I think two-thirds of my 100-hour practicers might get between 50 and 70 million. So I'll go with a $\sigma$ of 10 and see how that looks.

Finall, here's the actual code to produce a synthetic data set of 200 dancers. First, generate the practice times themselves:

```
num_hrs = np.random.normal(50,20,200).clip(0,500)
```

Perhaps your average dancer practiced 50 hours for the competition, with most of them within 20 hours of that, and no one who practiced less than 0 hours (not even me), or greater than 500 hours.

Then, we generate these players' scores:

```
score = num_hrs * .333 + 26.667 + np.random.normal(0,10,200)
```

I think it looks pretty decent (Figure 6.3).

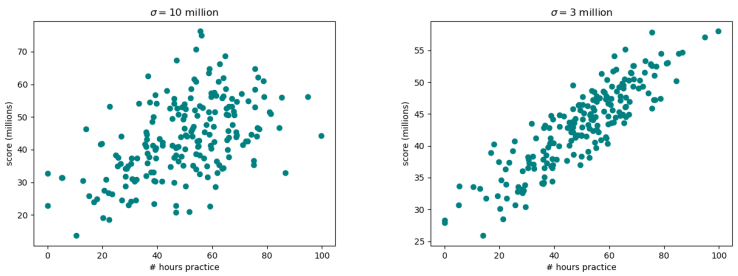



**Figure 6.3:** A scatter plot of two synthetic, partially-but-not-completely correlated numeric variables. In the left figure, the $\sigma$ for the noise was set to 10 million; in the right, to 3 million.

There's also a `multivariate_normal()` function in the `scipy.stats` package which can generate these kinds of correlated data sets more powerfully.

## 6.2 Two categorical variables

As with numeric variables, of course, a pair of categorical variables can be either uncorrelated, completely correlated, or "somewhat correlated." Let's generate examples all three types.

### Uncorrelated categorical variables

Let's generate a data set with 2000 registered voters in Fredericksburg, 54% Democrats and 46% Republicans. We'll also generate their pick for the Superbowl: the Chiefs (58%) or the 49ers (42%).

Since we want these variables to be uncorrelated, we just generate each one separately:

```
party = np.random.choice(['Democrat','Republican'], p=[.54,.46],
    size=2000)
superbowl = np.random.choice(['Chiefs','49ers'], p=[.58,.42],
    size=2000)
print(pd.crosstab(superbowl,party,margins=True))
print(scipy.stats.chi2_contingency(pd.crosstab(superbowl,party)))
```

```
         Democrat  Republican   All
49ers         461         383   844
Chiefs        595         561  1156
All          1056         944  2000
(1.81827219952, 0.177519079284, 1, array([[445.632, 398.368],
       [610.368, 545.632]]))
```

Don't be fooled by the heat map on the left side of Figure 6.4 (p. 52). It looks like the four categories have wildly different values, but that's because we didn't set the heat map's range explicitly, and so the color bar is all pinched to the range 400 to 600. We can tell Seaborn to use specific values by passing `vmin` and `vmax` arguments:

```
sns.heatmap(pd.crosstab(party, superbowl), vmin=0, vmax=2000)
```

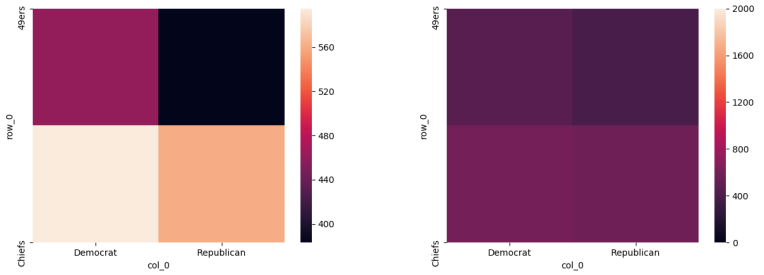



**Figure 6.4:** Two heat maps for a synthetic set of uncorrelated categorical variables. The left heat map looks like the four totals are very different, but that's because the scale was not explicitly set. In the right map, we pegged the color scale to the range (0,2000).

Here, the range 0 to 2000 makes sense, because that's as far as any one of our compartments could possibly range. The result is the right side of Figure 6.4.

As expected, a $\chi^2$ test's p-value shows no significant correlation (remember that the second entry is the $p$-value):

```
print(scipy.stats.chi2_contingency(party_sup))
```

```
(1.81827219952, 0.177519079284, 1, array([[445.632, 398.368],
       [610.368, 545.632]]))
```

## Completely correlated categorical variables

Now let's add a "`party_color`" categorical variable that gives the associated color of each voter's political party (blue for Democrats and red for Republicans). Note that this is *perfectly* correlated with `party`, and to enforce this, we need a different approach.

NumPy's `where()` function comes in handy here. It's tricky but powerful. `np.where()` takes three arguments – an array of booleans (`True`s and `False`s), and two other arguments which are used as substitutions. It produces an array *that includes the second argument in every position where the first is* `true`*, and the third argument everywhere it's* `false`*.* In the current example, we're saying

"for every place that the `party` array has a `'Democrat'` value, put `'blue'` in this new array you're making for me, and put `'red'` everywhere else."

The code looks like this:

```
party_color = np.where(party=='Democrat','blue','red')
```

As will be the case nearly every time we use `where()`, the first argument – the "array of booleans" – comes from a **query**. Remember that when we say something like "`party=='Democrat'`", we actually get back an array of `True`s and `False`s, one for each element in `party`:

```
print(party)
print(party=='Democrat')
```

```
['Republican' 'Republican' 'Democrat' ... 'Democrat' 'Republican']
[False False True ... True False]
```

Our call to `where()` effectively said "wherever `party=='Democrat'`, gimme a `True` (and thus take the second argument's value), otherwise gimme a `False` (and thus take the third argument's value). If we look at the first few values of our new array, we see that it worked:

```
print(party)
print(party_color)
```

```
['Republican' 'Republican' 'Democrat' ... 'Democrat' 'Republican']
['red' 'red' 'blue' ... 'blue' 'red']
```

Thus, we get perfect correlation between our two variables:

```
print(pd.crosstab(party, party_color))
print(scipy.stats.chi2_contingency(
    pd.crosstab(party, party_color)))
```

```
col_0        blue  red
row_0
Democrat     1056    0
Republican      0  944
(1995.989429141519, 0.0, 1, array([[557.568, 498.432],
       [498.432, 445.568]]))
```

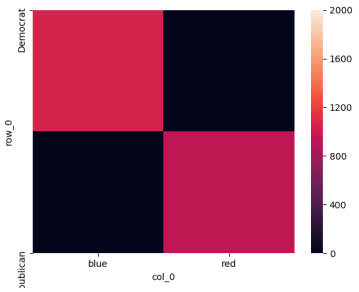



**Figure 6.5:** Two completely correlated categorical variables.

### Somewhat correlated categorical variables

And now let's create a "`gun_owner`" categorical variable which has the value `'gun'` or `'no gun'` for each voter. According to data I Googled, approximately 44% of our synthetic Republicans should own guns, and about 20% of our Democrats should. For this, we can go back to our friend `np.where()`:

```
gun_owner = np.where(party=='Democrat',
    np.random.choice(['gun','no gun'],p=[.2,.8],size=2000),
    np.random.choice(['gun','no gun'],p=[.44,.56],size=2000))
```

This time, our second and third arguments to `np.where()` are *themselves arrays*. We're saying, "in every position where `party` has a

`'Democrat'`, use the corresponding value from our random array that has 20% guns. Otherwise, use the corresponding value from a different random array that is 44% guns."

Checking, we do get the desired correlation:

```
print(pd.crosstab(party, gun_owner, margins=True))
print(scipy.stats.chi2_contingency(
    pd.crosstab(party, gun_owner)))
```

```
             gun  no gun
Democrat     208     848
Republican   394     550
(114.034337674, 1.28071376464e-26, 1, array([[317.856, 738.144],
       [284.144, 659.856]]))
```

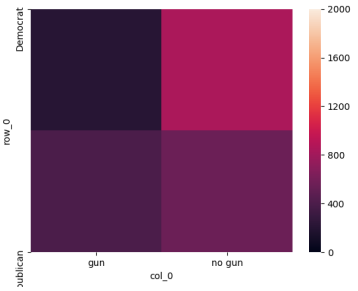



**Figure 6.6:** Two partially correlated categorical variables.

## 6.3 Intermission: stitching it all together

By the way, in all of the examples above, we simply generated two separate NumPy arrays. Even though these arrays were implicitly related to each other – they were the same length, and corresponding elements referred to aspects of the same student/dancer/citizen/whatever – they weren't actually in a `DataFrame` together. How can we make them so?

The syntax seems a little strange if you've never seen a Python "dictionary" before, but this helpful little data structure will come

up a lot later (*e.g.*, in Chapters 7-8.) You can think of a dictionary as a stripped-down, less-feature-rich version of a Pandas `Series`. In other words, it's a repository of key-value pairs. To create one, you use a pair of **curly braces**, inside of which you list the key-value pairs, each pair separated by a comma, and the key and value separated by a colon. An example would be:

```
teams = { 'Washington':'Mystics', 'Los Angeles':'Sparks',
    'Seattle':'Storm' }
```

You can then treat it like a `Series`, using boxies (`[]`) to get/set elements, although none of the advanced Pandas features won't work.

Anyway, the reason I mention this is that the easiest way to create a `DataFrame` out of a bunch of NumPy arrays is to pass the `DataFrame()` function a dictionary, where the keys are the column names you want, and the values are the arrays.

```
citizens = pd.DataFrame({'party': party, 'color': party_color,
    'prediction': superbowl, 'gun_owner': gun_owner})
print(citizens.iloc[0:8])
```

```
         party color prediction gun_owner
0   Republican   red      49ers       gun
1   Republican   red     Chiefs    no gun
2     Democrat  blue     Chiefs    no gun
3     Democrat  blue      49ers       gun
4     Democrat  blue      49ers    no gun
5   Republican   red     Chiefs    no gun
6     Democrat  blue      49ers    no gun
7     Democrat  blue      49ers    no gun
```

It's a snap!

## 6.4 One categorical & one numeric variable

Okay, back to our synthetic data creation. Our third and final case is a data set with one variable of each kind: numeric and categorical. Let's use professional athletes as our running example for this case.

### Completely uncorrelated

Let's create a synthetic data set with information about professional athletes in three sports: baseball, football, and basketball. I'm going to guess that players in each of these sports, on average, train about the same number of hours per week. That would make `sport` (categorical) completely uncorrelated with `training_hours` (numeric). So, we just generate them independently. Let's go with:

```
sport = np.random.choice(['baseball','football','basketball'],
    p=[.35,.45,.2], size=1000)
training_hrs = np.random.normal(35,10,1000)
print(sport[0:6])
print(training_hrs[0:6])
```

```
['football' 'basketball' 'basketball' 'football' 'football' 'baseball']
[26.24722 57.79145 51.44831 26.75212 21.95934 41.5458 30.76964]
```

Looks to be in the ballpark of what we want (pun intended). Let's put this info in a `DataFrame` and then generate a box plot:

```
athletes = pd.DataFrame({'sport': sport,
    'training_hrs': training_hrs})
athletes.boxplot("training_hrs", by="sport")
```

As expected. (Figure 6.7.)

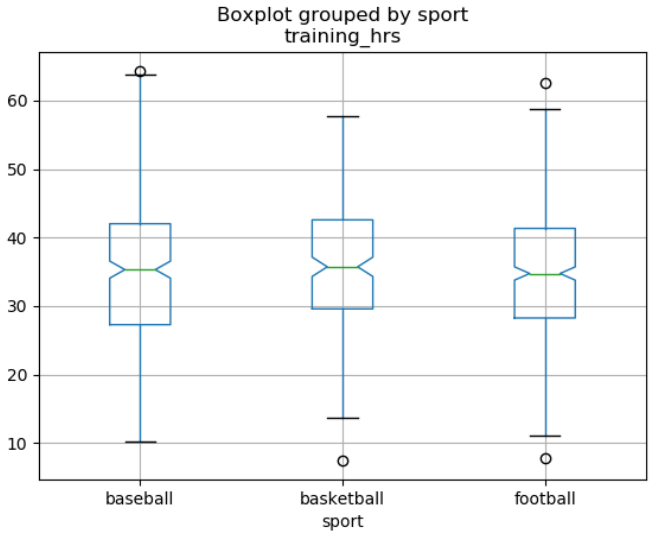



**Figure 6.7:** Synthetic mixed variables: uncorrelated.

## Completely correlated

It's kind of hard to think of an example with two completely correlated variables, one categorical and one numeric. This would mean that the value of the categorical variable *completely* determines the numeric value for that individual. So all baseball players must have the exact same value, and the same for all football players, and for all basketball players. What is like that? Just to have a complete set of examples, how about we use "the year the sport was invented."

We'll use good ol' `np.where()` again, although there's a bit of a catch (pun intended) since we have *three* different values for `sport` instead of just two. The key is to use **nested** function calls. Check it out:

```
year_inv = np.where(athletes.sport == 'baseball', 1869,
    np.where(athletes.sport == 'football', 1920, 1946))
```

If you follow the logic, it makes sense. This code says:

1. Make a new array, same size as `athletes.sport`.
2. For every place where `athletes.sport` has the value `'baseball'`, use the value 1869.
3. For every place where it has some other value, use...
    a) ...a new array, same size as `athletes.sport`.
    b) For every place where `athletes.sport` has the value `'football'`, use 1920.
    c) For every place where it has some other value, use 1946.

Get it? It's kind of like a sequence of nested `if` statements. Just make sure all your bananas line up.

We'll add this new column to our `DataFrame`, and take it for a spin:

```
athletes['year_inv'] = year_inv
athletes.boxplot("year_inv", by="sport", notch=True)
```

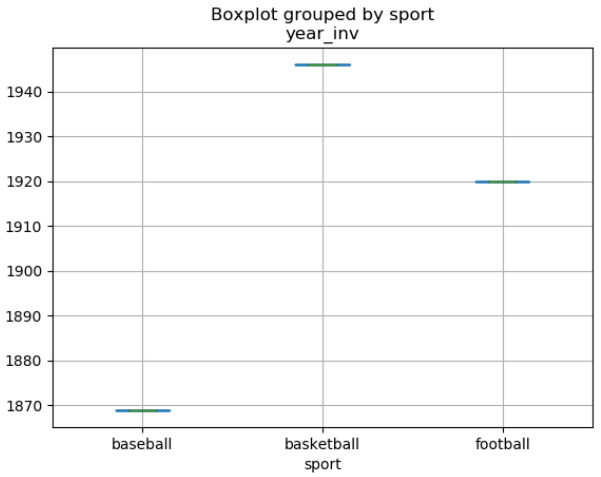



**Figure 6.8:** Synthetic mixed variables: completely correlated.

Figure 6.8 looks odd at first, but it's correct: every single baseball player plays a sport that was invented in exactly 1869, and so forth. So of course each "box" is collapsed to just a single line.

### Partially correlated

And finally, the case where the categorical variable partially, but not completely, determines the value of the numeric variable. Salaries for professionals in the three areas differ a great deal, even considering only male athletes: Major League Baseball players earn on average $4.1 million annually, NBA players a whopping $7.7 million, and NFL players, along with dealing with concussions, get a lowly $2.7 million a year. Who knew?

This data isn't truly normally distributed, you may realize, since there are a few Tom Bradys and LeBron Jameses who are paid astronomical amounts, skewing the average for everyone else. But just to finish this long chapter, let's assume normality, along with some reasonable-sounding standard deviation, and be done with it:

```
salary = np.where(athletes.sport == 'baseball',
    np.random.normal(4.1,1,1000),
    np.where(athletes.sport == 'football',
        np.random.normal(2.7,1,1000),
        np.random.normal(7.7,2,1000)))

salary = salary.clip(.4,100000)

athletes['salary'] = salary
athletes.boxplot("salary", by="sport", notch=True)
```

It's `np.where()` again. This time, we're generating three complete sets of 1000 synthetic salaries: one each to represent baseball, football, and basketball players. But then our `where()` call says "if the `sport` is `'baseball'`, take the value from the first one; if it's `'football'`, take it from the second one; otherwise, take it from the third one.

After creating this array, we clip it to make sure that no athlete is making less than $400,000 per year (which Google tells me is legit).

The result is in Figure 6.9, which looks as we expected. Go team!

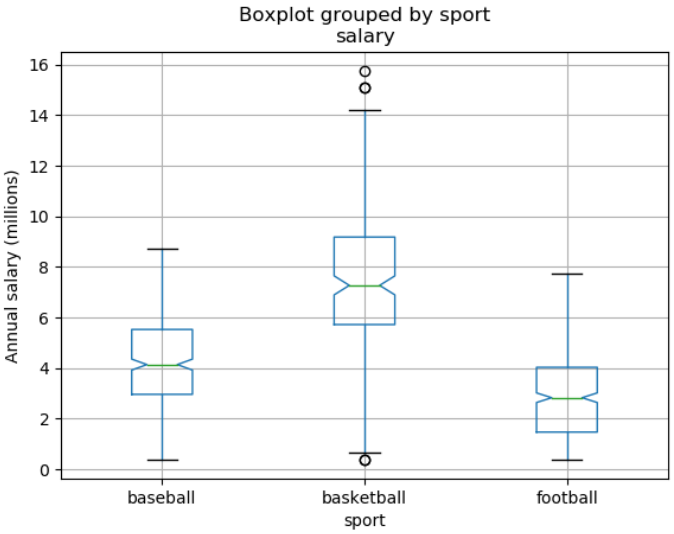



**Figure 6.9:** Synthetic mixed variables: partially correlated.

# Chapter 7

# JSON (1 of 2)

JSON (pronounced like the name "Jason") is a simple, human-readable text file format that is very commonly used for information storage and interchange. (It stands for "JavaScript Object Notation," but don't be fooled: it doesn't have much to do with the JavaScript language except historically. *Any* language, including Python, can read/write JSON data.)

In this chapter, we'll learn about how to read and navigate through JSON data. First, though, a word about a couple of Python essentials I omitted from DATA 101 for brevity and simplicity.

## 7.1 Lists and dictionaries

Last semester, we spent a lot of time learning how to use NumPy `ndarray`s and Pandas `Series`es. These are the preferred implementations of arrays, and associative arrays, respectively, in the Python Data Science ecosystem. As you know, a NumPy array holds a numbered sequence of items (indexed starting from 0), and a `Series` holds a set of key-value pairs.

For any serious data work, you want to use those tools, because they are lightning-fast, super-efficient, feature-rich, and optimized to the task.

As it turns out, plain-ol' Python has stripped-down, feature-poor,

but easy-to-type versions of these data structures as well, which are baked in to JSON and also important to know about in their own right. They're called **lists** and **dictionaries**.

### Lists

If, instead of writing this:

```
crew = np.array(["Ed","Kelly","Alara","Bortus","John",
    "Claire"])
```

you simply wrote this:

```
crew = ["Ed","Kelly","Alara","Bortus","John","Claire"]
```

then you get a plain-ol **list** instead of a NumPy array. It isn't nearly as fast, nor can it store nearly as many items, and you can't do broadcasting operations and such with it, but it does the basic job. For example:

```
print("Captain {} initiating roll call for {} officers:".format(
    crew[0], len(crew)))
for member in crew[1:len(crew)]:
    print("{} reporting for duty, sir!".format(member))
print(crew[0])
```

```
Captain Ed initiating roll call for 6 officers:
Kelly reporting for duty, sir!
Alara reporting for duty, sir!
Bortus reporting for duty, sir!
John reporting for duty, sir!
Claire reporting for duty, sir!
```

Working with small lists of items is very, very similar to working with NumPy arrays, so I'm sure you'll pick this right up.

Incidentally, we've actually used lists several times already, without knowing it. For instance, this very line of code:

```
good = np.array(["Janet","Chidi","Eleanor","Michael","Tahani"])
```

is actually first creating a *list*, and then passing that list as an argument to `np.array()`. And this code:

```
alter_egos = pd.Series(['Hulk','Spidey','Iron Man','Thor'],
    index=['Bruce','Peter','Tony','Thor'])
```

creates two separate lists, one for the data and one for the index, and passes those to `pd.Series()` to build a `Series` out of them. Lists are super-lightweight and super-common.

### Dictionaries

As mentioned in section 6.3 (p. 55), **dictionaries** are like stripped-down Pandas `Series`es, in the same way that lists are like stripped-down NumPy arrays. Dictionaries contain key-value pairs, accessed in the same sort of way (with the boxie `[]` syntax). You create a dictionary by using the syntax from p. 56:

```
alter_egos = { 'Bruce':'Batman', 'Dick':'Robin',
    'Diana':'Wonder Woman', 'Clark':'Superman' }
```

Then, just like with `Series`es, you can retrieve the value for a key, change the value for a key, add a new key-value pair, and so forth:

```
caped_crusaders = [ alter_egos['Bruce'], alter_egos['Dick'] ]
alter_egos['Clark'] = 'Man of Steel'
alter_egos['Victor'] = 'Cyborg'

print("There are {} heroes, {} of whom are the caped crusaders.".
    format(len(alter_egos), len(caped_crusaders)))
print("The dynamic duo is: {} and {}!".format(caped_crusaders[0],
    caped_crusaders[1]))
for key, value in alter_egos.items():
    print("Psssst, {} is really {}...".format(key,value))
```

```
There are now 5 heroes, 2 of which are the caped crusaders.
The dynamic duo is: Batman and Robin!
Psssst, Bruce is really Batman...
Psssst, Dick is really Robin...
Psssst, Diana is really Wonder Woman...
Psssst, Clark is really Man of Steel...
Psssst, Victor is really Cyborg...
```

### Nesting...and nesting, and nesting...

All that was easy so far. The only thing left to tell you – and man, it can pack a whammy when you first see it – is that both lists and dictionaries can be **nested** indefinitely. This means that one of a list's elements might well be another list, or a dictionary. And the value for one of a dictionary's keys might well be a list, or another dictionary.

Sometimes you have to stare hard at the printout of a nested structure to figure out how to unpack it. Here are some examples:

```
a = [ 7, 1, [9, 5], 6 ]
```

The `a` variable is a list (you can tell because it starts with a boxie) and one of its elements happens to be another list (ditto). Stare hard at that, and then stare hard at this output, and make sure you see why it's so:

```
print("a[1] is {}".format(a[1]))
print("len(a) is {}".format(len(a)))
print("a[3] is {}".format(a[3]))
print("len(a[2]) is {}".format(len(a[2])))
print("a[2][1] is {}".format(a[2][1]))
```

```
a[1] is 1
len(a) is 4
a[3] is 6
len(a[2]) is 2
a[2][1] is 5
```

The first one was a warmup. But the second output may have surprised you: aren't there *five* numbers in that list, not four? The answer is *no*, there are exactly four:

- Item #0 is the number 7.
- Item #1 is the number 1.
- Item #2 is a list, which has two elements: 9 and 5.
- Item #3 is the number 6.

Once you grasp that, you can probably understand the other outputs from that example as well. Of particular note is the last one: `a[2][1]` means "get element #2 from `a`, and since it is itself a list, get element #1 from *that*." And since all lists are numbered starting with 0, that's effectively the second element of the third element of `a`, which is the number 5.

Next one:

```
b = { "apple": 54, "banana": [14, 67], "cherry": { "bing":
[ 13, 17, 21], "rainier": { "sweet": "yes", "juicy":
"yes" } } }
```

The `b` variable is a dictionary (you can tell because it starts with a curly) and it contains several key-value pairs. How many, you ask?

```
print(len(b))
```

```
3
```

The three key-value pairs are:

- `"apple"`, whose value is the number 54.
- `"banana"`, whose value is a list, whose elements are 14 and 67.
- `"cherry"`, whose value is another dictionary. *That* dictionary has two key-value pairs:
  - `"bing"`, whose value is a list with 13, 17, and 21.
  - `"rainier"`, whose value is yet another dictionary, with keys `"sweet"` and `"juicy"`.

Now test yourself and make sure you can predict the right output from these lines of code:

```
print("b['apple'] is {}".format(b['apple']))
print("b['banana'] is {}".format(b['banana']))
print("len(b['banana']) is {}".format(len(b['banana'])))
print("len(b['cherry']) is {}".format(len(b['cherry'])))
print("len(b['cherry']['bing']) is {}".format(
    len(b['cherry']['bing'])))
print("b['cherry']['bing'][0]) is {}".format(
    b['cherry']['bing'][0]))
print("b['cherry']['rainier']['sweet']) is {}".format(
    b['cherry']['rainier']['sweet']))
```

```
b['apple'] is 54
b['banana'] is [14, 67]
len(b['banana']) is 2
len(b['cherry']) is 2
len(b['cherry']['bing']) is 3
b['cherry']['bing'][0]) is 13
b['cherry']['rainier']['sweet']) is yes
```

Remember, `len()` plays several roles. When called on a list or array, it gives the number of elements; on a dictionary or `Series`, the number of key-value pairs; on a string, the number of characters; and on a `DataFrame`, the number of rows. That's why `len(b['banana'])` and `len(b['cherry'])` both return 2, even though they're very different types of things.

Note this general rule, too: every time the thing you have is a *list*, you must follow it with an *integer* in boxies. Every time the thing you have is a *dictionary*, you must follow it with a *key* (often a string) in boxies. Always.

And now's a good time to mention how to find out what type of thing something *is* – the `type()` function:

```
print("b['apple'] is a {}".format(type(b['apple'])))
print("b['banana'] is a {}".format(type(b['banana'])))
print("b['cherry'] is a {}".format(type(b['cherry'])))
print("b['cherry']['rainier']['juicy'] is a {}".format(
    type(b['cherry']['rainier']['juicy'])))
```

```
b['apple'] is a int
b['banana'] is a list
b['cherry'] is a dict
b['cherry']['rainier']['juicy'] is a str
```

This is super useful when plunging deep through nested data sets.

One last example:

```
c = [ { 'x': 5 }, [ 14, 'bob', [ 11, { 'duck': 'donuts',
'five': 'guys' }, [ 17, 6 ] ] ] ]
```

Can you visually line up all those boxies? If so, then you can probably get these answers correct:

```
print("len(c) is {}".format(len(c)))
print("c[0]['x'] is {}".format(c[0]['x']))
print("c[1][1] is {}".format(c[1][1]))
print("c[1][2][1]['five'] is {}".format(
    c[1][2][1]['five']))
print("c[1][2][2][1] is {}".format(c[1][2][2][1]))
```

```
len(c) is 2
c[0]['x'] is 5
c[1][1] is bob
c[1][2][1]['five'] is guys
c[1][2][2][1] is 6
```

## 7.2 JSON

Okay, now about JSON proper.

The really nice things about JSON are (1) it's a simple format, and relatively easy on the eyes (unlike binary formats, or XML), and (2) it structures information in nested list-ish, dictionary-ish, string-ish type elements that are exactly like what we covered in the previous section. A JSON "document" is, in fact, *essentially a Python list or dictionary with embedded contents.*

Here's an example file in JSON format:

```
{"name": "Luke Skywalker", "rank": "Jedi", "lightsaber color":
"blue", "episodes": ["IV", "V", "VI", "VIII", "IX"], "relations":
{"Leia": "sister", "Han": "friend", "Artoo": "servant",
"Threepio": "servant", "Rey": "student"}}
```

Its structure is instantly apparent: a dictionary whose values are strings, lists, and other dictionaries, as appropriate.

Probably the best thing about JSON is that once we read and parse a JSON file or other information source, we have a bona fide Python variable that we can treat in the ordinary way.

In Python, we have the `json` package, which you can import like any other:

```
import json
```

There are four functions that matter:

- `json.dump`(*someVariable*, *aFile*) - Dump the Python variable to a file in JSON text format.
- `json.dumps`(*someVariable*) - Dump the Python variable to a string in JSON text format (and return it).
- `json.load`(*aFile*) - Build and return a Python variable from the contents of the JSON text file.
- `json.loads`(*someString*) - Build and return a Python variable from the JSON text string.

When I refer to "*aFile*" in the above list, I'm talking about a Python **file object**, which pros normally obtain using the somewhat weird-looking "`with`" syntax. It works like this:

```
with open('whatever.json','r') as f:
    ...do stuff with the file object f...
```

The name of the file we're opening here is "`whatever.json`", and like all files, it must be in the same folder as our Python `.py` file in order for Spyder to find it. The rest of that line is just a pattern to memorize. Importantly, the line(s) immediately underneath the "`with`" in which you use the file object "`f`" are *indented*, just like in a `for` loop or `if` statement or function `def`inition.

So, to load a file `info.json` into a Python variable called "`my_stuff`", we'd write this code:

```
with open('info.json','r') as f:
    my_stuff = json.load(f)
```

And we could parse and access our Luke Skywalker file just like this:

```
with open('luke.json','r') as f:
    luke = json.load(f)
print(luke['lightsaber color'])
blue

print(luke['episodes'][2])
VI
```

### "Pretty printing"

One thing I think you'll find useful is the ability to "**pretty print**" a nested Python structure, like one you read from a JSON file. Instead of a monolithic wall of text, like many `.json` files look out of the box, a pretty printer attempts to format, indent, and put linebreaks in, so that you can more readily perceive its structure and figure out how to pick out the parts you want.

A good package for this is the `pprint` package. First, you have to do the import:

```
from pprint import pprint
```

From then on, instead of `print()`ing a variable, you can `pprint()` it. I think you'll agree, the latter is easier to make sense of:

```
print(luke)
```

```
{"name": "Luke Skywalker", "rank": "Jedi", "lightsaber color":
"blue", "episodes": ["IV", "V", "VI", "VIII", "IX"], "relations":
{"Leia": "sister", "Han": "friend", "Artoo": "servant",
"Threepio": "servant", "Rey": "student"}}
```

```
pprint(luke)
```

```
{'episodes': ['IV', 'V', 'VI', 'VIII', 'IX'],
 'lightsaber color': 'blue',
 'name': 'Luke Skywalker',
 'rank': 'Jedi',
 'relations': {'Artoo': 'servant',
               'Han': 'friend',
               'Leia': 'sister',
               'Rey': 'student',
               'Threepio': 'student'}}
```

As a bonus, it even puts dictionary keys in alphabetical order, so you can find them more easily.

## 7.3 "Hierarchical" vs. "flat" data

So you see that the JSON file format is essentially a textual representation of an Python variable with arbitrarily nested inner structure. This variable can be a list or a dictionary, and have embedded lists and dictionaries to any level of nesting. Here's another example:

```
[{"prefix": "DATA", "num": 219, "creds": 3, "instructor": "Davies",
"meetings": [{"time": {"day": "TR", "time": "12:30pm"}, "location":
{"bldg": "Farmer", "room": "B6"}}], "roster": [{"first": "Lady",
"last": "Gaga", "email": "lgaga@umw.edu"}, {"first": "The", "last":
"Rock", "email": "trock@umw.edu"}, ...
```

When you disentangle this, you'll realize that what you have is:

A list, each element of which is:

- a dictionary, with key/value pairs:
  - `prefix`: a string
  - `num`: an int
  - `creds`: an int
  - `instructor`: a string
  - `meetings`: a list, each element of which is:
    - a dictionary, with key/value pairs:
      - `time`: a dictionary, with key/value pairs:
        `day`: a string
        `time`: a string
      - `location`: a dictionary, with key/value pairs:
        `bldg`: a string
        `room`: a string
  - `roster`: a list, each element of which is:
    - a dictionary, with key/value pairs:
      - `first`: a string
      - `last`: a string
      - `email`: a string
  - ...and possibly other stuff...

This kind of structure is called **hierarchical** data. This is in contrast to so-called **flat** data, like a CSV:

```
Prefix,Num,Instructor,Creds,Bldg,Room,Day,Time
DATA,219,Davies,3,Farmer,B6,TR,12:30pm
ENGL,286,Rigsby,3,Combs,112,MWF,11am
CPSC,305,Finlayson,4,Farmer,B52,MWF,8am
```

It should be clear that hierarchical data is intrinsically *more expressive* than flat data. Rather than each data record being a strict, identical-length sequence of values, the whole nested structure communicates order and relationships between subcomponents, like an outline.

It's not even always possible, let alone straightforward, to convert from a hierarchical format to a flat format. Consider the JSON file on p. 73: it permits any number of `meetings` for a single course, each of which has embedded structure. In this case, the structure for each meeting is regular, since it's apparently composed of a fixed number of fields with unique names. (This won't always be the case, and if it's not, we would *lose information* in collapsing it to a flat format.) Even so, though, it's not clear what to do with the multiple meeting times/locations for a course. Do we make each `Bldg/Room/Day/Time` group into its own set of headings in the flat format? This brings with it its own problems, such as:

1. How do we associate each group of buildings/rooms/days/times together, since they're now all individual top-level fields? (Naming conventions seem like the only solution, and it's awkward.)
2. How do we know the maximum number of such meetings, so as to specify the width of the table?
3. What do we do for rows which don't have the maximum number of meetings? Leave the others blank?
4. How do we perform standard queries like "find all courses that have at least one meeting in Farmer?" (We have to split this up into an awkward query that separately queries each of the columns and unions the answer.)

There are better ways to organize such data, such as the **relational model** that has been ubiquitous in database schema design since Ted Codd invented it in the 1960's. It allows us to "normalize" such data sets and represent them in multiple, interrelated tables. We'll take a look at this when we look at SQLite later in the course. Some irregular structures defy even the relational model, however, which is why some newer database paradigms (like NoSQL databases) have been developed to get around its limitations.

One important fact to grasp, however, is that at the present state of technology, *almost all machine learning algorithms are based on a **flat** data structure.* There are some quite advanced, cutting-edge exceptions to this, but really the field of mining hierarchical (and other non-flat) data formats is still in its infancy. Lots of opportunity to make a name for yourself here!

# Chapter 8

# JSON (2 of 2)

In this chapter we'll cover some common techniques for dealing with JSON data. Most often, what you end up doing is writing Python code that combs systematically through the data, surgically extracting the parts you need for analysis. These parts can then be assembled in NumPy arrays, Pandas `DataFrame`s, or whatever, and probed as you're accustomed to.

Let's go back to the college courses example from p.73, pretty printed here:

```
[{'creds':3,
  'instructor':'Davies',
  'meetings':[{'location':{'bldg':'Farmer', 'room':'B6'},
               'time':{'day':'TR', 'time':'12:30pm'}}],
  'num':219,
  'prefix':'DATA',
  'roster':[{'email':'lgaga@umw.edu', 'first':'Lady', 'last':'Gaga'},
            {'email':'trock@umw.edu', 'first':'The', 'last':'Rock'},
            ...,
            ...]
 },
 ...
]
```

The first brute fact to grasp is that whatever its internal complexities, this whole thing is *a list of dictionaries*. Not a list of lists, or a dictionary of dictionaries, or a dictionary of lists, but: a list of dictionaries. How do we know this? Because the first character is a boxie ("`[`") and the second one is a curly ("`{`").

## 8.1 Printing a class roster

As a first example of working with this data set, let's say we wanted to simply print the full names of all the students in the 17th course in this list. First, let's load the `.json` file into Python:

```
import json

with open("courses.json") as f:
    c = json.load(f)
```

Here we've called the outermost structure "`c`", which stands for "courses" but is shortened since we'll type it a lot. (Remember that `c` is a list – a very long and complicated list, but still a list.)

And then we do a deep think. Printing all the names clearly requires a loop. But what exactly do we want to loop through? The answer, after scrutinizing the above structure, is: we need to find the value of the `"roster"` key of the 17th dictionary in the `c` list. That in turn will be a list, and it will contain dictionaries, one for each student. (Pause before continuing, look at the JSON contents from p. 77, and see if you agree with every word of this paragraph.)

So, the loop we want is something like this:

```
for student in c[16]['roster']:
    print("{} {} is in {} {}.".format(student['first'],
        student['last'], c[16]['prefix'], c[16]['num']))
```

```
Lady Gaga is in DATA 219.
The Rock is in DATA 219.
Obi-wan Kenobi is in DATA 219.
Amy Klobuchar is in DATA 219.
...
```

Success. (Don't worry if you don't get this loop right the first time; it often takes some tweaking and refinement before it works.) Notice how this code operates:

1. We dig fairly deep into `c` (which is a list), finding its 17th element (at index 16 of course), which is a dictionary. Then we get the value of that dictionary's `"roster"` key. As you can see above, that key's value is a list.
2. Every time through the loop, the "`student`" variable is set equal to the next element of this list. And that element, as you can see above, is a dictionary. The dictionary has two items of interest: `"first"` and `"last"`. We then print the values of these two keys, plus the course prefix and number. (Note that the course prefix and number come directly from the `c[16]` dictionary itself, whereas the first and last names come from keys of the elements of the inner `"roster"` list that we're iterating through.)

## 8.2 Printing *all* the class rosters

That printed the roster for one class. What about printing the roster for *all* the classes?

If you think about it, the structure is much the same – except that instead of merely iterating through class #17's list of dictionaries, we want to do it for every class.

You'll probably realize that this necessitates *another* loop. All the stuff we did for class #17, we now want to do for all the classes, one after another. So in essence, we wrap the previous code in a nested, outer loop which will perform it once for each course. Check out the following:

```
for course in c:
    roster = course['roster']
    for student in roster:
        print("{} {} is in {} {}.".format(student['first'],
            student['last'], course['prefix'], course['num']))
```

Observe the nested structure (a `for` within a `for`), and the use of a temporary helper variable (`"roster"`) to make the code clearer. Also notice how the `print()` statement includes information from both the `student` and `course` variables, as appropriate.

This is just the right thing. However, when we run it, we get an error after a while:

```
Lady Gaga is in DATA 219.
The Rock is in DATA 219.
Obi-wan Kenobi is in DATA 219.
...
Elizabeth Jennings is in PSCI 401.
Stan Beeman is in PSCI 401.
Phillip Jennings is in PSCI 401.
...
Tyrion Lannister is in ENGL 101.
Jon Snow is in ENGL 101.
Daenerys Targaryen is in ENGL 101.
...
Han Solo is in CHEM 211.
Poe Dameron is in CHEM 211.
---------------------------------------------------------------
KeyError                    Traceback (most recent call last)
     77 for student in roster:
     78   print("{} {} is in {} {}.".format(student['first'],
---> 79     student['last'], course['prefix'], course['num']))
     80

KeyError: 'last'
```

Whoaaaa, what's *dat*?

### Encountering erroneous/missing data

This kind of error will happen all the time when you're working with JSON. The first step is not to panic. The second step is to calmly observe that apparently, everything was working fine up to a point...and then it suddenly broke. The third step is to look at that error message and see if you can make sense out of it. (Often, you can.) And the fourth step is to introduce some tactical debugging messages into your code, so that you can narrow down the source of the error.

I assume you've done those first two steps. On to the third: the error message. It says, quote:

```
KeyError: 'last'
```

and it evidently happened on line 79, which was in the middle of the `print()` statement. Put 2 and 2 together and you'll realize that when we attempted to extract the value of the `"last"` key for one of the dictionaries, *it wasn't there.* That's what "`KeyError`" turns out to mean: you asked for a particular key but there wasn't one in the dictionary.

The fourth step is crucial. It marks the difference between fledgling, flailing novices and cool, critical-thinking experts. We need to insert (temporarily) one or more `print()` statements into our loop, so that *right before the program crashes,* we get some crucial insight into what was about to go wrong.

This takes some practice and some intuition, but in this case let me simply observe what it makes sense to do. If we were about to access a non-existent key from a dictionary, it might illuminate things if we printed out the dictionary immediately before trying that stunt. That way, we'll see the state of affairs just before the error.

Here's the key line, inserted into the inner loop:

```
for course in c:
    roster = course['roster']
    for student in roster:
        print("The dict is: {}".format(student))
        print("{} {} is in {} {}.".format(student['first'],
            student['last'], course['prefix'], course['num']))
```

Now look at the revised output, below:

```
The dict is: {'email':'han.solo@corellia.gov', 'first':'Han',
    'last':'Solo'}
Han Solo is in CHEM 211.
The dict is: {'email':'dameron@resistance.org', 'first':'Poe',
    'last':'Dameron'}
Poe Dameron is in CHEM 211.
The dict is: {'email':'root@dagobah.net', 'first':'Yoda'}
---------------------------------------------------------------
KeyError                         Traceback (most recent call last)
     78  print("The dict is: {}".format(student))
     79  print("{} {} is in {} {}.".format(student['first'],
---> 80      student['last'], course['prefix'], course['num']))
     81

KeyError: 'last'
```

Aha! Our problem is `Yoda`, a student in CHEM 211 who doesn't have a last name.

It takes practice and experience to get a feel for where to insert meaningful debugging statements. The key question to ask is: "what do I wish I had known right before the error occurred?" Add lines of code to shed light on that question.

## Dealing with erroneous/missing data

Once you've discovered the absence of something you were looking for, you need to ask yourself what the implications are of it being missing. Sometimes it's a bona fide data error that means you need to investigate the source of the information, discard some data points, or something else. Other times (as in the Yoda case)

it's innocuous – not everyone has a last name, after all – but you still have to *deal* with the problem somehow so your program can continue.

In the case of a missing key which you can sensibly ignore, you can code around it as follows:

```
for course in c:
    roster = course['roster']
    for student in roster:
        if 'last' in student:
            print("{} {} is in {} {}.".format(student['first'],
                student['last'],course['prefix'],course['num']))
        else:
            print("{} is in {} {}.".format(student['first'],
                course['prefix'],course['num']))
```

The important line is the fourth one: "`if 'last' in student:`". The "`in`" keyword checks to see whether a dictionary has a certain key or not. In this case, if there is no `"last"` key, we want to simply print the first name and go on, not crash. The output is now satisfactory:

```
...
Han Solo is in CHEM 211.
Poe Dameron is in CHEM 211.
Yoda is in CHEM 211.
Emperor Palpatine is in CHEM 211.
Chewie is in CHEM 211.
Rey is in CHEM 211.
...
```

The appropriate way to deal with an error like this varies depending on the situation. This is why you need to back away from the keyboard, take a walk, and ask yourself, "what does it *mean* when this value is absent or corrupt? Does that imply that I need to throw out that data point? Or that something deep and sinister is going on? Or is there a way to safely ignore it?"

## 8.3 Analyzing class sizes

Let's end this chapter with a real-life analysis example. At universities (including our own) administrators keep close tabs on class sizes, for two reasons: classes that are too small are an inefficient drain on teaching resources, and classes that are too large diminish students' learning outcomes.

Suppose we were in the Provost's office, and had this JSON data set at our disposal. How could we use it to answer the following question: "how do class sizes compare among the various disciplines?"

You could answer this lickety-split if you only had a `DataFrame` with `prefix` and `size` columns. You'd just create a box plot with `prefix` as your categorical variable and `size` as your numeric one. The question is how to get such a `DataFrame` from this complex, hierarchical JSON data set?

It's really the same kind of thing we did in the previous examples: you create loops to sift through the data, extracting exactly what you want. In this case, for each course in the list, we simply need two things:

1. its `prefix`, and
2. the length of its `roster` list.

```
for course in c:
    roster = course['roster']
    for student in roster:
        print("{} {} is in {} {}.".format(student['first'],
            student['last'],course['prefix'],course['num']))
```

Now you'll recall from back in section 6.3 (p. 55) that if you have two NumPy arrays, you can stitch them together into a `DataFrame` by using a dictionary that names each array as a column. So our challenge boils down to the problem of creating two arrays: one with the prefix of each class, and the other with the size of each roster.

In this case, we start out knowing exactly how many elements these arrays will have; namely, however long our `c` list is. The best thing to do is create two initially-empty arrays, and then fill them up with values in the loop. Here we go:

```
prefixes = np.empty(len(c), dtype=object)
sizes = np.empty(len(c), dtype=int)
```

The NumPy `empty()` function says "make me an array of the right type but with no particular initial values, because I'm going to fill them up myself with what I want." You may remember that "`dtype`" stands for "data type," and that "`object`" is the way we say "strings, please." (Props if you do.)

Then, we write a loop that iterates through all the courses, setting each `prefixes` value to the `"prefix"` key of the corresponding course, and each `sizes` value to its roster size. See if you can follow this code which does that:

```
for x in np.arange(0,len(c)):
    prefixes[x] = c[x]['prefix']
    sizes[x] = len(c[x]['roster'])
```

Remember that "`np.arange()`" is a way of generating all the successive from one extreme to another. In this case, we want `x` to go from 0 (the first time through the loop) to `len(c)-1` (the last time). For each value of `x` (0, 1, 2, ..., 200) we extract the appropriate part of the `c` structure and fill in our two arrays' values.

Printing these verifies it worked:

```
print(prefixes)
```

```
['DATA' 'CPSC' 'CPSC' 'SOCG' 'MATH' 'CPSC' 'PHYD' 'CLAS' 'SPAN' 'BIOL'
 'PSCI' 'PHYD' 'PHYD' 'CPSC' 'BIOL' 'CPSC' 'ENGL' 'DATA' 'ENGL' 'CLAS'
 'BIOL' 'CLAS' 'STAT' 'BIOL' 'PHYD' 'PHYD' 'STAT' 'MATH' 'SOCG' 'SPAN'
 'CLAS' 'CPSC' 'PHYD' 'DATA' 'DATA' 'MATH' 'MATH' 'PHYD' 'MATH' 'STAT'
 'MATH' 'BUAD' 'DATA' 'DATA' 'PSCI' 'BIOL' 'CPSC' 'DATA' 'MATH' 'PSCI'
 'CLAS' 'BUAD' 'MATH' 'BIOL' 'SPAN' 'PHYD' 'DATA' 'PHYD' 'ENGL' 'STAT'
 'MATH' 'ENGL' 'DATA' 'ENGL' 'STAT' 'PSCI' 'SPAN' 'BUAD' 'PHYD' 'PSCI'
 'CPSC' 'CPSC' 'BUAD' 'SPAN' 'BIOL' 'SPAN' 'STAT' 'BIOL' 'BIOL' 'PHYD'
 'PSCI' 'BUAD' 'BUAD' 'SPAN' 'BUAD' 'BUAD' 'BUAD' 'MATH' 'BUAD' 'PSCI'
 'DATA' 'PHYD' 'PHYD' 'STAT' 'BUAD' 'PHYD' 'CPSC' 'MATH' 'DATA' 'PHYD'
 'BUAD' 'STAT' 'SPAN' 'ENGL' 'CLAS' 'CLAS' 'SOCG' 'ENGL' 'MATH' 'SOCG'
 'PSCI' 'MATH' 'SPAN' 'BUAD' 'BUAD' 'BUAD' 'SPAN' 'BIOL' 'DATA' 'CPSC'
 'PSCI' 'CPSC' 'SOCG' 'BIOL' 'PSCI' 'STAT' 'PHYD' 'SOCG' 'SPAN' 'BUAD'
 'PSCI' 'MATH' 'MATH' 'CLAS' 'STAT' 'MATH' 'SPAN' 'CPSC' 'SPAN' 'DATA'
 'PSCI' 'SPAN' 'CLAS' 'PHYD' 'CPSC' 'CPSC' 'SOCG' 'PSCI' 'SPAN' 'PSCI'
 'PSCI' 'CPSC' 'STAT' 'PHYD' 'BIOL' 'BIOL' 'STAT' 'CLAS' 'STAT' 'MATH'
 'BUAD' 'PHYD' 'BUAD' 'BIOL' 'DATA' 'SPAN' 'CPSC' 'ENGL' 'CPSC' 'PHYD'
 'BUAD' 'BUAD' 'ENGL' 'SOCG' 'PSCI' 'STAT' 'DATA' 'ENGL' 'CPSC' 'DATA'
 'STAT' 'SPAN' 'SOCG']
```

```
print(sizes)
```

```
[35 29 28 14 25 30 20  7 15 21 22 25 14 18 28 22 28 23 22 23 10 25 24 10 13
 19 18 16 23 22 15 26  8 30 22 29 21 22 12 25 22 12 26 12 25 19 26 12 21 26
 12 18  7 18 23 20 22 16 21 25 16 21 18 20 20 19 29 24 25 24 17 16 22 23 19
 28 22 15 22 17 17 21 21 19 17 25 15 24 16 25 21 16 24 19 15 15 28 19 23 20
 12 29 19 30 17 15 23 24 15 18  9 19 12 21 13 15 15 12 20 15 15 22 17 16 23
 27 21 22 25 20 24 22 20 15 24 15 23 17 22 12 25  8 13 15 17 30 18 25 18 24
 17 18 26 27 16 13 16 22 19 18 29 14 18 21 21 24  6 13 15 17 13 23 21 24 29
 26 23 28 15  4 20 15 25 15 14 17 28 22 30 19 13 22 18 21]
```

Now we just create our `DataFrame`:

```
course_info = pd.DataFrame({'prefix':prefixes, 'size':sizes})
print(course_info)
```

```
     prefix  size
  0     DATA    35
  1     CPSC    29
  2     CPSC    28
  3     SOCG    14
  4     MATH    25
  ..     ...   ...
```

and do our box plot:

```
course_info.boxplot("size", by="prefix")
```

Figure 8.1 gives the goods. Looks like our university's Computer Science (CPSC) and Data Science (DATA) classes have the highest enrollment (no surprise), while Classics (CLAS) is lagging behind the others.

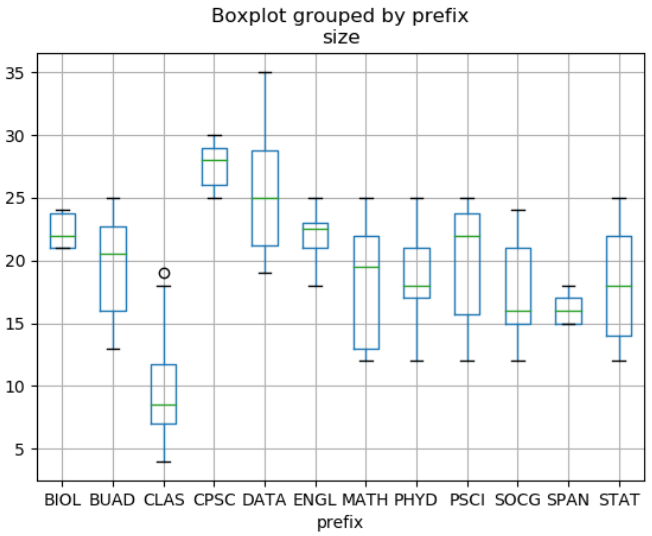



**Figure 8.1:** A straightforward analysis, culled from JSON data.

By the way, in this case it was clear from the outset how many rows would be in our `DataFrame`, because the `c` list had one element in it for each class, and each class would obviously result in one prefix and one size. Sometimes, you don't know how many elements it will have until you're done sifting through the JSON. In that case, you could use this pattern instead:

```
prefixes = np.empty(0, dtype=object)
sizes = np.empty(0, dtype=int)

for course in c:
    prefixes = np.append(prefixes, course['prefix'])
    sizes = np.append(sizes, len(course['roster']))
```

You see how this works: instead of starting off with arrays of the proper length, we start off with *zero* length, and simply `append()` a value to each of them as we go. Warning, however: this approach is *way* slower if the data size is large. Doing a bunch of appends forces Python to create a whole new array each time through the loop, copying the contents! It's always faster to **pre-allocate** arrays of the proper length – or perhaps, of a safe "large enough" length which we can then truncate at the end with a slice – than to do this repeated-appending approach.

Bottom line: once you get your data into a `DataFrame`, you can bring all your powers to bear upon it. Getting it into one is largely a matter of looping and selectively extracting.

# Chapter 9

# LOWESS

A common exploratory technique for bivariate, numerical data involves finding a smooth curve to approximate a noisy data set. The structure of the data – and whether there even is a relationship between the two variables at all – may be more easily visible from such a curve than from a raw splattering of points.

## 9.1 Best-fit line: "parametric"

In your stats class, you probably learned how to compute the best-fit line to a set of bivariate numerical data points, where "best fit" was taken in a "least squares" sense (*i.e.*, the line that minimizes the sum of the squared deviations of the line from the actual data points). It will not surprise you that it's easy to do this in Python as well, as shown in Figure 9.1 (p. 90).

NumPy's "`polyfit()`" function stands for "polynomial fit." You'll recall from high school algebra that a polynomial is a function that involves only *powers* of your $x$ variable: squares, cubes, and so forth (no sines, cosines, logarithms, "$e$-to-the's" or anything else). Also permitted are a plain-old $x$ term (since that's $x^1$, or "$x$ to the first power") and a constant term (since that's $x^0$, or "$x$ to the zeroth power"). And any of these things can be multiplied by any coefficient you like. So, one example polynomial would be:

$$y = 4.3x^3 - 29.4x^2 + 6x - 13.8$$

The **degree** of a polynomial is the highest exponent it contains; this example has degree 3.

```
# Create x points and some crazy, noisy y function of them.
x = np.random.uniform(0,100,100)
x.sort()
y = 4*x - .2 * x**2 + np.random.normal(0,120,100)

# Get the slope and intercept of the best-fit line.
m, b = np.polyfit(x, y, 1)

# Heck, while we're at it let's find the best-fit quadratic too.
a1, a2, a3 = np.polyfit(x, y, 2)

# Plot the points and the approximations.
plt.scatter(x,y)
plt.plot(x, m*x + b,color="green")
plt.plot(x, a1*x**2 + a2*x + a3,color="purple")
```

**Figure 9.1:** Finding and plotting the best-fit (least-squares) line. (Note that we have to `.sort()` the $x$ points since we draw line plots based on them, and you get crazy zig-zags if you don't sort your $x$ values first.)

Now the `polyfit()` function asks: which polynomial can I pick (of a given degree) that will get the closest to the data points – *i.e.*, minimize the squared distances between the polynomial's value and the points? It takes three arguments: an array of $x$ values, an array of $y$ values, and the degree. It returns the coefficients for the best-fit polynomial of that degree. So in the Figure 9.1 code, this line:

```
m, b = np.polyfit(x, y, 1)
```

says "please give me the coefficients of the best-fit 1-degree polynomial to these `x` and `y` points." Since a 1-degree polynomial is a straight line, we got two coefficients back, which we named `m` and `b`, as is traditionally done. Plotting the actual line was accomplished with this code:

```
plt.plot(x, m*x + b,color="green")
```

which says "For each $x$ value in the data set, plot $x$ versus $mx + b$." And that, of course, plots the line with slope `m` and $y$-intercept `b`. Similar code plots the best-fit quadratic function (2-degree polynomial), or any degree we like.

No matter what degree we use, these approximations are called **parametric** models because they're based on (global) parameters: a slope and an intercept, say, or three coefficients in the case of the quadratic. In each case, we assume the data fit an overall particular "functional form" (like a line, or a quadratic) and say, "given that we feel like these data are 'really' a line, what parameters that describe a line would give us the best line?"

Figure 9.2 (p. 92) shows the best-fit line and best-fit quadratic (function with an $x^2$ term) for the points generated by the code in Figure 9.1.

## 9.2 LOWESS: "non-parametric"

A more sophisticated technique for this task is called "**LOWESS**" (sometimes "**LOESS**"[1]), which (sorta) stands for "Locally Weighted Estimated Scatterplot Smoothing." LOWESS tries to capture the overall trend of a messy set of data – but what distinguishes it from a best-fit line is that it operates *locally* rather than globally. When you crunch the numbers to find the best-fit least-squares line to a data set, you're asking, "what values of slope and intercept

[1]Some authors make a very fine distinction between the LOESS and the LOWESS techniques, which is too nitpicky to even get into here. We'll treat the two terms as synonymous.

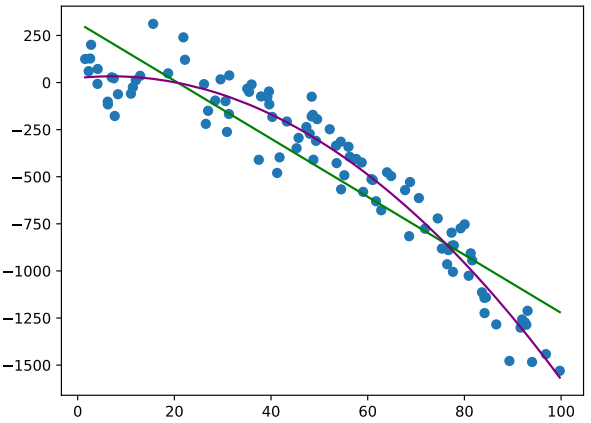



**Figure 9.2:** The best-fit line, and best-fit quadratic, to the set of points generated by the code in Figure 9.1.

for a *single* line across the *entire* data set will give me the lowest *overall* deviation from the points?" (The same is true for a best-fit quadratic, cubic, *etc.*) In other words, you're attempting to fit a single model over the entire range of data, and penalizing inaccuracies equally everywhere.

By contrast, the LOWESS technique approximates the data *locally*. This means that it weights the data points in such a way that points close to the location of interest contribute more strongly than do data points farther away. It does this by fitting a linear (or polynomial) regression to each $x$ point of interest, but using a weighted contribution from only the nearby points.

Here's how it works. We start with a bunch of $(x, y)$ points, and we want to compute a "locally smoothed" $y$ for every one of the $x$'s.

First, we have a parameter $\alpha$ that specifies *what fraction of the data* to take into account (at all) for each estimate. This can be any value from 0 to 1. You might guess that the smaller it is, the more wiggly it'll allow our smoothed estimate to be, since we'll be considering only a small number of points. This is true, as we'll see.

Then, once we've fixed $\alpha$, we're going to find a bunch of best-fit, least-squares lines, one at each $x$ value. This is just like in regular old linear regression. The catch is that instead of minimizing the *sum* of squared differences, we're going to minimize the **weighted** sum. And we'll place a greater weight on the errors for $x$ points close to the one we're evaluating. This will have the effect of allowing the curve to bend closely to our actual data points while ignoring stuff that's far away.

Written in equations, the ordinary best-fit line approach finds an $m$ and $b$ that minimize the overall sum of squared deviations (or "residual sum of squares"):

$$RSS = \sum_i (y_i - (mx_i + b))^2$$

But with LOWESS, we calculate this separately for every $x$ point, and we weight this with a **weight function** $w$:

$$RSS(x) = \sum_i w(x - x_i) \cdot (y_i - (mx_i + b))^2$$

Note how the weight function is given the distance between the $x$ value of interest and the locations of the actual data points. Since we want to weight close-by points more heavily, the $w$ should be higher for values closer to zero.[2]

This is **non-parametric** because when we're done, if somebody asked, "hey, I like your LOWESS curve – what parameters did you use for it?" the answer would be "uh...there really aren't any parameters." The curve is a messy combination of a bunch of different shifting approximations that we calculated as we went through the

[2] If you're really on your game, you might observe that the weight function is much like the *kernel* for KDEs: in fact, it really is basically a kernel. Thus we can use a Gaussian for it, just like we did for KDEs, although it's more common with LOWESS to use the so-called "tri-cube" kernel: $w(\Delta x) = (1 - |\Delta x|^3)^3$ for $|x| < 1$ (and 0 otherwise).

whole data set. We didn't choose parameters to plug into a particular model; in fact, we didn't really *have* a model.

Like KDEs, this technique wasn't computationally possible until the age of computers. Hence it's one of the newer kids on the block. Here's how to do it in Python with the `statsmodel` library:

```
from statsmodels.nonparametric.smoothers_lowess import lowess

l = lowess(y,x,frac=1/3)
plt.plot(l[:,0],l[:,1],color="red")
```

The "`frac`" parameter is our $\alpha$. The resulting curve for two different values of $\alpha$ is shown in Figure 9.3. Notice how $\alpha = \frac{1}{3}$ gives a much smoother line than $\alpha = \frac{1}{10}$, since it is using more points to do the smoothing. In fact, the former is quite close to the best-fit quadratic in this case. This is a manifestation of the classic "bias-variance trade-off" we'll look closely at in Chapter 24.

LOWESS might not appear to have much of an advantage over just a plain old line. But Figure 9.4 (p. 96) shows a data set where neither the line nor the quadratic are even in the ballpark, yet where LOWESS does quite well. Intuitively, if the data *aren't* ultimately generated by something linear (or close to it), a linear model will be hard-pressed to capture the curve.

In general, LOWESS is a better *exploratory* technique than best-fit parametric curves are. This is true for a couple of reasons:

- When exploring a data set, you're looking for patterns that stick out, and you want to let the data speak for itself. You're not coming to the data with a pre-established model choice and wanting to fit it. LOWESS lets you be model-agnostic and yet see the forest instead of just trees.
- LOWESS (and non-parametric methods in general) are "robust," meaning they aren't as adversely affected by outliers. Consider fitting a least-squares line to a set of data, and then introducing a couple of outliers near one of the far ends. This

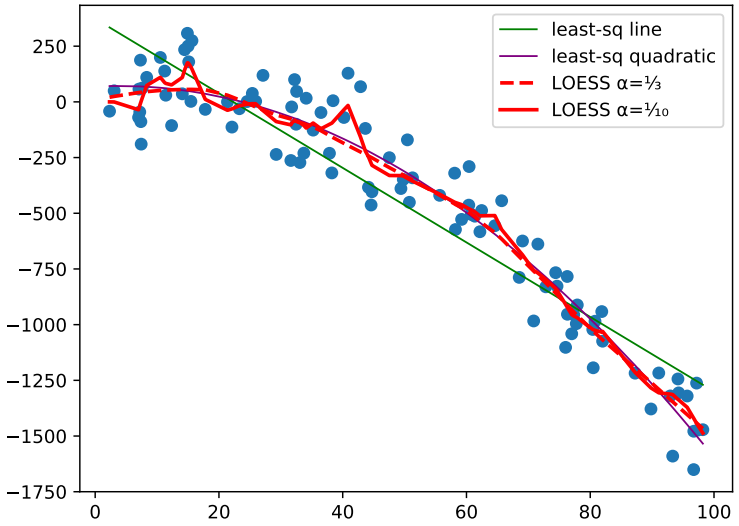



**Figure 9.3:** Various attempts to plot the "true, underlying pattern" of our noisy data set.

is going to force your global-error-minimizing best-fit line to swing radically away from the bulk of the data (which it may describe fairly adequately) in order to try and reach those outliers. Clearly this isn't a good fit for the data! LOWESS, however, will only "reach" for those outliers in the $x$ range when it gets near those outliers.

By the way, although we fit a *linear* function to each local point, we could fit a quadratic, cubic, or anything else. Here's something to think about: if we replaced the linear "$mx+b$" function with just a constant "$b$", then LOWESS becomes simply a weighted moving average. Oooo, deep.

Finally, remember to play with the $\alpha$ parameter just as you played with the kernel width and bin size in other exploratory techniques. Remember: changing this will give you different views on the data, and different views are good.

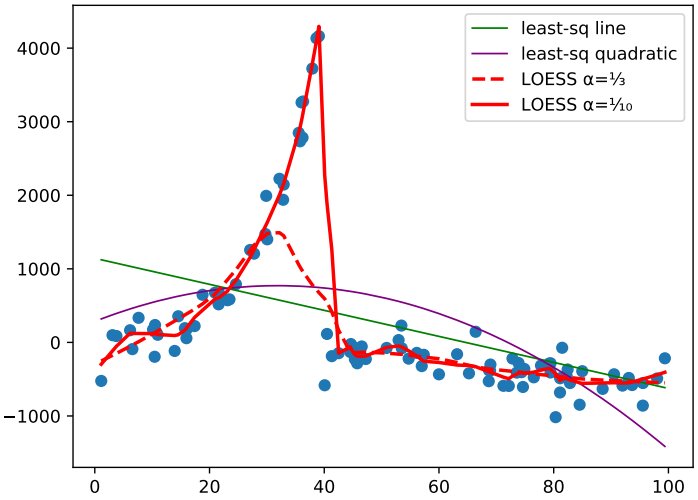



**Figure 9.4:** A decidedly non-linear data set, for which LOWESS (and particularly LOWESS with a low $\alpha$) does quite well.

# Chapter 10

# Data fusion

In this chapter we'll introduce the sexy-sounding technique of **data fusion**. Data fusion means combining and integrating multiple data sources into a single data set. This can give you richer, more useful information than any of the individual data sets could on their own.

## 10.1 Merge operations

On the ground, data fusion usually necessitates merging multiple tables together. As we've learned, the *lingua franca* of the data science world is the rectangular table perfectly reflected by a CSV file: it has (heterogeneous) rows, it has (homogeneous) columns, and is otherwise flat. In Pandas we speak of this structure as a `DataFrame`, of course.

More complicated data sets sometimes consist of *multiple* such tables. This is especially true if there are different aspects to the data, each of which is deserving of its own table. The tables are often implicitly related, as we'll see, through some piece of common information that links them together logically.

Moreover, there will be times in your career when you want to integrate multiple *different* data sets in some way, perhaps because each gives you information on some related aspect of a common phenomenon. Imagine if you found a data source giving vote totals for various political candidates, and a different data source docu-

menting the financial donations that their campaigns received. An obvious question would be: "to what extent do a candidate's contributions relate to his/her vote count?" This kind of analysis is only possible if the two data sets can be merged in a coherent way, so that the vote totals for a candidate are properly associated with the contributions to that same candidate's campaign.

We'll use the term **merge** (or **join**) to describe the operation of connecting two tables/`DataFrame`s into one, based on a common linking piece of information. The term **fusion** is usually restricted to the case described in the previous paragraph; namely, when the two tables to be joined are from different data sets entirely.

## 10.2 Merging in Pandas

The basic idea is that in order to meaningfully merge two `DataFrames`, one (or more) columns in the first table must be logically linked to one (or more) columns in the second. "Logically linked" usually means "having the same values in them."

For example, consider Figure 10.1, which contains two `DataFrame`s from a data source like IMDB. There are clearly questions we'd like to ask which involve both `DataFrame`s together, rather than each in isolation. For instance, "have actor salaries been going up over time?" or "how often have various actors worked with specific directors?"

Merging here is simple: we simply identify *the common column* which unites rows from the two tables. Clearly, it's the film title: we know that Scarlett Johansson was directed by Joss Whedon because a `Johansson` row in the `roles` table has the same film name as a `Whedon` row in the `movies` table.

In database parlance, we call the `title` column of the `movies` table its **primary key** (PK), and we call the `film` column of the `roles` table a **foreign key** (FK). The primary key / foreign key relationship is supposed to suggest that for every row in the `roles` table, its `film` value *will* appear in one row of the `movies` table (namely, in that row's `title` column).

roles:

| actor | film | salary (millions) |
|---|---|---|
| Downey Jr. | The Avengers | 50 |
| Johansson | The Avengers | 20 |
| DiCaprio | Inception | 59 |
| Hanks | Forrest Gump | 70 |
| Bullock | Gravity | 77 |
| Downey Jr. | Iron Man 3 | 51 |
| Hanks | Saving Private Ryan | 40 |
| . . . | | |

movies:

| title | director | year |
|---|---|---|
| Inception | Nolan | 2010 |
| The Avengers | Whedon | 2012 |
| Forrest Gump | Zemeckis | 1994 |
| Gravity | Cuaron | 2013 |
| Star Wars | Lucas | 1977 |
| . . . | | |

**Figure 10.1:** Two DataFrames from an IMDB-like source.

To "join" these two DataFrames all in one fell swoop, we execute a command like this:

```
roles_movies = pd.merge(roles, movies, left_on="film",
    right_on="title")
```

This produces a new DataFrame that contains (1) all the columns of the two, and (2) a row for each pair of original rows that match on their movie title. Notice we had to specify *two* arguments (besides the table names) to pd.merge(): "left_on" (for the name of the merging column in the first DataFrame) and "right_on" (for the second). If these two columns had the same name, we could just specify a single argument called "on" for the two.

The `roles_movies` table will look like this:

```
                          roles_movies:
actor       film          salary     title          director     year
-------------------------------------------------------------------------
Bullock     Gravity        77        Gravity        Cuaron       2013
DiCaprio    Inception      59        Inception      Nolan        2010
Johansson   The Avengers   20        The Avengers   Whedon       2012
Downey Jr.  The Avengers   50        The Avengers   Whedon       2012
                               . . .
```

(The sequence of the rows is not in general reliable, and you should not depend on them being in the order you expect.) This `DataFrame` can be used to answer either of the questions we posed above, and others.

Note that our new table has some redundant information (the `film` and `title` columns are identical) which you can remove using normal Pandas operations if you wish.

## 10.3 Odds and ends

1. Sometimes we want to merge on more than one column:

   ```
   df = pd.merge(votes, contribs,
       left_on=['first_name','last_name'],
       right_on=['candidate_first','candidate_last'])
   ```

   This gives us rows in the result only when the values in *both* the `first_name` and `last_name` columns of `votes` match the `candidate_first` and `candidate_last` columns of `contribs`.

2. If we're lucky, the name(s) of the column(s) we want to merge on are named exactly the same in both `DataFrame`s. In this case, we don't have to specify `on`, `left_on`, or `right_on`: we can just do the `merge()` with two arguments:

```
merged_df = pd.merge(df1, df2)
```

This is called a "**natural join**," and also has the benefit of only including the joined column(s) once in the result, rather than preserving duplicates.

3. The default merge operation we've been doing so far is sometimes called an "**inner join**". This means that *if there is no corresponding match for a row in one of the `DataFrames`, there will be no associated row in the result.* This is normally what we want. In the movies example, if we don't have a row in the `movies` table for a particular film, then we don't know the year for that film, and it's (perhaps) pointless to include any of the actors in that film in the resulting merged `DataFrame`.

   Sometimes, we want to make sure that every row in the left (or right, or both) `DataFrame` appears in the result *at least once*, though, with corresponding null values if necessary. We can do this by specifying `'left'`, `'right'`, or `'outer'` as the value of the `'how'` argument to `pd.merge()`:

```
df = pd.merge(votes, contribs, left_on=['first_name',
    'last_name'], right_on=['candidate_first',
    'candidate_last'], how='outer')
```

4. Sometimes merging two `DataFrames` will result in column **name collisions**. Say that our `roles` table had also had a `year` column indicating the birth year of the actor:

```
                        roles:
actor           year    film                    salary
-----------------------------------------------------
Downey Jr.      1965    The Avengers              50
Johansson       1984    The Avengers              20
DiCaprio        1974    Inception                 59
Hanks           1956    Forrest Gump              70
Bullock         1964    Gravity                   77
                      . . .
```

Then the resulting `DataFrame` would need to have two columns named "`year`", with different meanings. Pandas solves this by renaming the conflicting columns with a "`_x`" or "`_y`" suffix, corresponding to the left/right tables in the join:

```
                              roles_movies:
actor      year_x   film       salary   title      director   year_y
-------------------------------------------------------------------
Bullock    1964     Gravity    77       Gravity    Cuaron     2013
DiCaprio   1974     Inception  59       Inception  Nolan      2010
```

(which you can rename via "`roles_movies.columns`" if you want, of course.)

## 10.4 One-to-many vs. many-to-many relationships

The above examples have featured "**one-to-many**" relationships between the two tables. This means that one of the `DataFrame`'s columns (the one with the primary key) has only *one* row for each matching value: *many* actors star in *one* movie, for instance. But sometimes we have a "**many-to-many**" relationship, in which both `DataFrame`s can have multiple rows with values that match the other. Consider the Halloween costumes data set below, with `costumes` and `children` tables:

```
print(children)
```

```
        child  age   costume
0     Allison   12      Elsa
1       Kiara    8  Princess
2       Mason   12    Batman
3       Jenny   12    Wizard
4     Wendell   11   Student
5  Betty Lou   10  Princess
6    Hermione   11    Wizard
7       Faith   13    Wizard
8       Julie   11      Elsa
```

```
print(costumes)
```

```
        accessory      costume
0           crown     Princess
1            wand     Princess
2           dress     Princess
3          helmet  Darth Vader
4           boots  Darth Vader
5     lightsaber  Darth Vader
6            cape  Darth Vader
7            cape         Elsa
8            wand         Elsa
9     lightsaber          Rey
10  utility belt       Batman
11         boots       Batman
12          cape       Batman
13          mask       Batman
14          cape         Anna
15           wig         Anna
16         boots         Anna
17          sack        Ghost
18    pointy hat       Wizard
19          wand       Wizard
```

In order to represent all these children in their chosen costumes, we need multiple matches from both `DataFrame`s for each costume value. This is because each `Princess` has more than one accessory, and there are also multiple children who want to *be* princesses. Therefore, we can potentially end up with a lot of rows in our result.

```
children_costumes = pd.merge(children, costumes,
    on="costume")
print(children_costumes)
```

```
         child  age   costume     accessory
0      Allison   12      Elsa          cape
1      Allison   12      Elsa          wand
2        Julie   11      Elsa          cape
3        Julie   11      Elsa          wand
4        Kiara    8  Princess         crown
5        Kiara    8  Princess          wand
6        Kiara    8  Princess         dress
7    Betty Lou   10  Princess         crown
8    Betty Lou   10  Princess          wand
9    Betty Lou   10  Princess         dress
10       Mason   12    Batman  utility belt
11       Mason   12    Batman         boots
12       Mason   12    Batman          cape
13       Mason   12    Batman          mask
14       Jenny   12    Wizard    pointy hat
15       Jenny   12    Wizard          wand
16    Hermione   11    Wizard    pointy hat
17    Hermione   11    Wizard          wand
18       Faith   13    Wizard    pointy hat
19       Faith   13    Wizard          wand
```

Btw, notice that poor `Wendell` was left out of the merged `DataFrame` entirely, since his costume did not have any accessories. We can include him by doing a "**left join**" (or even a full "**outer join**") like this:

```
children_costumes = pd.merge(children, costumes, on="costume",
    how="left"))
print(children_costumes)
```

This produces the output below. `Wendell`'s entry can now be found on line 11. The "`NaN`" is the placeholder Pandas uses for rows that didn't match when doing a left/right/outer join.

```
          child  age   costume     accessory
0     Allison   12      Elsa          cape
1     Allison   12      Elsa          wand
2       Kiara    8  Princess         crown
3       Kiara    8  Princess          wand
4       Kiara    8  Princess         dress
5       Mason   12    Batman  utility belt
6       Mason   12    Batman         boots
7       Mason   12    Batman          cape
8       Mason   12    Batman          mask
9       Jenny   12    Wizard    pointy hat
10      Jenny   12    Wizard          wand
11    Wendell   11   Student           NaN
12  Betty Lou   10  Princess         crown
13  Betty Lou   10  Princess          wand
14  Betty Lou   10  Princess         dress
15   Hermione   11    Wizard    pointy hat
16   Hermione   11    Wizard          wand
17      Faith   13    Wizard    pointy hat
18      Faith   13    Wizard          wand
19      Julie   11      Elsa          cape
20      Julie   11      Elsa          wand
```

We're now in a position to perform our analyses. For instance, we could assemble a grand shopping list:

```
print(children_costumes.accessory.value_counts())
```

```
wand           7
cape           3
pointy hat     3
crown          2
dress          2
mask           1
utility belt   1
boots          1
Name: accessory, dtype: int64
```

If the wand product turns out to have a safety hazard, we could find all children younger than a certain age who were issued wands:

```
print(children_costumes[(children_costumes.age < 10) &
    (children_costumes.accessory=="wand")])
```

```
          child  age   costume     accessory
   3      Kiara    8  Princess          wand
```

Or, if we had another `DataFrame` with `accessory` prices:

```
print(accessories)
```

```
       accessory  cost
 0          boots    14
 1           cape    11
 2          crown    12
 3          dress    22
 4         helmet    20
 5     lightsaber     9
 6           mask    10
 7     pointy hat    12
 8           sack     1
 9   utility belt     9
 10          wand     6
 11           wig    12
```

we could merge *this* `DataFrame` with our previously merged one, thereby producing a three-way merge:

```
full = pd.merge(children_costumes, accessories, on="accessory")
print(full)
```

```
        child  age   costume     accessory  cost
 0     Allison   12      Elsa          cape    11
 1       Mason   12    Batman          cape    11
 2       Julie   11      Elsa          cape    11
                      . . .
```

Now we could, say, compute the total cost of clothing these trick-or-treaters:

```
print("These kids will cost a total of ${}.".format(
    full.cost.sum()))
```

```
These kids will cost a total of $212.
```

Ouch. Consider these costs when contemplating family size.

## 10.5 "By the way...why?"

At this point you may be asking, "if we just have to merge the `DataFrame`s to do our analysis, why were they stored that way in the first place? Why not just have everything in one big CSV file?"

The answer has to do with **redundancy of information**. Consider the merged table on p. 100. It's not the most compact way of expressing the information, because certain pieces of data are repeated unnecessarily.

For instance, *The Avengers* was released in 2012. Our data source needs to record that. But in the merged table, this year would be repeated *for every actor/actress in the movie.* The same is true for the director of the film. By performing the merge, we have duplicated lots of values. In database terms, the data set has become **unnormalized**. This isn't always a bad thing, and in terms of performing standard ML (machine learning) algorithms, it's necessary. But you can see why we wouldn't want the data permanently stored that way. It consumes extra storage, plus it opens a Pandora's Box of possible contradictions: what if `Downey Jr.`'s `Avengers` row said 2012, while `Johansson`'s said 2014. Who would we believe?

Database normalization is a larger topic than we have time to fully cover in this class, but the basics are very simple. Conceptually: *each piece of information should be stored in one and only one place.* Generally speaking, when that's true, you have a **normalized** data set, which is most appropriate for storage and for communication to

other potential users. Analysts will proceed to unnormalize select parts of it in order to perform certain analyses.

# Chapter 11

# Long, wide, and "tidy" data

## 11.1 Wide form data

Consider the following `DataFrame` (called "`g`"), which contains a professor's grade book for his students:

```
print(g)
```

```
      name year   Q1   Q2   Q3   Q4   Q5   Q6   Q7   Q8
0  Beyonce   So  9.0 10.0  7.0 10.0  8.0 10.0  9.0 10.0
1    Jay-Z   Jr  7.0 10.0  4.0 10.0 10.0  8.0  3.0 10.0
2   Bortis   Sr  8.0 10.0  7.0  3.0  7.0  7.0  7.0  9.0
3      Han   So  NaN  1.0  NaN 10.0  7.0  8.0  7.0  2.0
4      Mal   Jr  5.0  4.0  9.0  NaN  7.0  2.0  5.0 10.0
5    Inara   Jr  3.0  3.0  4.0 10.0  6.0  4.0  7.0  5.0
6  Obi-wan   So  5.0 10.0  9.0  4.0  1.0  4.0  NaN  2.0
7     Finn   Jr  6.0  3.0  5.0  6.0 10.0  NaN  NaN  3.0
```

It's not hard to tell what's going on: each student's name and year in school is recorded, as is their grade on the eight class quizzes. Some students took zeroes on one of more quizzes (like `Han` did for quizzes 1 and 3), and the quiz grades range from 0 to 10.

The structural style for this kind of `DataFrame` is called **wide form**. Each piece of a student's data is in its own column, making the `DataFrame` quite "wide," and comparatively not very long (tall).

Now there's nothing wrong with wide form. All the data is there, and it allows us to ask many questions easily, like:

- What was Inara's score on Quiz #5? `g[g.name=="Inara"].Q5`
- The high score on Quiz #3? `g.Q3.max()`
- Mal's average quiz score? `g[g.name=="Mal"].mean(axis=1)`

Other kinds of questions, though, defy easy answers, like these:

- What was the overall average score (for all quizzes)? (?)
- How did class performance compare between the first half of the semester (quizzes 1-4) and the second half (quizzes 5-8)? (?)
- How did freshmen, sophomores, juniors, and seniors compare? (?)

The reason these questions are difficult are that we have quiz scores spread across different columns. As long as we're happy treating them in groups like that, it's easy, but as soon as we want to carve up the quiz scores in some other way, it becomes hard.

## 11.2 Long form data

The solution is to convert the `DataFrame` to a structure which collapses all the quiz data into a single column. For this, we use the `melt()` function from the Pandas package:

```
gl = pd.melt(g, ["name","year"], var_name="quiz",
    value_name="score")
```

Now this is kind of complicated so pay attention.

- The first argument is the name of the wide-form `DataFrame` you want to "melt."
- The second argument is a list of the columns *that you want to leave alone.* In other words, a list of "off-limits" columns that you want Pandas *not* to melt.
- The third argument, named `var_name`, is *the name you want for your new column whose values will be the old column names.* It can be hard to get your head around this one. You have to imagine all the current column names that you're

melting being put in a column, and ask yourself: "what is the right name for that new column?" In this case, since we're melting `Q1`, `Q2`, *etc.*, the right name for the column is something like "`quiz`," since those are the quiz numbers.

- Finally, the fourth argument, named `value_name`, is *the name you want for your new column whose values will be the old column's values.* You have to ask yourself: "what are those 'things' that are currently values in the `Q1`, `Q2`, *etc.* columns?" A reasonable answer would be "`score`," since each one is a quiz score.

We set the result of the `melt()` call to a variable called `gl` (where "`l`" stands for "long.") Here's what it looks like:

```
print(gl)
```

```
        name year quiz  score
0   Beyonce   So   Q1    9.0
1     Jay-Z   Jr   Q1    7.0
2    Bortis   Sr   Q1    8.0
3       Han   So   Q1    NaN
4       Mal   Jr   Q1    5.0
5     Inara   Jr   Q1    3.0
6   Obi-wan   So   Q1    5.0
7      Finn   Jr   Q1    6.0
8   Beyonce   So   Q2   10.0
9     Jay-Z   Jr   Q2   10.0
10   Bortis   Sr   Q2   10.0
11      Han   So   Q2    1.0
12      Mal   Jr   Q2    4.0
13    Inara   Jr   Q2    3.0
14  Obi-wan   So   Q2   10.0
15     Finn   Jr   Q2    3.0
16  Beyonce   So   Q3    7.0
              . . .
60      Mal   Jr   Q8   10.0
61    Inara   Jr   Q8    5.0
62  Obi-wan   So   Q8    2.0
63     Finn   Jr   Q8    3.0
```

This is called **long form**, for obvious reasons. We now have one row for every single quiz score. It might seem wordy, and I'll admit it's not as easy to locate and eyeball a single result. However, all our "hard" questions from above can be easily answered:

- What was the overall average score (for all quizzes)?
  `gl.score.mean()`
- How did class performance compare between the first half of the semester (quizzes 1-4) and the second half (quizzes 5-8)?
  `gl[gl.quiz.isin(["Q1","Q2","Q3","Q4"])].mean()`
- How did freshmen, sophomores, juniors, and seniors compare?
  `gl.groupby("year").score.mean()`

Turning what were column headings into *values* gave us all the flexibility we needed. We can still treat all the scores individually by quiz if we want to, but we can also treat them as a whole, or aggregate them in other ways (like by school year).

As an aside, one thing I'd probably do to this `DataFrame` is get rid of the leading "`Q`" before each `quiz` value, and convert that column to integers to boot:

```
gl.quiz = gl.quiz.str[1]
gl.quiz = gl.quiz.astype(int)
print(gl)
```

```
       name year  quiz  score
0   Beyonce   So     1    9.0
1     Jay-Z   Jr     1    7.0
2    Bortis   Sr     1    8.0
3       Han   So     1    NaN
4       Mal   Jr     1    5.0
5     Inara   Jr     1    3.0
6   Obi-wan   So     1    5.0
7      Finn   Jr     1    6.0
8   Beyonce   So     2   10.0
9     Jay-Z   Jr     2   10.0
10   Bortis   Sr     2   10.0
11      Han   So     2    1.0
12      Mal   Jr     2    4.0
13    Inara   Jr     2    3.0
14  Obi-wan   So     2   10.0
15     Finn   Jr     2    3.0
16  Beyonce   So     3    7.0
17    Jay-Z   Jr     3    4.0
18   Bortis   Sr     3    7.0
```

The "`.str`" suffix, you'll recall, lets us perform standard string operations (like `len()`, `contains()`, or indexing) on entire `DataFrame` columns. Here, by saying "`gl.quiz.str[1]`", we're requesting only the *second* character (character #1) of each string, which extracts the "`1`" from "`Q1`" and so forth.

Treating quiz numbers like the integers they are is conceptually correct, and also allows us to do things like query for things like "quizzes after quiz #3" instead of having to list a bunch of categorical values.

## 11.3 "Tidy" data

The term "tidy" to describe a data set has sprung into prominence recently as a result of the excellent paper by Hadley Wickham (of R fame) who neatly captured the perils of various data formatting choices. Hadley first defined these terms:

- **variable** – a category of something, for which individual objects have a value. Examples: name, height, gender, center field distance.
- **value** – an actual individual piece of data corresponding to a variable for one object. Examples: Kylo Ren, 5'6", female, 390 feet.
- **observation** – a particular measurement that comprises all the information necessary to interpret that measurement. Examples: Jeff's weight was 165 lbs., Jenny's golf score at Field & Cross Links in the rain was 88. (In the first example, "all the information necessary" includes "Jeff" and "165"; in the second, it includes "Jenny", "Field & Cross Links", "rainy", and "88".)
- **observational unit** – a collection of all the observations of a particular type. ("Golf performances" would be an observational unit, separate from a "golfers" unit which contains information about golfers themselves, not their particular performances.)

Then, he outlined one simple rule. A data set is considered **tidy** if and only if:

1. Each observational unit is in its own table.
2. In each table, each observation forms a row.
3. In each table, each column header is a variable, and the column contains values.

Point #1 is essentially the same as "normalized," from section 10.5 (p.107). Points #2 and #3 are essentially "long form," as described in the previous section. Hence, I usually think of "tidy" as meaning "normalized and long."

Our `gl` grade book was long, but not tidy, because it had repeated information in it: namely, every student's `year` was repeated for every one of their quiz scores. To normalize it, we'd want to divide it into two tables; say, `student_years` and `grades`:

```
student_years = gl[['name','year']].drop_duplicates()
grades = gl.drop('year',axis=1)
```

The `.drop_duplicates()` method gets rid of identical rows, retaining only one. The `.drop()` method keeps all columns except for one, which is convenient if you don't want to type all the names of the ones you want to keep. ("`axis=1`" means "I'm talking about columns here, not rows.")

Our two remaining (tidy!) `DataFrames` are now:

```
print(student_years)
```

```
      name year
0  Beyonce   So
1    Jay-Z   Jr
2   Bortis   Sr
3      Han   So
4      Mal   Jr
5    Inara   Jr
6  Obi-wan   So
7     Finn   Jr
```

```
print(grades)
```

```
      name  quiz  score
0  Beyonce     1    9.0
1    Jay-Z     1    7.0
2   Bortis     1    8.0
3      Han     1    NaN
4      Mal     1    5.0
5    Inara     1    3.0
6  Obi-wan     1    5.0
7     Finn     1    6.0
8  Beyonce     2   10.0
9    Jay-Z     2   10.0
10  Bortis     2   10.0
11     Han     2    1.0
12     Mal     2    4.0
13   Inara     2    3.0
14 Obi-wan     2   10.0
15    Finn     2    3.0
16 Beyonce     3    7.0
17   Jay-Z     3    4.0
18  Bortis     3    7.0
          . . .
```

Every piece of information in one and only one place. Very tidy indeed.

### Messy data sets

Some data sets don't make it easy on us. Check out this decidedly *un*tidy one, which contains survey results about income and religious affiliation:

```
   religion   <$10k   $10-20k  $20-30k  $30-40k   $40-50k  $50-75k
0  Agnostic      27        34       60       81        76      137
1   Atheist      12        27       37       52        35       70
2  Buddhist      27        21       30       34        33       58
3  Catholic     418       617      732      670       638     1116
4     Other      15        14       15       11        10       35
...
```

As before, the problem here is that *the column headings are actually values, not variables.* Think about it: "`$10-20k`" isn't the name of a variable which might have actual values, but the value (range) itself of some variable.

Again the two questions: (1) What would the variable be for these column values? Answer: *Income.* (2) What are the cells themselves representing? Answer: *Frequency.* (*i.e.*, the number of people polled in the survey who had that religion and that income level.)

Now we can tidy this with `melt()`:

```
tdf = pd.melt(df, ['religion'], var_name='income',
    value_name='frequency')
```

```
        religion    income  frequency
    0    Agnostic     <$10k         27
    1     Atheist     <$10k         12
    2    Buddhist     <$10k         27
    3    Catholic     <$10k        418
   ...
```

By the way, the inverse operation of "melt" is often called "**pivot**". To reverse the above transformation in Pandas, you can use the `pivot()` function:

```
df = pd.pivot(tdf, index='religion', columns='income',
    values='frequency')
```

and get back your original wide form `DataFrame`.

# Chapter 12

# Dates and times

One of the most common categories of information you'll ever deal with are those dealing with various aspects of *time*. It turns out this is considerably more complex than you might think at first. For one thing, the English word "time" can mean several different things – a point in time (12:05pm on Feb. 20, 2021), an abstract wall clock time (12:05pm), a duration of time (1 hour and 15 minutes), and possibly other things.

For another, the clock and calendar systems that humans have devised are just plain weird. Why does the break between "am" and "pm" occur between 11 and 12 (11am, 12**p**m, 1pm) instead of between 12 and 1 where any sane person would put it? Why do some months have more days than others? Heck, they don't even follow the moon. And why do some *years* have more days than others? And why doesn't every month start over on a Monday? And so forth. There are good answers to some of these questions, and lousy answers to others, but they all make dealing with time a major pain.

## 12.1 The `datetime` package

Python helps deal with the pain through the `datetime` package. You have to import it, of course, which I usually do via:

```
import datetime as dt
```

The package has these goodies:

- **The `timedelta` type**. Variables of this type represent *durations in time*. You can create them like this:

  ```
  one_semester = dt.timedelta(weeks=15)
  one_year = dt.timedelta(weeks=52)
  this_class = dt.timedelta(hours=1, minutes=15)
  finger_snap = dt.timedelta(seconds=.1)
  ```

  You can also use `days`, `milliseconds`, and `microseconds`. Anything else is ambiguous. (Ask yourself: why?)

  Don't think of the `timedelta` variable you create as being intrinsically "in" any particular unit – just think of it as an "amount of time," which could then be expressed in any units.

  `timedelta`s can be positive or negative, by the way, and you can add or subtract them to/from each other to get other `timedelta`s:

  ```
  print(one_semester - this_class)
  print(this_class + finger_snap)
  print(one_semester - one_year)
  ```

  ```
  104 days, 22:45:00
  1:15:00.100000
  -259 days, 0:00:00
  ```

  After printing the number of whole days (if any), the rest of the output gives time in *hours*:*minutes*:*seconds*:*microseconds*. Note that the last of these three outputs is negative, since `one_semester` is obviously shorter than `one_year`.

- **The `date` type**. Each `date` variable represents a date in an idealized Gregorian calendar. You can create them via:

```
election_day = dt.date(year=2020, month=11, day=3)
primary_day = dt.date(year=2020, month=3, day=4)
here_we_are = dt.date.today()
```

If you *subtract* two `date`s, you get a `timedelta`. If you *add* a `date` to a `timedelta`, you get another `date`.

```
print(type(election_day - primary_day))
print(election_day - primary_day)
print(type(primary_day + one_semester))
print(primary_day + one_semester)
```

```
datetime.timedelta
244 days, 0:00:00
datetime.date
2020-06-17
```

Note that if your `timedelta` has precision more granular than days, it is lost in these operations:

```
if dt.date.today() == dt.date.today() + finger_snap:
    print("It'll still be the same day a finger snap from now.")
if dt.date.today() == dt.date.today() + this_class:
    print("It'll still be the same day one lecture from now.")
if dt.date.today() == dt.date.today() + one_semester:
    print("It'll still be the same day one semester from now.")
```

```
It'll still be the same day a finger snap from now.
It'll still be the same day one lecture from now.
```

You can also compare dates with comparison operators like `<` and `>=`:

```
if primary_day < election_day:
    print("The primary occurs before the election, duh!")
else:
    print("Wuuuut??")
```

```
The primary occurs before the election, duh!
```

- **The `time` type.** A "time," by itself, represents an abstract wall clock time, independent of any particular day. It doesn't mean "5pm this afternoon" but rather "5pm's in general."

```
start_of_class = dt.time(hour=12, minute=35)
dinner_time = dt.time(hour=18, minute=0)
```

These can also be compared in expected ways, but *not* added or subtracted (which actually wouldn't make sense – why?)

- Finally, we have **the `datetime` type**, which as its name suggests, combines features of both dates and times. In fact, a `datetime` variable represents *an absolute, specific point in history*. Creation options include:

```
this_exact_moment = dt.datetime.now()
terrorist_attack = dt.datetime(2001, 9, 11, 10, 33)
print("Right now it's: {}".format(this_exact_moment))
print("A horrible thing occurred at: {}".format(
    terrorist_attack))
```

```
Right now it's: 2021-03-10 09:33:57.015432
A horrible thing occurred at: 2001-09-11 10:33:00
```

We can also use the `datetime`'s `.combine()` method to put a `date` and a `time` together into a `datetime`:

```
todays_class = dt.datetime.combine(here_we_are,
    start_of_class)
print("Today's lecture is at: {}".format(todays_class))
```

```
Today's lecture is at: 2021-03-03 12:35:00
```

`datetime`s can be subtracted from each other, and `timedelta`s can be added or subtracted to/from them to produce other `datetime`s. They can also be compared. Finally, `.time()` and `.date()` methods will produce the constituent parts as `time` or `date` variables, accordingly.

## 12.2 Parsing and formatting

Now most of the time we won't be creating `datetime` variables using the techniques above. Instead, we'll be *parsing* them from string data.

There are a seemingly unlimited number of ways that dates and times can be expressed in strings. Just consider a few possibilities:

- Feb. 29, 2021 4pm
- Feb 29, 2021 4:00pm
- Feb 29, 2021 4:00 P.M.
- 4/29/21 4:00 P.M.
- 4/29/21 16:00
- 02/29/21 16:00:00
- 29-Feb-2021 4:00pm
- 2021-Feb-29 16:00:00
- ...

and on it goes. It's a testimony to the power of the human mind that we can look at these and at a glance infer what date/time was intended. Getting a computer to automatically do so is somewhat of a challenge.

### Pandas' auto-parsing

The great news is that in many cases, Pandas can auto-parse common date formats and convert strings into the proper kinds of objects. There are two ways of doing this: as you're loading a file with `read_csv()`, and after the fact.

### Parsing dates with `read_csv()`

With `read_csv()`, you can pass an argument called `parse_dates`, whose value should be a *list* of the columns you want it to auto-parse. Suppose we had a CSV file that looked like this:

```
Donor,Date,Amt,Party
Barack X. Tyrell,Tue 09/05/17,$3370,I
Gandalf A. Trump,Tue 07/18/17,$70,R
Jay-Z G. Targaryen,18-Dec-2017,$170,D
Brad T. Bolton,Thu 01/26/17,$1840,R
Luke T. Obama,29-Sep-2017,$4230,D
Matt Y. Kenobi,Sun 12/25/16,$3695,I
Gandalf Z. Pitt,07-Jun-2017,$6375,I
            .  .  .
```

This is a record of campaign contributions from various donors, which includes the date of the donation as well as the amount. Both columns are going to be problematic for us: the amount because of the leading dollar sign, and the date because it's in a god-awful mixed format.

If we just read it normally, we'd get this:

```
contribs = pd.read_csv("contribs.csv")
print(contribs)
```

```
                   Donor          Date    Amt Party
0       Barack X. Tyrell  Tue 09/05/17  $3370     I
1       Gandalf A. Trump  Tue 07/18/17    $70     R
2     Jay-Z G. Targaryen   18-Dec-2017   $170     D
...                  ...           ...    ...   ...
7181      Katy I. Tyrell  Thu 11/02/17   $140     R
7182     Brad T. Baggins  Fri 01/22/16  $1255     R
7183    Taylor E. Thrace  Sun 02/26/17  $3235     D
```

This has all the information in it, but not in a format we can do anything with. See, the dates and the amounts are just strings:

```
print(contribs.Date)
```

```
0    Tue 09/05/17
1    Tue 07/18/17
2     18-Dec-2017
3    Thu 01/26/17
4     29-Sep-2017
Name: Date, dtype: object
```

```
print(contribs.Amt)
```

```
0    $3370
1      $70
2     $170
3    $1840
4    $4230
Name: Amt, dtype: object
```

(Recall that "`object`" – as we saw on p. 85 – is just a dumb way of saying "string." Both these columns, therefore, are strings.)

It might not be obvious to you what the problem is with that. After all, isn't `str` the correct type for text sequences like "`Tue 07/18/17`" and "`$1840`" and "`18-Dec-2018`"?

Sure it is, but realize that we can't *do* anything interesting with dates or amounts if they're in that format. For example, we can't do any of the following:

- take the average or add up all the amounts (because they're not numbers!)
- sort the transactions chronologically (because you can't simply alphabetize strings like "`Tue 07/18/17`" and get chronological order!)
- ask basic questions like "how did the average donation amount change before and after the 2016 Presidential election?"
- ...

The problem is that even though a human looks at a string like "`Mon 05/14/19`" and instantly recognizes a date (and a string like "`$1800`" and recognizes a numerical amount in dollars), we don't actually *have* dates or amounts to work with. We have sequences of characters.

So we fix all this in an instant by simply passing a `parse_dates` argument with the names of the column(s) we want it to parse:

```
contribs = pd.read_csv("contribs.csv", parse_dates=['Date'])
```

Now, our `Date` column looks like this:

```
print(contribs.Date)
```

```
0   2017-09-05
1   2017-07-18
2   2017-12-18
3   2017-01-26
4   2017-09-29
Name: Date, dtype: datetime64[ns]
```

which, as you can see by the `dtype`, is full of useful `datetime` variables instead of useless strings.

Now we can do stuff like sort by dates:

```
print(contribs.sort_values(['Date']))
```

```
                      Donor       Date   Amt Party
6698         Wash T. Thrace 2015-06-28  1365     I
2561       Frodo X. Tyrell 2015-06-28  3500     R
4149     Katy U. Skywalker 2015-06-28  1855     I
...                    ...        ...   ...   ...
5651        Rey U. Aniston 2021-02-21  2915     D
2408       Tyrion M. Perry 2021-02-21  4755     I
6735      Taylor W. Tyrell 2021-02-21  2780     D
```

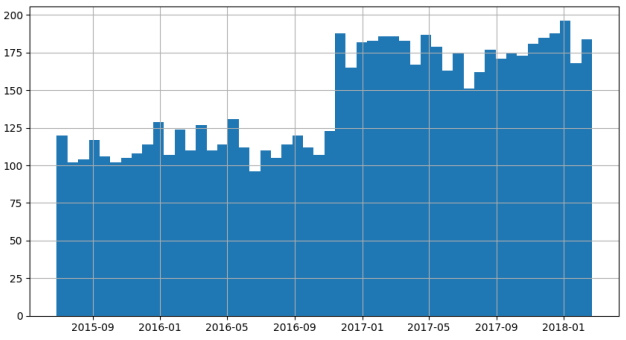
or query by dates:

```
print(contribs[contribs.realdate < dt.date(year=2016,
    month=11, day=8)])
```

```
                  Donor        Date   Amt Party
8         Wash Q. Thrace 2016-05-24  1475     D
9      Matt I. Skywalker 2016-09-12  7215     R
10         Matt K. Stark 2015-09-06   405     R
11         Tywin X. Pitt 2016-04-06  5530     R
12         Zoe T. Tyrell 2016-04-08  4610     D
                    .   .   .
```

or even do a date-based histogram:

```
contribs.Date.hist(bins=50)
```




Looks like donations spiked sharply immediately following the 2016 election, and stayed that way through the end of the data set.

Btw, if you're wondering how to fix the `Amt` column, you can do so with the same `.str` suffix we used on p. 113:

```
contribs.Amt = contribs.Amt.str[1:].astype(int)
```

The "`1:`" in the boxies says "take characters 1 through the end of each value"; since the first character (character #0) is the "`$`" sign, this gets rid of it. We then convert the column type from string to `int`, and we're able to treat donation amounts as the numerical quantities they actually are.

### Converting strings to dates with `to_datetime()`

The above technique works if you're reading dates directly from a `.csv` file. But if you already have some data in memory that consists of strings in date format, you need a different solution.

Pandas' `to_datetime()` method is that solution. All you have to do is pass it a `Series` (or NumPy array) with your strings, and it returns the `datetime` equivalents:

```
revolutions_strings = pd.Series(["March 8, 1917", "4-July-1776",
    "5/5/1789", "Jan. 5 2011"])
revolutions_actual_dates = pd.to_datetime(revolutions_strings)
print(revolutions_actual_dates)
```

```
0   1917-03-08
1   1776-07-04
2   1789-05-05
3   2011-01-05
dtype: datetime64[ns]
```

## Parsing with `.strptime()`

Sometimes you're not so lucky. Perhaps the string data you're blessed with has some ungodly format to it that can't be automatically recognized. In these cases, you have to do it manually.

The `date`, `time`, and `datetime` types all have a (somewhat clunky) method called "`.strptime()`" that you can call, passing (1) a string representing a date, time, or datetime, and (2) a formatting string telling the method how to interpret it. This is best seen through an example:

```
s = "4/30/2021 12:35"
last_class = dt.datetime.strptime(s, "%m/%d/%Y %H:%M")
print(last_class)
```

```
2021-04-30 12:35:00
```

This example demonstrates a full "round-trip" operation: we started with a `string`, parsed it into a `datetime`, and then printed it back to the screen as a `string`. Note that the format of the printout didn't match the format of "`my_string`"; this is okay. What matters internally to our program is that our date & time variables *represent* the right things, not that they are printed in certain ways.

Now what are all those funky percent signs and junk in the second argument to `.strptime()`? They all have a special meaning. Figure 12.1 shows some common ones (others are in the docs).

You have to be really careful here and just go slow. Examine the date and/or time input that you have in your data set, and work out which bits of info, combined with which literal characters (like "`/`" and "`:`" in the example above), appear in which order.

### Formatting with `.strftime()`

Complementary to `.strptime()` is "`.strftime()`". (Note that the "p" stands for "**p**arse," while the "f" stands for "**f**ormat.") This is the reverse operation: given a `date`, `time`, or `datetime` variable, spit it out as a string of characters. This isn't used nearly as often, but it occasionally is, and it's useful to know as a translation mechanism.

```
print(start_of_class.strftime("%A, %B the %dth at %I%p."))
```

| | |
|---|---|
| `%a` | Weekday (abbreviated): Sun, Mon, *etc.* |
| `%A` | Weekday (full): Sunday, Monday, *etc.* |
| `%w` | Weekday (number): 0, 1, ..., 6 |
| `%d` | Day of month (number): 0, 1, ..., 31 |
| `%b` | Month (abbreviated): Jan, Feb, *etc.* |
| `%B` | Month (full): January, February, *etc.* |
| `%m` | Month (number): 01, 02, ..., 12 |
| `%y` | **Two**-digit year: 00, 01, ..., 99 |
| `%Y` | **Four**-digit year: ..., 1999, 2000, 2001, ... |
| `%H` | Hour on **24-hour** clock: 01, 02, ..., 23 |
| `%I` | Hour on **12-hour** clock: 01, 02, ..., 12 |
| `%p` | AM/PM (only used in conjunction with **%I**) |
| `%M` | Minute: 01, 02, ..., 59 |
| `%S` | Second: 01, 02, ..., 59 |

**Figure 12.1:** Common date/time indicators used by `.strptime()` and `.strftime()`.

```
Tuesday, February the 20th at 02PM.
```

One common error: note that you call `.strptime()` directly on the *type* (`date`, `time`, or `datetime`), passing two arguments:

```
a_datetime = dt.datetime.strptime(my_birthday_string,
    "%m/%d/%Y %H:%M")
```

but you call `.strftime()` on the variable in question (a specific `date`, `time`, or `datetime` variable), passing one argument:

```
a_string = my_birthday_datetime.strftime("%m/%d/%Y %H:%M")
```

# Chapter 13

# Using logarithms

Recall that the logarithm is the inverse operation of exponentiation. What is $10^3$? 1,000. So what is the log of 1,000? 3. It's really that simple. Instead of asking, "what is ten to this particular power?" I'm asking "what power would I raise 10 to in order to get this particular number?"

(This is assuming we're using "base-10 logarithms," notated as $\log_{10}$. You can use any other base as well: common choices are 2 (sometimes $\log_2$ is abbreviated "lg"), $e$ ($\log_e$, the "natural" logarithm, is usually abbreviated "ln"), and 10 ($\log_{10}$ is often just plain "log".))

The role of the logarithm is to mercilessly crush numbers down to size.

| $x$ | $\log x$ |
|---|---|
| 1 | 0 |
| 10 | 1 |
| 100 | 2 |
| 1,000 | 3 |
| 10,000 | 4 |
| 100,000 | 5 |
| ... | ... |

Enormous numbers – in the millions – get squished down to single digits, and *the squashing gets more dramatic as the size of the*

*number grows.* Jumping from 1 to 10 (a difference of 9) netted us one higher in terms of logarithm, but jumping from 10 all the way to 100 (a difference of *90*) *also* only got us one higher. It's this property that makes logarithms useful.

Another way to think of logarithms is "the logarithm of $x$ is the order of magnitude of $x$."

One property of logarithms that is extremely important to know is this:

$$\log(xy) = \log(x) + \log(y)$$

Thus logarithms effectively *turn multiplications into additions.* One practical implication of this truth is leveraged in natural language processing systems: we often find ourselves multiplying minuscule quantities (very close to zero). As we multiply these, we get closer and closer to zero, and eventually Python doesn't have enough precision to even represent a number that low. But by dealing with logarithms, we're adding instead of multiplying and avoid that problem completely.

A natural consequence of the above property is this one:

$$\log(x^a) = a \log(x)$$

## 13.1 Logarithmic plots

A common plotting technique is to use not the raw values of the independent variable on the $x$ axis, but rather their logarithms. If we do this, we have a **semi-log plot**. If we do this for both the $x$ and the $y$ axis, we have a **log-log plot**.

Why would we do this? There are three reasons:

1. **It reins in large variations in the data.** If some of our data points are orders of magnitude larger than others, the detail of the smaller points gets completely swamped in trying to plot the larger points. Plotting orders-of-magnitude

instead of raw values solves this problem, though you have to remember you did this when interpreting the plot!

Here's a (fictitious) example of some American and British celebrities, and their total Instagram "likes":

```
plt.plot(uk, linestyle='None', color="red", marker=".",
    label="UK")
plt.plot(us, linestyle='None', color="green", marker=".",
    label="US")
plt.legend()
plt.show()
```

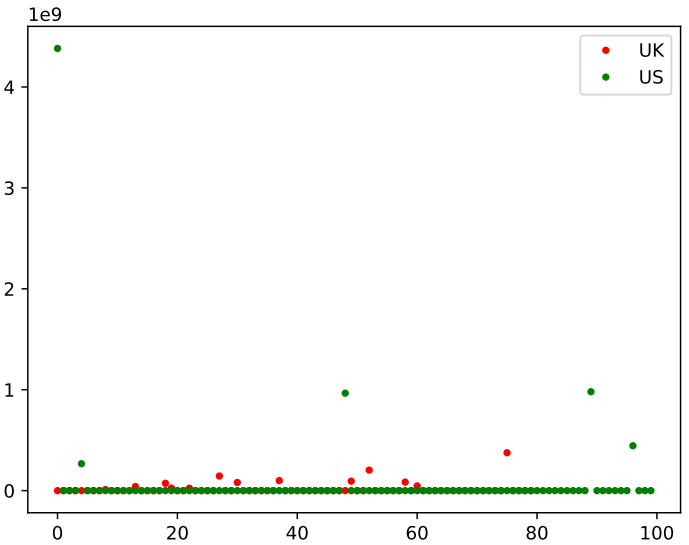



**Figure 13.1:** A regular (non-logarithmic) plot of celebrity "likes."

The scatterplot is shown in Figure 13.1. It has limited use, because there are a few uber-celebrities (Justin Bieber, *etc.*) who have far more "likes" than anyone else. Hence most people are crushed against the bottom of the plot and we can't (say) compare the UK people with the US people easily.

We can dramatically improve the readability and analyzeability by plotting the $y$ axis on a log scale. Just add this line before `plt.show()`:

```
plt.yscale('log')
```

and voila, Figure 13.2. It's imperative that when you do this, however, you remember that the $y$-axis no longer represents number-of-likes, but log-number-of-likes.

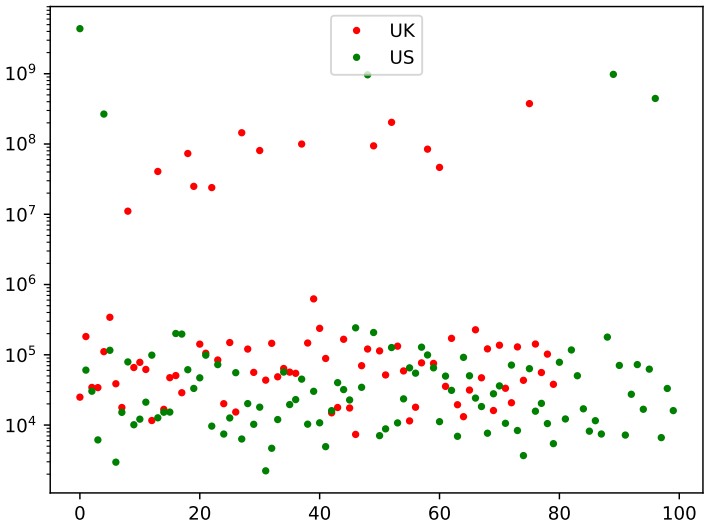



**Figure 13.2:** A logarithmic plot of the same data from Figure 13.1.

2. **A semi-log plot shows relative (multiplicative) changes instead of absolute (additive) changes.** Consider Figure 13.3, whose (ordinary, not logarithmic) plot depicts a fictional company's stock price over time. Two significant events occurred in this company's history: one in April 2015 and the other in March 2017. Both caused the stock's value to jump. Question: would you rather have bought stock immediately

before event A and sold it immediately after, or done the same before/after B?

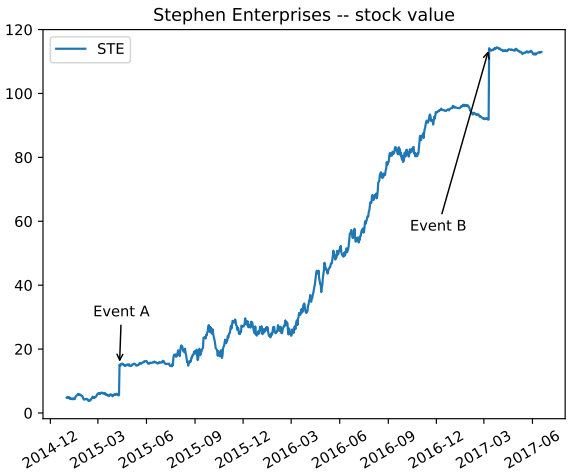



**Figure 13.3:** A regular (non-logarithmic) plot of a company's stock price.

From Figure 13.3, it may look like event B is the better bet: after all, it looks like the jump was higher. But this is an *absolute* distance: in other words, the total number of dollars per share jumped higher for event B. But for something like an investment, you actually don't care about this absolute number, but the *relative* number.

Look carefully at event A: before the jump, the stock was selling at about \$5 per share, and afterwards, at about \$15. This means that if you timed this right, you *tripled your money*! (Buy \$1000 worth of stock in April 2015, and you sell it for \$3000 the following day.) Compared to event B, this is a way better deal. Consider that at event B, the stock went from \$90 to \$110. Sure, \$20 is more than \$10 in absolute dollar terms, but if you bought \$1000 worth of stock in March 2017 and sold it the following day, you'd have sold it for $\$1000 \times \frac{110}{90} = \$1222$. Nice, but not nearly the windfall of event A.

For this reason, stocks and other investments are nearly always shown on a semi-log plot, like the one in Figure 13.4.

it has the advantage that *same-size increases on the (log) y axis correspond to identical relative (multiplicative) increases of the stock.* In other words, if the stock rises an inch somewhere on the plot, and it rises an inch somewhere else, these represent equal gains for investors *no matter how high the stock value is in absolute terms.* Such is the magic of logs.

In this example, you can easily see from the semi-log plot that event A was a bigger windfall for investors than event B.

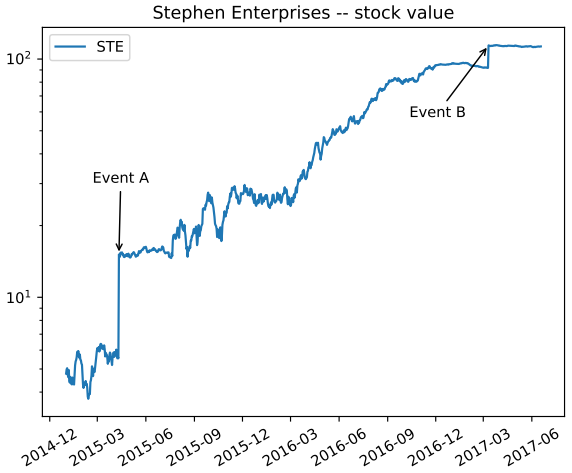



**Figure 13.4:** A semi-logarithmic plot of a company's stock price.

3. **It reveals exponential and power-law relationships.** This requires a little math to understand. Suppose we have two variables, $x$ and $y$, and they are related according to something like this:

$$y = p \cdot e^{qx}$$

where $p$ and $q$ are just numbers. For example,

$$y = 5.2 \cdot e^{2.96x}$$

Now if we plot $x$ vs $y$ on a standard plot, we get a curvy exponential function that is very difficult for the human eye

to distinguish from other curvy functions. But suppose we plot not $y$, but the *logarithm* of $y$?

Let's take the natural log (ln) of both sides of the equation. Using our properties from above, we get:

$$\begin{aligned}\ln y &= \ln(5.2 \cdot e^{2.96x}) \\ &= \ln(5.2) + \ln(e^{2.96x}) \\ &= 1.649 + 2.96x\end{aligned}$$

This is just a linear equation with a slope ($m$) of 2.96 and a $y$-intercept ($b$) of 1.649. So plotting this relationship on a semi-log plot will give us a straight line.

Why do we care? Because it turns out that exponential relationships like this come up a lot in the world. One ubiquitous pattern is that of exponential growth or decay: any time that *the rate of increase of a quantity* (like the number of new baby rabbits added to a rabbit population) is proportional to *the quantity itself* (the number of existing rabbits), we have exponential growth. And any time that the rate of *de*crease of a quantity (like the number of mechanical parts that wear out) is proportional to the quantity itself (the total number of mechanical parts owned by the company), we have exponential decay.

Another important kind of relationship is often mistaken for exponential growth, but is emphatically *not*. It's called a "power-law" relationship, and has caused much buzz in the scientific community over the past decade or so. It occurs when we have a simple polynomial relationship:

$$y = p \cdot x^q$$

where $p$ and $q$ are just numbers. For example,

$$y = 3.9 \cdot x^{-2.45}$$

Again, some math: if we take the logarithm of both sides, we get:

$$\ln y = \ln(3.9 \cdot x^{-2.45})$$
$$\ln y = \ln(3.9) + \ln(x^{-2.45})$$
$$\ln y = 1.361 - 2.45 \ln(x)$$

If we plot not $y$ vs $x$, but $\ln y$ vs $\ln x$ (in other words, a **log-log plot**, we will get a straight line. (You can see this by mentally substituting your letter of choice for $\ln x$ and another letter of your choice for $\ln y$. Now you have a plain old linear equation with a slope of -2.45 and an intercept of 1.361.)

To see how the logarithmic plots reveal this, consider Figure 13.5, each of which is a plot of the same three synthetic data sets. The blue points are linear in $x$, the red points are exponential, and the green points are power-law (with an exponent of 6).

In the linear plot, the blue points can be seen to be a straight line. In the semi-log plot, the red points are. In the log-log plot, the green points are. This is a powerful tool for recognizing these important kinds of relationships at a glance.

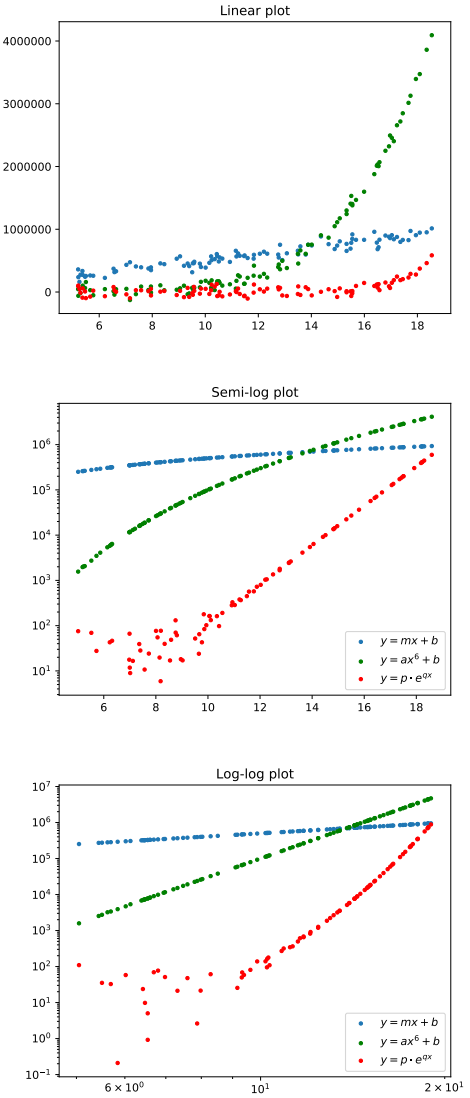



**Figure 13.5:** A linear, semi-log, and log-log plot of the same three data sets: blue (linear), red (exponential), and green (power-law).

# Chapter 14

# Accessing databases

"Database" is a very loose term for "a repository of information that can be readily accessed." When we use that term in Data Science, we mean a data source that is managed by a piece of software called a **DBMS**, or **database management system**. (True, plain-old lists, dictionaries, or Pandas `DataFrame`s are also "repositories of information that can be accessed," but when we use the term **database** we're not talking about that.)

There are principally two reasons to learn how to access data from databases:

- Sometimes, our data is simply available in that form only. We may want to import it into Python/Pandas and deal with it using the techniques from the first half of the semester, but in order to get it in there, we need to (briefly) interface with the database and issue the proper commands.
- Sometimes, our data is just flat *big*. There's a limit to how much data Spyder can store in memory and deal with on the spot. Suppose you had to analyze all the eBay transactions over the past two years? Or all the tweets made in the world over the last month? That stuff can't remotely fit in your system's memory. Hence, we have to access it through a database which will manage the sheer size and scope for us, and work with it a little at a time.

## 14.1 Two kinds of databases

There are essentially two kinds of databases in the world: **relational**, and **NoSQL**.

Previously this semester, we've worked with data spread across multiple `DataFrame`s that we need to join together in some way. This structure is extremely common, so much so that most of traditional database schema theory is based directly on it. A **relational database** is a repository of information in which the data is stored in **tables** (a table is pretty much *exactly* a `DataFrame` in spirit), and on which the language **SQL**[1] can be used to query it and manipulate it. A software system that enables a user to create and work with relational databases is called an **RDBMS**, or **relational database management system**.

There are many, many RDBMS's out there: Oracle, Sybase, Microsoft SQL Server, MySQL, MariaDB, PostgreSQL, and literally dozens of others. They all work in very much the same way: they store data in tables, and they are manipulated via SQL. Ever since Ted Codd invented the relational model in 1970, this organizational paradigm has proven to be so powerful and computationally efficient that it has dominated the database world. Only recently have some alternate paradigms gained some traction (so-called "NoSQL" databases), but even so, the majority of the world's structured data is all in relational databases of some sort.

Relational DBMS's are much more similar to each other than NoSQL systems are to each other. The wide variety of NoSQL DBMS's (Cassandra, MongoDB, Redis, Neo4j, *etc.*) means that learning how to use one doesn't give you much knowledge about how to use one of the others. Some store key/value pairs; others store objects and binary data; some store information as a graph (network). Part of the great power of the relational model is that SQL has proven to be a common, flexible, broadly-applicable query language that many different vendors have adopted and which suits many data needs.

[1] Some people pronounce the acronym SQL as the three letters "ess-queue-ell," and others as the word "sequel." Either one is acceptable (I do the former).

## 14.2 SQLite

SQLite is a really slim, trim RDBMS that stores all of its data *in a single file.* When you work with SQLite (or any RDBMS), though, you don't think in terms of files, but in terms of tables. The fact that the tables are stored in file(s) in some strange format is invisible to you as the user of the data, and this is in fact one of the great powers of the relational model: separating the conceptual data from the storage implementation.

### Interfacing to SQLite

"**Connecting**" to a relational database basically means establishing a communication path over which you can talk SQL. In Python, this is pretty easy:

```
import sqlite3

conn = sqlite3.connect('my_local_file.db')
```

SQLite-compatible files typically have a `.db` extension (for "database") or a `.sqlite` extension.

The return value from `connect()` that we're calling `conn` is "a connection to the database." We'll use it every time we want to perform an **SQL query**. SQL is a new language, but it's not nearly as complex as something like Python because it's not a programming language, but a **query language**. You don't write entire programs in it; you merely specify queries in it. This means that the range of things you can do in SQL is much more restricted, and hence the language is easier to learn.

### Browsing the tables

The first thing you'll normally want to do is figure out which tables exist in the database. You can run this command:

```
print(pd.read_sql(
    "SELECT name FROM sqlite_master WHERE type='table'", conn))
```

to find out. If this were the output:

```
          name
0        songs
1       albums
2      artists
3       labels
```

that would tell us that the SQLite database has four tables in it, named `songs`, `albums`, `artists`, and `labels`. Each one can be queried using SQL statements, or simply imported wholesale into a Pandas `DataFrame` (see below).

## 14.3 Querying the database

By far the most common thing you'll do with a relational database like SQLite is execute an SQL query, and get a `DataFrame` back:

```
df_name = pd.read_sql("YOUR SQL QUERY GOES HERE", conn)
```

The string inside the call to `pd.read_sql()` is called "an embedded SQL statement." This means we have code in one language (SQL) "embedded" inside another (Python). Do not be alarmed at this.

### The easy case: inhaling an entire table

Now *if* the data is small enough to load into memory, you don't need to know much SQL at all. You can simply use this one-liner:

```
df = pd.read_sql("SELECT * FROM table_name", conn)
```

This reads one of the database's tables (whose names you learned from the command in Section 14.2) into a new, fully-fledged `DataFrame`, with column names, a reasonable guess at their types, *etc.*

That's literally all you need to know about working with a (small-ish) SQLite database. Just to connect to it, get all the table names, read each one into a `DataFrame`, and continue in Pandas Land, forgetting all about SQLite. You can then leverage all the knowledge you've learned up to this point. Bingo!

### The harder case: more complex SQL

Sometimes, however, the data is too large to do this. So it's worth learning a little SQL so you can make the RDBMS do some of the heavy lifting, and give you trimmed results for your Python program to work with.

The workhorse is the SQL `SELECT` statement. Here are some common variants:

- To compute the *number* of rows, or individual values, without returning the entire result, use `COUNT(*)`, `MAX()`, `MIN()`, *etc.*:

```
SELECT COUNT(*) FROM table_name
SELECT MAX(col1) FROM table_name
```

- To get only the first few rows (similar to Pandas' `.head()` operation) tack on a "`LIMIT`" expression:

```
SELECT * FROM table_name LIMIT 10
```

- To get only certain columns, change the "`*`" to a comma-separated list of column names:

```
SELECT col1 FROM table_name
SELECT col1,col2,col3 FROM table_name LIMIT 10
```

- To get only certain rows, add a "`WHERE` clause" after the table name:

```
SELECT * FROM table_name WHERE col1==val1
SELECT col2 FROM table_name WHERE col1==val1 AND col2>val2
SELECT c1,c2 FROM t WHERE c1==val1 AND NOT c2>val2 LIMIT 10
```

(The usual boolean operations work with keywords `AND`, `OR`, and `NOT`, and parentheses for grouping.)

- The "`IN`" keyword can be useful in a `WHERE` clause for querying membership in a set:

```
SELECT * FROM table_name WHERE col1 IN (val1,val2)
SELECT col1,col2 FROM table_name WHERE col1==val1 AND
            NOT col2 IN (val1,val2,val3) LIMIT 10
```

- To get only unique rows (like Pandas' `.drop_duplicates()` gives) use the word `DISTINCT` before the column names:

```
SELECT DISTINCT * FROM table_name
SELECT col1,col2 FROM table_name WHERE NOT col1 IN
            (val1,val2,val3) OR col2!=val4 LIMIT 5
```

  The `DISTINCT` option is useful in conjunction with `COUNT()`:

```
SELECT COUNT(DISTINCT col1) FROM table_name
```

- You can have SQLite do sorting with "`ORDER BY`":

```
SELECT * FROM table_name ORDER BY col1
SELECT DISTINCT c1,c2 FROM table_name WHERE c1==val1
            ORDER BY c2,c1 DESC LIMIT 5
```

  As you can see, you can sort on multiple columns, and sort in reverse order with the `DESC` keyword.

- SQL supports a "GROUP BY" operation very much like Pandas' `.groupby()` method:

```
SELECT col1,count(*) FROM table_name GROUP BY col1
SELECT col1,max(col2) FROM table_name WHERE col3==val1
            GROUP BY col2 ORDER BY col1 DESC LIMIT 5
```

- Finally, to do a merge/join operation, use the `JOIN` keyword:

```
SELECT * FROM table_1 join table_2 ON col1==col2
SELECT c1,c2 FROM t1 join t2 ON t1.x==t2.q
            WHERE c2>val1 LIMIT 5
```

  The `JOIN` keyword supports `LEFT`, `RIGHT`, and `OUTER` options.

There are many, many other options as well. See the online documentation at `https://www.sqlite.org/docs.html`. Again, one of the great things about SQL is that with the exception of the initial commands to connect and to list all table names (p. 141), *all relational databases use essentially identical syntax.* So if you ever need to query an Oracle, Sybase, Informix, MySQL, PostgreSQL, or SQL Server database, you'll discover that everything in this section applies nearly identically.

# Chapter 15

# Screen scraping (1 of 2)

Welcome to the worst of all possible worlds[1]: when the data you want to analyze is on a human-readable but machine-unfriendly website somewhere. It's there, you can see it...but getting it from a pretty web page into a Pandas `DataFrame` is a non-trivial proposition.

Usually this situation occurs when the provider of the data, and the designer of the website, didn't envision anyone using the data for any purpose other than viewing it through the website itself. Sometimes there is another reason: that the organization wanted to deliberately make this operation difficult so that you *couldn't* easily use it for other purposes. Either way, though, as long as the data is accessible and visible through your browser, it is at least theoretically extractable into the form we need to do our magic.

## 15.1 HTML

(Most) web pages look snazzy and colorful when you view them: the word "code" doesn't jump immediately to mind. When you load a web page, though, what you're actually getting from the server you specify is a plain-text file written in a language called **HTML**, or **hypertext markup language**. It consists of a combination

[1] Actually, the *second*-worst; the very worst is when the data you seek isn't even in electronic form at all.

of content and formatting/structural commands (or "markup") to instruct the browser how to **render** the page. ("Rendering" a page means "interpreting all that HTML formatting stuff and actually presenting a pretty page formatted the way it specifies.)

The first thing to be aware of is that HTML is *not* a programming language. (That is, you can't write a program in it.) It's strictly a formatting syntax for specifying how text and graphical elements should be laid out. If you ever ask someone whether they've done computer programming, and they say, "yeah, I've done programming in HTML," you know they're lying.

The second thing to know is that it is *hierarchical*, not flat. This makes it more like JSON than CSV. Even though every HTML file is a single sequence of characters, it encodes a tree-like structure in which elements can exist inside other elements, which can exist inside other elements, *etc.*, with no limit to the amount of nesting.

The basic building block of HTML is the **element**, which is delimited by starting and ending **tags**. Tags are key words, most of which indicate something structural or stylistic, enclosed in wakkas ("`< ... >`"). The ending tag has a slash ("`/`") immediately before the keyword, showing that it matches the corresponding opening tag. So one pair of starting and ending tags might be "`<title>`" and "`</title>`".

Note that the entire contents of the *element* is (1) the starting tag, (2) the ending tag, and (3) *everything in between*, which could be text in addition to other elements.

## An example HTML file

Figure 15.1 shows a very simple, but complete, example. Lots going on there. The first way to get your bearings is to start visually lining up starting tags with their corresponding ending tags and perceive the structure. Notice that this entire page begins with "`<html>`" and ends with "`</html>`". This is in essence the "root node" of the page's entire hierarchical tree[2] It has two immediate "children": a

[2]I'm using the term **tree** here in much the same way as the **decision tree**s from volume I of this series. Remember that they start at the top with a **root**,

`head` element, and a `body` element. Each of those have starting and ending tags as well. Inside the `head` element is a `title` element, *etc.*

As you can guess, each of these tags is interpreted by the browser to mean a particular kind of structure/formatting. "`h1`" means "top-level heading" which in practicality means "render it in a large font, with some extra space around it." The "`b`" element means to put something in boldface. The "`table`" element means to construct a table-like structure, with rows ("`tr`") and cells within rows ("`td`"). *Etc.* HTML is in general a big mess of things that are supposed to indicate structure (like `table` and `h2`) and things that specify specific formatting (like `i` and `u`). All of this is eminently look-up-able online.

Some starting tags (not ending) contain additional information called **attributes**. You can see this with the `a` and `img` tags from the example:

```
<a href="http://buildings.umwblogs.org/james-farmer-hall/">Farmer Hall</a>
```

The `a` tag stands for "anchor" and is the most common way of embedding a hyperlink (which you can click on to go to another page) in a document. Note that the words that will appear in the page are the **contents** of the element, not part of the tag itself. The tag, in addition to the required "`a`" has a key/value pair where the key is the string `href` and the value is the URL the user will be directed to if they click on the link. This key/value pair is called an **attribute**.

```
<img src="http://clipart.com/prof.jpg" width=200 />
```

In the `img` example, we have *two* attributes: one for the filename of the image, and the other for some specific formatting suggestions (in this case, a width of 200 pixels). An element can have many different attributes, in any order.

(By the way, the sharp-eyed reader may have noticed something else odd about the `img` example, above: an extra slash before the

and branch out wider and wider as they are drawn down the page.

```
<html>
<head>
    <title>All About Stephen</title>
    <style>
        img { width:150px; }
        td { border-width:1px; }
    </style>
</head>
<body>
<h1>Stephen Davies, Esquire</h1>

<p>Deep in the bowels of
<a href="http://buildings.umwblogs.org/james-farmer-hall/">James Farmer
Hall</a> resides a carbon-based life form known to outsiders only as
<b>Stephen</b>. This mysterious being fulfills several roles <u>not</u>
widely known to humankind.</p>

<p><i>Some</i> of these functions are delineated below. Please memorize
them and then immediately destroy this page upon reading it.</p>

<h2>Areas of operation</h2>

<table border=2 cellpadding=15>
    <tr><td class="pic"><img src="http://clipart.com/prof.jpg" width=200 />
        </td>
        <td class="role">College professor</td>
        <td class="description">Stephen teaches computer science and data
    science to willing undergraduates, shaping them into the heroes of
    tomorrow.</td>
        <td><ul><li>Super rewarding</li>
            <li>Exciting</li>
            <li>Ever-changing</li>
            <li>Fun</li></ul></td>
        <td><b>50%</b> of total time</td>
    </tr>
    <tr><td class="pic"><img src="http://clipart.com/dad.png" width=200 />
        </td>
        <td class="role">Dad</td>
        <td class="description"> With a wife, three teenagers, and two cats
        (one of whom throws up a lot), Stephen's home life is a constant
        source of love, anxiety, and Hallmark moments.</td>
        <td><ul><li>Amazing</li>
            <li>Loving</li>
            <li>Complicated</li>
            <li>Surprising</li></ul></td>
        <td><b>30%</b> of total time</td>
    </tr>
    ...
</table>
</body>
</html>
```

**Figure 15.1:** A sample HTML page.

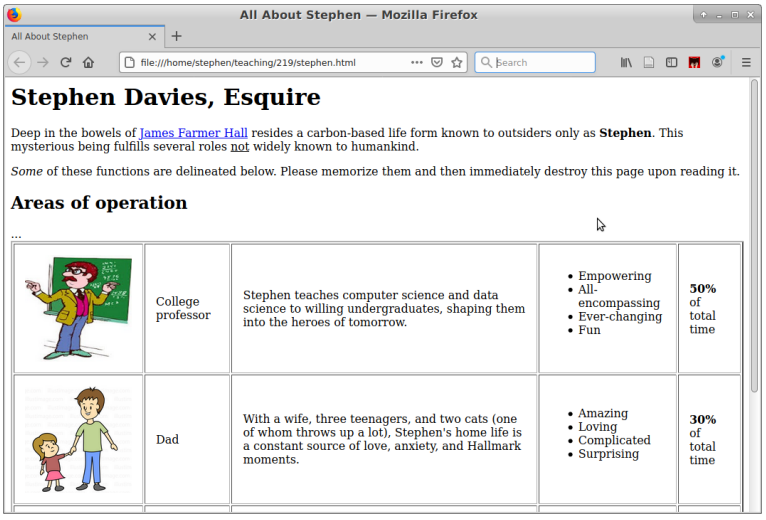
ending "`>`". This is an HTML shorthand for "starting and ending the element all within a single tag, since it has no content anyway." Whenever you have something of the form "`<x></x>`" you can replace it with the equivalent "`<x/>`" to save typing and file size.)

Lastly, I'll point out that near the top of this example, there's a bunch of stuff which looks a bit visually jarring; it doesn't look like HTML. And it's not. I'm referring to this:

```
<style>
    img { width:150px; }
    td { border-width:1px; }
</style>
```

This code is called **CSS** (or **Cascading Style Sheets**) which is sort of a companion technology to HTML to give additional formatting control. (Originally, HTML was supposed to strictly delineate document *structure*, and CSS could then be used to specify the formatting of that structure. This strict separation of concerns, which was a good idea, has gotten very muddy in the intervening years, however.)

The whole thing, once rendered, looks something like this:



## 15.2 The easy case: reading from `<table>`s

From the point of view of Data Science, we don't care very much about all this formatting stuff. To us, it's clutter. On the page is some important data we'd like to analyze, and the goal is to sift through all this HTML and CSS crapola looking for it and extracting it. This is called by the evocative term "**screen scraping**."

Now just like with relational databases (recall p. 142), there's both an easy scenario and more challenging ones. The more challenging ones we'll postpone until the next chapter. The easy one is when the data you want to scrape *is all inside* ***HTML tables***.

An HTML table is the contents between an opening <**table**> tag and its corresponding </**table**> tag. Look carefully again at Figure 15.1 on p. 150. *If* the information we care about scraping is all inside the "areas of operation" table (which begins about half-way down the page; squint until you see the word `table`), then we're in the easy case, thank heavens. We can use Pandas' `read_html()` function as follows:

```
the_tables = pd.read_html("http://theURLtoTheWebpage.html")
```

This function takes just one argument: the **URL** of the page we want to scrape. (A URL – which stands for Uniform Resource Locator – is another word for a web page's address, or "link.") Sometimes you'll find it more convenient to first download the page to your local computer, so that you're not dependent on a network connection (and latency) while you're working on scraping it. This will normally put a `.html` (or `.htm`) file on your computer, which you can store in the same directory/folder as your `.py` file, just as you do with `.csv` or `.db` files. You'll then pass the simple filename (like "`allAboutStephen.htm`") as the argument to `read_html()`.

The return value of this function is *a list of `DataFrames`, one for each `<table>` on the page.* Read that sentence once again slowly. In particular, note that the return value is not *a* `DataFrame`, which many students seem to expect. This is of course because the web

page may well contain *multiple* `<table>`s, and therefore `read_html()` would need to return multiple `DataFrame`s.

Let's try this approach with `allAboutStephen.html`:

```
the_tables = pd.read_html(
    "http://stephendavies.org/allAboutStephen.html")
print(len(the_tables))
```

```
1
```

There is apparently only one `<table>` on the page. Let's put it in its own variable ("`areas`" for "Areas of operation") and take a look at it:

```
areas = the_tables[0]
print(areas)
```

```
    0  ...                   4
0 NaN  ...  50% of total time
1 NaN  ...  30% of total time
2 NaN  ...  10% of total time
3 NaN  ...   5% of total time
4 NaN  ...   5% of total time

[5 rows x 5 columns]
```

This is a bit confusing at first, for several reasons. One is that the columns don't have names, as we're used to – just numbers. Another is that most of the information is omitted from the display (with just "..." placeholders). Another is that the first column is entirely `NaN` values[3].

[3]The value `NaN`, you'll recall, stands for "not a number." But that phrase is misleading here. Of *course* the value is not a *number*: why would we expect text on a web page to necessarily be a number? Really it means "not a value Python could do anything with."

The root causes of these conundrums are as follows:

1. The `DataFrame` columns don't have names because HTML `<table>`s often don't have header cells (delimited with `<th>` cells in the first `<tr>` row), and so `read_html()` has no idea what to name the columns.
2. Most columns are omitted from the `print()` output because they're just too long to fit. (Look at p. 151: that third column has paragraphs in it.)
3. The first column has `NaN`s because the first column of the `<table>` has images in it, not text (again see p. 151).

We can *give* the `DataFrame` meaningful column names with:

```
areas.columns = ['pic','role','description','adjectives',
    'allocation']
```

and we can get rid of the columns we don't care about (the image, and perhaps the descriptions) with a Pandas operation:

```
areas = areas[['role','adjectives','allocation']]
```

Now we can see better what's going on:

```
print(areas)
```

```
              role                          adjectives          allocation
College professor   Empowering  Important  Fun  ...   50% of total time
Dad                            Amazing Fun Impor...   30% of total time
Kids Club Leader    Cute  Exhausting  Character-...   10% of total time
Secret Agent        Thrilling  High-impact  Dang...    5% of total time
Jedi Master         Important  Thrilling  Challe...    5% of total time
```

### Some text cleaning stuff

At this point, we're out of screen-scraping-land and into ordinary-Python land. What we do next depends on what we want to analyze. One interesting question I could imagine asking is: "how much of Stephen's total time does he spend doing 'fun' things? 'important' things? 'exhausting' things?

To do this, we'll have to deal with that messy `adjectives` column. I say it's "messy" because all Pandas knew to do was take each bulleted list – comprised of a `<ul>` element ("unordered list") and nested `<li>` elements ("list elements") – and concatenate all the contents into a single string.

My strategy to dealing with it is to split these up, putting each role's adjective in its own row of a new table that looks like this:

```
                role           adjective
   College professor          Empowering
   College professor           Important
                 Dad             Amazing
    Kids Club Leader           Important
               . . . etc . . .
```

We can do this with a loop. Since we don't know at the beginning how many rows this table will have, we'll use a slightly different technique than we did on p. 85. We'll just create two *zero*-length NumPy arrays, and repeatedly `append()` to them for each new adjective we encounter:

```
roles = np.array([], dtype=object)
adjs = np.array([], dtype=object)

for row in areas.itertuples():
    for adjective in row.adjectives.split():
        roles = np.append(roles, row.role)
        adjs = np.append(adjs, adjective)
```

Two other notable things about this code:

- It's a *nested* `for` loop. This is because (1) we have to go through all the rows of our `areas DataFrame`, and (2) for each of those rows, there will be *multiple* adjectives.
- We use the very handy `.split()` method here. When you call `.split()` on a string, you get back all its individual words in a list. You can also pass an argument to `.split()` giving the string **delimiter** that you want it to divide the string on. So calling `"needles/yarn/scissors".split("/")` would return the list `["needles", "yarn", "scissors"]`, and calling `"Stephen".split("e")` would return the list `["St", "ph", "n"]`.

Now all we have to do is stitch together our arrays into a `DataFrame`, just like we did on p. 55:

```
adjectives_df = pd.DataFrame({'role':roles, 'adjective':adjs})
```

and voilà! The resulting `adjectives_df` is in Figure 15.2.

And now that we've done that, we can get rid of the old, awkward, separated-by-spaces column:

```
areas = areas[['role','allocation']]
```

Okay. The other thing we need to do is change those ridiculous human-readable strings like "`30% of total time`" to integers like `30`. We'll use the `.split()` method again, this time passing a delimiter:

```
percentages = np.array([], dtype=int)

for row in areas.itertuples():
    percentages = np.append(percentages,
        int(row.allocation.split("%")[0]))

areas.allocation = percentages
```

| | role | adjective |
|---|---|---|
| 0 | College professor | Empowering |
| 1 | College professor | Important |
| 2 | College professor | Fun |
| 3 | College professor | Cool |
| 4 | College professor | All-encompassing |
| 5 | College professor | Ever-changing |
| 6 | Dad | Amazing |
| 7 | Dad | Fun |
| 8 | Dad | Important |
| 9 | Dad | Challenging |
| 10 | Kids Club Leader | Cute |
| 11 | Kids Club Leader | Exhausting |
| 12 | Kids Club Leader | Character-building |
| 13 | Kids Club Leader | Important |
| 14 | Secret Agent | Thrilling |
| 15 | Secret Agent | High-impact |
| 16 | Secret Agent | Dangerous |
| 17 | Secret Agent | Cool |
| 18 | Secret Agent | Daring |
| 19 | Jedi Master | Important |
| 20 | Jedi Master | Thrilling |
| 21 | Jedi Master | Challenging |
| 22 | Jedi Master | Daring |
| 23 | Jedi Master | Cool |
| 24 | Jedi Master | Lit |

**Figure 15.2:** The `adjectives_df` `DataFrame` we constructed with our nested `for` loop.

What does "`int(row.allocation.split("%")[0])`" mean? Let's break it down. For each row, we first get the allocation column's value (which is a string), then split it on the "`%`" sign. This will give us a list of two values in each case, the first of which has digits like "`30`" and the second of which has the rest of the text ("`of total time`"). Putting `[0]` after it gets the first element of this list. Then, by wrapping the result in "`int(...)`", we convert it from a string of digits to an actual number, which we can do something with.

The last step in that code was to reassign the `DataFrame`'s `allocation` column to be our new percentages. The result is now:

```
print(areas)
```

```
                    role  allocation
0  College professor          50
1                Dad          30
2   Kids Club Leader          10
3       Secret Agent           5
4        Jedi Master           5
                    . . .
```

where the right-most column actually has numbers.

### The analysis

Finally (whew!) we're in a position to perform our analysis of Stephen's time. We have two `DataFrames` – `areas` and `adjectives_df` – both of which are needed to answer our key question. So it makes sense to merge them. It now sucks to have the role be the index of the `areas` `DataFrame`, so let's make it a regular column again and then do the merge:

```
df = pd.merge(areas, adjectives_df)
print(df)
```

```
                  role  allocation           adjective
0   College professor          50          Empowering
1   College professor          50           Important
2   College professor          50                 Fun
3   College professor          50                Cool
4   College professor          50    All-encompassing
5   College professor          50       Ever-changing
6                 Dad          30             Amazing
7                 Dad          30                 Fun
                            . . .
```

And at last, after all this data cleaning, we can get the goods. The *number* of different roles Stephen plays that have various adjectives is as follows:

```
print(df.adjective.value_counts())
```

```
Important             4
Cool                  3
Fun                   2
Thrilling             2
Challenging           2
Daring                2
High-impact           1
Amazing               1
Ever-changing         1
Cute                  1
Lit                   1
Exhausting            1
Empowering            1
All-encompassing      1
Character-building    1
Dangerous             1
```

And the *percentage* of time he spends with these adjectives is:

```
perc_of_time = df.groupby('adjective').allocation.sum()
print(perc_of_time.sort_values(ascending=False))
perc_of_time.plot(kind='bar')
```

```
Important             95
Fun                   80
Cool                  60
Ever-changing         50
Empowering            50
All-encompassing      50
Challenging           35
Amazing               30
Thrilling             10
Exhausting            10
Daring                10
Cute                  10
Character-building    10
Lit                    5
High-impact            5
Dangerous              5
```

which is represented in Figure 15.3.

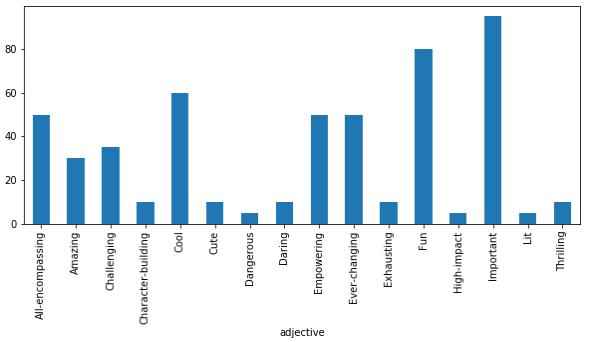



**Figure 15.3:** Good news: Stephen spends a lot of time doing important stuff!

I know that might seem like a lot of work for "the easy case." But the wild wild world has lots of messiness, and if you want the data shown on a web page you have to put in some elbow grease to bend it to your will. The good news is that as far as scraping the actual *page*, all we needed was one command: `pd.read_html()`. If the data you want from a page isn't in `<table>`s, though, you're in for the tougher case in Chapter 16. Stay tuned!

# Chapter 16

# Screen scraping (2 of 2)

## 16.1 The harder case: picking through the HTML tree

Chapter 15 was the "easy" screen scraping case: if the data on the web page that you want to import is in `<table>` rows, you can (relatively) simply use Pandas' `read_html()` function to suck it in to Python.

For anything else, you'll have to comb through the HTML structure, figuring out how to surgically extract what you seek. It's a major pain, but there is a Python library by the outrageous name "BeautifulSoup" which makes it just a little bit less painful. This chapter contains an overview of how to work with it.

## 16.2 Web Developer Tools

First, let me say that Firefox, Chrome, and several other browsers come equipped with very sophisticated "web developer tools" that let you browse the HTML, CSS, and rendered page, and figure out what elements got rendered via which portions of the screen. They're very handy, and when screen scraping you should get into the habit of using them. In Firefox, they're available via the "Tools | Web Developer | Toggle tools..." menu option. In Chrome, you go to the little three vertical dots, then choose "More Tools | Developer

Tools."

## 16.3 Parsing with BeautifulSoup

As I mentioned on p. 152, it's generally recommended to *download* the web page you want to parse rather than having Python read it for you over the network. This eliminates one more possible source of error. (Exception: if you need a Python program to act as a **web crawler** and read pages on demand as it discovers their URLs. More on that later.) Note that you can still open the page in your browser even after downloading it: just go to "File | Open File..." or the equivalent operation in your browser.

Once you've done this, and now have your HTML in a file called (say) "`myfile.htm`", you can then parse it with BeautifulSoup using:

```
from bs4 import BeautifulSoup
soup = BeautifulSoup(open("myfile.htm"), "html.parser")
```

By convention, the variable for this parsed structure is called "`soup`". The second argument to the `BeautifulSoup` function tells it which **parser** we want to use to analyze the code; there are other choices here, but stick with `"html.parser"` for now.

One possibly useful command (though limited if your web page is large) is:

```
print(soup.prettify())
```

This "pretty prints" out the entire contents of the page, but in a way that is properly indented according to the HTML's structure, rather than how it was indented in the raw page. You may have noticed that the HTML file may or may not be physically indented and spaced in a way reflective of the structure. The BeautifulSoup parser is smart enough to discern the implied structure from the

tag sequence, and thus prints it how it will "really" be seen by a browser.

At this point, I generally take one of two approaches: either I navigate the structure **top-down** looking for where the data I'm interested in is situated, or I find the data by searching through the file, and use a **bottom-up** approach to get it from there. You typically have to combine the two approaches to get your screen-scraping dirty work done.

### The top-down approach

By using "`soup.contents`", you get the immediate descendants of the root node of the HTML hierarchy. Each of these could be examined for its type, like this:

```
for child in soup.contents:
    print(type(child))
```

```
bs4.element.Tag
bs4.element.NavigableString
```

So our entire document is composed of an element (misleadingly named "Tag" here, but w/e) and a "`NavigableString`" which essentially just means "string of literal text". For elements, it's useful to print out their "`.name`". For strings, it's useful to print them out verbatim. Here, we see:

```
print(soup.contents[0].name)
print(soup.contents[1])
```

```
'html'
'\n'
```

So the first child is the entire `html` element in all its embedded glory, and this is followed by a single, pesky newline. Now you know.

Drilling down another level, we see:

```
html_children = soup.contents[0]
for child in html_children:
    print(type(child))
```

```
bs4.element.NavigableString
bs4.element.Tag
bs4.element.NavigableString
bs4.element.Tag
bs4.element.NavigableString
```

Two tags, with three strings interleaved. Let's examine them:

```
print(html_children.contents[0])
print(html_children.contents[1].name)
print(html_children.contents[2])
print(html_children.contents[3].name)
print(html_children.contents[4])
```

```
'\n'
'head'
'\n'
'body'
'\n'
```

You're starting to see a pattern: a lot of the strings are just newline characters that split up the HTML text file and make it more readable. What we really care about is the content under the tags. Let's dig one deeper:

```
head_children = html_children.contents[1].contents
print(head_children[0])
print(head_children[1].name)
print(head_children[2])
print(head_children[3].name)
print(head_children[4])
```

```
'\n'
'title'
'\n'
'style'
'\n'
```

Okay, you get the idea. We can drill down to whatever level we want just by following the appropriate children. To get the title of the page, we could do:

```
print(head_children[1].contents[0])
```

```
'All About Stephen'
```

(This is because the second element (element #1) of the `<head>` element is the `<title>` element, and its only child is the string `'All About Stephen'`.)

Sometimes a quicker method to find your way through the forest is to use this syntax[1] at the interactive console:

```
print([ x.name for x in body_children ])
```

```
[None, 'h1', None, 'p', None, 'p', None, 'h2', None, 'table', None]
```

[1] That thing in the boxies – "`[ x.name for x in body_children ]`" – is called a "**list comprehension**," by the way, and is an advanced Python technique that is sometimes very useful.

You can better see at a glance what's what. Now that we know the first "p" (paragraph) is element #3 of the body, we could find that hyperlink via:

```
print([ x.name for x in list(body_children)[3] ])
```

```
[ None, 'a', None, 'b', None, 'u', None]
```

and grab it via:

```
dat_hyperlink =  list(list(body_children)[3])[1]
```

BeautifulSoup lets you access the attributes of an HTML element by treating the element as a dictionary. Pretty cool. We can snag the actual link, then, with:

```
print(dat_hyperlink['href'])
```

```
'http://buildings.umwblogs.org/james-farmer-hall/'
```

### The bottom-up approach

Sometimes, when you try to dive from the top of the document all the way to what you want, you can find yourself in a tangled mess. In these cases it's easier to search for the data you want using BeautifulSoup's search facilities.

Let's illustrate this by creating a simple `DataFrame` that contains each role and its percentage allocation of Stephen's time. We want `df` to look something like this:

```
                role  perc
0  College professor  50.0
1                Dad  30.0
           . . .
```

To find our way through the forest, we search through the HTML with developer tools, locating one of the pieces of data we know is there – for instance, the number `50`, which we can see on the page is one of the percentages. When we click on this (or just search for it in a text file), we find ourselves in the middle of the HTML content in Figure 16.1.

```
...
<table border=2 cellpadding=15>
<tr><td class="pic"><img src="a.jpg"></td>
    <td class="role">College professor</td>
    <td class="description">Stephen teaches computer science and data
    science to willing undergraduates, shaping them into the heroes of
    tomorrow.</td>
    </td>
    <td>
    <ul>
    <li>Super rewarding</li>
    <li>Exciting</li>
    <li>Ever-changing</li>
    <li>Fun</li>
    </ul>
    </td>
    <td>
    <b>50%</b> of total time
    </td>
</tr>
...
```

**Figure 16.1:** Using a bottom-up approach – locating the text "`50`" in the HTML file (stare towards the bottom of that HTML text) and getting one's bearings regarding where it is in relation to other elements.

Looks like the role name we want is the text under a `td` element whose class[2] is "`role`". And it looks like the percentage we want is (*groan*) in a boldface (`b`) tag, underneath the last `td` tag of the row, which has no `class`.

[2]In HTML, a "**class**" is an attribute used to classify certain elements to be picked up by CSS formatting instructions. If this were a Web development textbook, it would talk about when and how to use "`class`". But for our purposes, it's just one of many handy things we might hook on to in order to find our data in the morass.

BeautifulSoup's `.find_all()` method makes this slightly less of a headache. To quickly grab all the `tr` elements in the document, we can do this:

```
trs = list(soup.find_all("tr"))
```

The variable `trs` is now a list of *elements* (BeautifulSoup "`Tag`" objects) each of which we can examine for (say) `td` children with a `role class` attribute. And you can call `.find_all()` on *any* tag (to search from that point in the hierarchy down), not just on the top-level `soup` element. So:

```
roles = np.array([], dtype=object)
trs = soup.find_all("tr")
for tr in trs:
    tds = tr.find_all("td")
    for td in tds:
        if "class" in td.attrs and "role" in td["class"]:
            ...
```

The "`.attrs`" syntax gives us a *dictionary* of key-value pairs which represent the attributes of an element. So by saying "`"class" in td.attrs`" we're first checking whether there is a `class` attribute in the current `td` element at *all* before then attempting to get its value using the dictionary syntax mentioned on p. 166.

Btw, one slight surprise in the above `if` statement might be that we're checking whether `"role"` is *in* `td["class"]` instead of simply being `==` to `td["class"]`. That's because in HTML, the `class` attribute of an tag can have *multiple* (space-separated) values, not just one, and so `td["class"]` is actually a *list*, not a single string.

Okay, now when we reach the body of that `if` statement, we have successfully found one of the desired `td` attributes. How do we then get the text under it? Just call `.get_text()` on it, and then append it to the list. This creates our desired list of roles that we can stick in our `DataFrame`.

```
            ...
            roles.append(td.get_text())
```

To get the percentages, we just need a slightly different approach: first, we're going to assume the percentage is in the *last* `td` tag, and second, we need to go inside that to retrieve the percentage from the embedded boldface tag. Adding this to our `for` loop almost gets us there:

```
percs = []
...
    the_bold = tds[-1].find("b")
    percs.append(the_bold.get_text())
```

although we'd like to also strip that percentage sign off and convert it to an actual numeric value, so we'll do this instead:

```
percs = []
...
    the_bold = tds[-1].find("b")
    percs.append(float(the_bold.get_text()[:-1]))
```

and now we can create our DataFrame with both columns. (Note that "`.find()`" does the same thing as "`.find_all()`" except that it only grabs the first matching element rather than all of them.) The complete code is shown in Figure 16.2.

### Other BeautifulSoup features

The BeautifulSoup library has a myriad of alternatives for navigating and searching the tree. Here are a few.

```
roles = []
percs = []

trs = soup.find_all("tr")
for tr in trs:
    tds = tr.find_all("td")
    for td in tds:
        if 'class' in td.attrs and 'role' in td['class']:
            roles.append(td.get_text())
    the_bold = tds[-1].find("b")
    percs.append(float(the_bold.get_text()[:-1]))

df = pd.DataFrame({'role':roles, 'perc':percs})[['role','perc']]
```

**Figure 16.2:** The complete code example to screen scrape the roles and percentages from the web page in Figure 15.1 (p. 150).

### Searching by id or class

`.find()` and `.find_all()` each have optional `id` and `class_` (note the trailing underscore!) parameters that can be used to restrict a search to only elements with matching attributes.

```
soup.find_all("td", class_="pic")
```

### Using the Python "dot" syntax

If we know the names of the tags, we can navigate a structure by using a Pandas-like "dot" syntax. Check it out:

```
print(soup.head.title)
print(soup.head.name)
print(soup.head.title.string)
print(soup.body.table.td.img['src'])
```

```
<title>All About Stephen</title>
title
'All About Stephen'
'a.jpg'
```

### Accessing all attributes

As we've seen, in addition to treating an element ("`Tag`") as a dictionary to retrieve its element values, you can also use the "`.attrs`" syntax to get the dictionary directly:

```
print(soup.body.find("a").attrs)
print(soup.body.find("td").attrs)
```

```
{'href': 'http://buildings.umwblogs.org/james-farmer-hall/'}
{'class': ['pic']}
```

(As noted on p. 168, see how the value of the "`class`" attribute is a list here.)

### Getting just text with `.get_text()`

The aforementioned `.get_text()` method is actually a bit more powerful than just extracting the contents of a single plain text element underneath an element. It can also be used to get *all the text* from that point down in the hierarchy, ignoring all tags. Check it out:

```
soup.body.find("p").get_text()
```

```
'Deep in the bowels of Farmer Hall resides a\ncarbon-based life form
known to outsiders only as Stephen. This\nmysterious being fulfills
several roles not widely known to\nhumankind.'
```

### Finding more than one tag name at once

You can pass a *list* to `.find_all()` to match more than one type of tag in a search:

```
soup.find_all(["td", "th", "p"])
```

And if you know how to use **regular expressions** (outside the scope of this class) you can use them as arguments to `.find_all()` and friends:

```
import re
soup.find_all(re.compile("^q"))
soup.find_all(re.compile("r"))
soup.find_all(re.compile("s$"))
```

(finds all tags whose name begin with `q`, contain `r`, or end with `s`, respectively.)

### CSS selectors

Finally, if you're familiar with CSS selector syntax, you can do all that jazz by calling the `.select()` method:

```
soup.select("div#master, tr td.data")
```

# Chapter 17

# Probabilistic reasoning

**Probability theory** is an area of mathematics that deals with *quantifying uncertainty*. We may not be sure that something is going to happen, but we want to be precise about *how* sure we are, given everything else we may know.

It turns out that probability theory is a crucial concept in Data Science. We've already used some of it in Chapters 5 and 6 when we generated random values from distributions. In this chapter, we'll zoom out from programming language details and consider how to reason about the probabilities of various values occurring and the relationships between random variables.

## 17.1 Terms

Some terms: an **outcome** is something that may (or may not) happen. This varies widely depending on the domain: a child that's born may or may not be male; an airline passenger may or may not have red hair; a customer may or may not buy a particular product. "Male," "red," and "*The Girl on the Train*, hardback edition" are all outcomes in these examples.

An **event**, by contrast, is a *set* (group) of outcomes that we're interested in. Often we don't care so much whether or not the customer specifically bought "*The Girl on the Train*, hardback edition" as whether they bought *any* book by Paula Hawkins, or maybe any

hardback book, or maybe any book at all (as opposed to a DVD).

Sometimes we'll use the symbol $\Omega$ ("omega") to refer to the **sample space**, which is simply the set of *all possible outcomes*. This will vary depending on what's under consideration; it might be { male, female } in one case and { red, blond, brunette, bald, other } in another case.

We'll also use the notation $\overline{\ }$ (overbar) to mean "any outcome *except* something." For instance, $\overline{\text{red}}$ means "the airline passenger had a hair color *other than* red."

## 17.2 Probability measures

A **probability measure** is a function that tells us intuitively how likely an outcome is to occur. We'll use the simple notation "P(·)" for this[1], read as "the probability of (something)." The probability of any outcome is always *a number between 0 and 1.* 0 means it can never possibly occur, 1 means it will definitely occur, and there's a continuum in between. In our first example, we might say P(male) = .5, P(red) = .1, and P(*The Girl on the Train*, hardback edition) = .0001.

You can talk about the probability of an event too, of course, and it's simply the sum of the outcome probabilities. P(male-or-female) = 1, P(red or blonde or bald) = .6, P(any hardcover book) = .08. We'll say that P($\Omega$) will be 1: after all, *something* has to happen, even if it's "the customer didn't buy anything," an outcome to which we'll assign a probability.

## 17.3 "Joint" probability

Very commonly, we'll be considering the likelihood that two different events *both* occur. For instance, perhaps we're interested in the probability that an airline passenger is a red-headed female. We'll write this as P(red, female).[2] The comma signals **joint probabil-**

[1] Some authors use "Pr()" instead of "P()" for this. Same diff.

[2] You may also run across the notation "P(red^female)," which means the same thing.

**ity**, which simply means that both of these outcomes/events must occur in order for the combined event to be considered to have occurred. If we wrote P(red, $\overline{\text{female}}$), it would mean 'the probability that the passenger is a red-headed *non*-female."

If you think about it, you'll realize that the joint probability cannot be greater than either of the two individual probabilities. Adding another condition (not female) to the first (red-headed) can't possibly *increase* the chance of it happening. Other than that, we don't know how to compute the joint probability from the individual ones, though (yet).

Finally, note that P(A,B) is the same thing as P(B,A), guaranteed. Switching the order of terms in a *joint* probability doesn't change the answer. (This will *not* be true in the next section, so watch out!)

Sometimes we'll talk about "the full **joint distribution**" of a set of discrete random variables. This can be visualized as a normalized contingency table with the probability for all the combinations. The joint distro of our airline passenger variables might look like this:

| | bald | blonde | brunette | red |
|---|---|---|---|---|
| female | 0.000 | 0.154 | 0.192 | 0.064 |
| male | 0.141 | 0.128 | 0.256 | 0.026 |
| other | 0.013 | 0.000 | 0.026 | 0.000 |

This means that, for instance, 14.1% of our passengers are bald males, 6.4% of our passengers are red-headed females, there were no blonde "others," *etc.* Obviously, the sum of all the cells in this table will equal exactly 1, since they are both mutually exclusive and collectively exhaustive.

## 17.4 "Marginal" probability

As we've seen, when we have two different variables (like hair color and gender) we can talk about the probability of various combinations of these, like P(blonde, $\overline{\text{male}}$) and P($\overline{\text{brunette}}$, male). But sometimes we also need to talk just one of those variables at a time,

like P(female): "what's the probability that an airline passenger is female, and I don't care what her hair color is?"

This is sometimes called the **marginal probability**. It gets its name because its answer is really in the *margins* of the corresponding contingency table. If we add margins to the above table, we get:

| | bald | blonde | brunette | red | All |
|---|---|---|---|---|---|
| female | 0.000 | 0.154 | 0.192 | 0.064 | 0.410 |
| male | 0.141 | 0.128 | 0.256 | 0.026 | 0.551 |
| other | 0.013 | 0.000 | 0.026 | 0.000 | 0.038 |
| All | 0.154 | 0.282 | 0.474 | 0.090 | 1.000 |

We can now look at the right margin and discover that the marginal probability P(male) is .551, and we can look at the bottom margin and see at a glance that P(blonde) is .282. This sort of analysis illustrates that, for example:

$$\text{P(female)} = \text{P(bald,female)} + \text{P(blonde,female)} + \text{P(brunette,female)} + \text{P(red,female)}$$

and

$$\text{P(brunette)} = \text{P(brunette,female)} + \text{P(brunette,male)} + \text{P(brunette,other)}$$

To compute a marginal from the joint, we're really just adding up all the different cases. There are three different ways to be a brunette: you can be a female brunette, a male brunette, or some other kind of brunette. That's all a marginal probability really is.

## 17.5 "Conditional" probability

Another notion we'll use a great deal is **conditional probability**, written with a "pipe" (vertical bar) like P(unemployed | college degree). The pipe is normally pronounced "given." So this expression is read "the probability that someone is unemployed *given* that

they have a college degree." We call this "**conditioning on**" college degree.

Or to return to our previous example, consider P(red | $\overline{\text{female}}$). This quantity is the answer to the question: "if I know for a fact that the passenger is not female, what's the probability that they're red-headed?"

Notice this is very different than the joint probability. With conditional probability, we're assuming that the second event *does* occur, and then asking how that revises our original prediction. Unlike with joint probability, adding a vertical bar *can* make the answer increase.

Consider this example: what's the probability that a random U.S. citizen has a Pinterest account? Let's estimate that as P(pinterest) = .15. But what if we learned that the chosen person was female? What is P(pinterest | female)? Just to shamelessly stereotype, I'm going to go out on a limb and say it's higher; perhaps .26. On the other hand, what if we learned the person was male? What is P(pinterest | male)? I'll say it's more like .04. In both cases, we adjusted our estimated probability in light of additional information: up in one case, and down in the other.

This adjusting-our-estimates stuff is at the heart of what's called "**Bayesian reasoning**" (you'll see why in section 17.8, below).

Two other terms that come up frequently are "**prior probability**" and "**posterior probability**". The "**prior**" is the probability of an event *without* applying conditioning. In the previous example .15 was the "prior probability" that the person was a pinterest user. When we learned our subject was female, we revised that to the "**posterior**" of .26.

Finally, note that P(A|B) is ***not*** the same thing as P(B|A). I gave you a heads-up about this above. In general, P(A|B) and P(B|A) are very different numbers. Ask yourself this: if you chose a random American, and they turned out to be pretty tall (say, taller than average), what's the probability that they're also an NBA player? I think you'll agree that the number here would be very small indeed: perhaps P(NBA | tall) would be .00001. There just aren't that many

NBA players out there, so the chances of you randomly choosing one – tall or not – is miniscule. But consider the reverse question: if your random choice just happened to be an NBA player, what's the probability that they'd also be tall? This, by contrast, would be far greater: I'll bet P(tall | NBA) is close to .95, since nearly all professional basketball players are pretty tall.

Or continue the pinterest example. P(pinterest | female) might be .26 (*i.e.*, 26% of all females are pinterest users), but P(female | pinterest) might be .87 (87% of all pinterest users are females). These are easy to confuse but critical to distinguish. We'll quantify all this in the next section.

## 17.6 The relationship between joint and conditional

Mathematically, here's how these two concepts (joint probability and conditional probability) are related. If A and B are two events, then:

$$P(A|B) = \frac{P(A,B)}{P(B)}$$

In words: the conditional is the joint divided by the marginal of the thing being conditioned on.

Let's quantify this with our pinterest example. Here's the four values in our joint distribution:

| | pinterest | $\overline{\text{pinterest}}$ |
|---|---|---|
| male | .02 | .48 |
| female | .13 | .37 |

We can compute the four marginals by summing rows / columns:

$$
\begin{aligned}
P(\text{male}) &= .5 \\
P(\text{female}) &= .5 \\
P(\text{pinterest}) &= .15 \\
P(\overline{\text{pinterest}}) &= .85
\end{aligned}
$$

And then, using our definition above, we can calculate all the conditionals:

$$
\begin{aligned}
P(\text{male} \mid \text{pinterest}) &= \frac{.02}{.15} = .003 \\
P(\text{male} \mid \overline{\text{pinterest}}) &= \frac{.48}{.85} = .565 \\
P(\text{female} \mid \text{pinterest}) &= \frac{.13}{.15} = .867 \\
P(\text{female} \mid \overline{\text{pinterest}}) &= \frac{.37}{.85} = .435 \\
P(\text{pinterest} \mid \text{male}) &= \frac{.02}{.5} = .04 \\
P(\text{pinterest} \mid \text{female}) &= \frac{.13}{.5} = .26 \\
P(\overline{\text{pinterest}} \mid \text{male}) &= \frac{.48}{.5} = .96 \\
P(\overline{\text{pinterest}} \mid \text{female}) &= \frac{.37}{.5} = .74
\end{aligned}
$$

It would be worth your while to double-check all the above calculations to reinforce your understanding of how joint, conditional, and marginal probabilities all work together.

By the way, it's frequently much easier to estimate the conditional probabilities than it is to estimate joint probabilities. So we often run the equation at the start of this section "backwards" and get joints from conditionals. Either way, it works, though.

## 17.7 The Law of "Total Probability"

Now if there are only two sexes of newborn babies possible, then it should be pretty obvious that:

$$P(\text{male}) + P(\text{female}) = 1$$

And if there are only three possible ice cream flavors to order at Carl's, then the probabilities for each customer's order must add up to 1 as well:

$$P(\text{vanilla}) + P(\text{chocolate}) + P(\text{strawberry}) = 1$$

We don't even need to know how likely vanilla is to know that the sum of the three must equal 1. This is the simplest application of the **Law of Total Probability**.

Now the following is also obvious if you think it through, but maybe not so obvious at first glance. Suppose that each Carl's customer orders a small, medium, or large ice cream cone, in one of the three flavors. The nine possibilities for a customer's order are thus:

| | | |
|---|---|---|
| A small vanilla cone | A small chocolate cone | A small strawberry cone |
| A medium vanilla cone | A medium chocolate cone | A med strawberry cone |
| A large vanilla cone | A large chocolate cone | A large strawberry cone |

Let's say we knew all nine probabilities (which must add up to 1, of course). Now, how could we figure out the probability of a *chocolate* cone order, regardless of size? The answer is: you sum up all the mutually exclusive and collectively exhaustive cases which include chocolate as the flavor. In symbols:

$$\begin{aligned} P(\text{chocolate}) &= P(\text{chocolate, small}) + P(\text{chocolate, medium}) + \\ &\quad P(\text{chocolate, large}) \end{aligned}$$

In plain English: the probability of the next customer ordering a chocolate cone is the probability they'll order a small chocolate cone plus the probability they'll order a medium chocolate cone plus the probability they'll order a large chocolate cone.

And what's the probability that the customer will order a *medium* cone, regardless of flavor? Clearly, it's:

$$P(\text{medium}) = P(\text{vanilla, medium}) + P(\text{chocolate, medium}) + P(\text{strawberry, medium})$$

It's not rocket science – you just have to think about all the different cases. But it is pretty useful, since oftentimes we have joint probabilities and need the marginal. And if you think about it, in the one-variable case the Law of Total Probability really just *is* computing the marginal.

Sometimes we have more than one variable we're interested in computing the probability of. Let's say that Carl's has an additional option: sprinkles on top. So now, there are these eighteen possible orders:

| | |
|---|---|
| A plain small vanilla cone | A small vanilla cone with sprinkles |
| A plain medium vanilla cone | A medium vanilla cone with sprinkles |
| A plain large vanilla cone | A large vanilla cone with sprinkles |
| A plain small chocolate cone | A small chocolate cone with sprinkles |
| A plain medium chocolate cone | A medium chocolate cone with sprinkles |
| A plain large chocolate cone | A large chocolate cone with sprinkles |
| A plain small strawberry cone | A small strawberry cone with sprinkles |
| A plain medium strawberry cone | A med strawberry cone with sprinkles |
| A plain large strawberry cone | A large strawberry cone with sprinkles |

If we wanted to know (say) the probability of a small strawberry cone, we'd calculate:

$$P(\text{strawberry, small}) = P(\text{strawberry, small, plain}) + P(\text{strawberry, small, sprinkles})$$

And if we wanted to know the probability of the next customer wanting a large cone with sprinkles, we'd compute:

$$P(\text{large, sprinkles}) = P(\text{vanilla, large, sprinkles}) + P(\text{chocolate, large, sprinkles}) + P(\text{strawberry, large, sprinkles})$$

You get the idea.

## 17.8 Bayes' Rule

Knowing how joint and conditional probabilities are related, and knowing that P(A,B) = P(B,A), it's easy to derive the following law:

$$P(A|B) = \frac{P(B|A) \cdot P(A)}{P(B)}$$

This is called **Bayes' Rule** (sometimes **Bayes' Law** or **Bayes' Theorem**) after the 18th-century Presbyterian minister Thomas Bayes. It is one of the most influential (and controversial, actually) statements in statistics and even all of mathematics. It will come up prominently in Chapters 19 through 21.

## 17.9 Independence

We need one more background concept before we're ready to apply some of this stuff, and that is the **independence** of events. There are two flavors of independence: absolute, and conditional.

### Absolute independence

Simply put, two events are **absolutely independent** if *the value of one has no bearing either way on the value of the other*. It does *not* mean the events are mutually exclusive. It means that the probability of each one of them occurring has nothing to do with the other.

It's best seen through an example. Suppose I chose a random U.S. citizen, and I observe two things: whether or not they're white, and whether or not they're female. If I asked you for your estimate of the "prior" for the race question, you'd probably come up with something like P(white) = .6. Now I ask you: suppose, before observing their race, you learned your subject was female. Does this cause you to update your "prior" estimate to a more accurate "posterior"?

The answer is no. Whether or not someone is white is *independent* of whether they're female. If you thought the probability of this random person being white was .6 before, then you still think it's .6 after learning she's female. In symbols, you thought P(white) was .6, and you think P(white | female) is also .6. The opposite was true in the pinterest example: your estimate of their pinterest status *did* change when you learned about their gender. Therefore, those two events are *not* independent.

I'm sure you realize that "independent" is pretty much the same concept as "not associated." The way to test a data set for two of its variables being independent is essentially to run the appropriate test ($\chi^2$, t-test, or Pearson's) and see whether there's a significant association or not. If there's not, then we have no compelling evidence that they're *not* independent, so we cautiously conclude they are.

Both of the following mathematical identities are true ***only if*** the events $A$ and $B$ are independent:

***If*** $A$ and $B$ are independent, then:

$$P(A|B) = P(A)$$
$$P(A, B) = P(A) \cdot P(B)$$

The first of these is basically the definition of independence: if P(white | female) = P(white), we say they're independent. (And conversely, if P(male | pinterest) ≠ P(male), we say they're associated and therefore *not* independent.)

The second one is a useful multiplicative shortcut, again only valid if the variables in question are independent. It's okay to compute P(white,female) as P(white) · P(female) = .6 · .5 = .3 – yielding a 30% chance of randomly choosing a white female – *because* we know that race and gender are independent. (Conversely, it's *not* okay to compute P(pinterest,male) as P(pinterest) · P(male) = .15 · .5 = .075, because these two variables are not independent; as we saw on p.178, the true answer for P(pinterest,male) is only .02.)

### Conditional independence

And lastly, two variables can be **conditionally independent given a third variable** in addition to (or instead of) being absolutely independent.

What does this mean? Perhaps the best way to think of it is those **confounding factors** we learned about in the first volume of this text. You may remember that I had a different pinterest example in that one (Section 10.4.1) which featured three variables: a person's `hair` length, their `pinterest` activity, and their `gender`. After noticing that `hair` was associated with `pinterest`, and jokingly speculating as to whether long-hair caused pinterest-ness or vice versa, we hypothesized that perhaps gender was a confounding variable that was actually influencing them both. This theory would explain why long hair and pinterest usage tended to go together, without either of them being the cause of the other.

In this case, we would say that although `hair` and `pinterest` were not *absolutely* independent, they nevertheless were *conditionally* independent given gender. In symbols:

$$P(\text{long hair} \mid \text{pinterest}) \neq P(\text{long hair})$$

*(**no** absolute independence)*

$$P(\text{long hair} \mid \text{pinterest,female}) = P(\text{long hair} \mid \text{female})$$

*(yes, conditional independence)*

In other words, once we know the subject is female, whether she's on pinterest tells us nothing further about whether or not she will have long hair. The information in the pinterest variable that signals "strong possibility of long hair!" is completely subsumed in the gender variable, and once that's controlled for, the pinterest and hair variables are again independent.

# Chapter 18

# Causality

I must now ask you to reach in your memory banks allll the way back to Chapter 10 of the *previous* volume of this book series. That chapter, entitled "Interpreting Data," dealt with association vs. causality, confounding factors, controlled experiments vs. observational studies, and related topics. The key question we addressed was how to interpret a statistical association between variables. If two variables are correlated, then they're correlated...but how confident can we be that there's a **causal** relationship between them – which is what we usually care about?

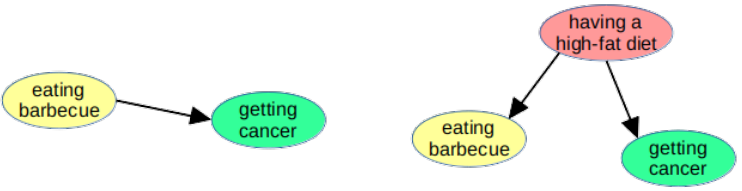



**Figure 18.1:** Causal diagrams, each expressing a hypotheses about the causality among variables.

The tool we used for this analysis was the **causal diagram**, examples of which appear in Figure 18.1. Each bubble represents one variable. Arrows pointing from one bubble to another asserts a causal relationship between the two: that the value of one is not merely *associated with*, but is partially *responsible for*, the value of the one pointed at.

If you remember that particular example, there was an observational study suggesting that eating barbecue can increase one's risk of various types cancer. Assuming that an association between the two variables was in fact discovered, the two sides of Figure 18.1 represent competing theories as to the reasons for that association.

The question we'll ask in this chapter is as follows: given a data set, is there any way to actually *tell* which of several competing causal theories is true? In other words, if we have more than one hypothesis giving alternate explanations for how the patterns in the data set arrived, can the *data itself* be used to judge between them?

And the answer is: sometimes. Let's learn when it can and can't.

## 18.1 The bad case: identical "skeletons"

Before I get you too excited, let me say right at the outset that there are times when the data fails us in our quest to nail this down. This happens when the **skeleton**s of the two causal models are identical.

The skeleton of a causal diagram is simply the diagram you get if you *remove the arrowheads*. Consider the two competing models in Figure 18.2. An observational study some years ago found an association between smoking cigarettes and experiencing clinical depression, and made the claim that therefore one of the many detriments to smoking (besides heart disease, lung cancer, and other things) was an emotional one. That represents the causal model on the left side of the diagram. But some objected and said, "wait a minute...couldn't it instead be the case that people who are going through depression are seeking ways to cope with it, and that substances like nicotine could be one of those ways?" This depression-causes-smoking hypothesis is on the right side.


**Figure 18.2:** Does smoking cause depression...or does depression lead to smoking?

Unfortunately there is no way to resolve this by looking at the data alone. This is because if you remove the (one) arrowhead, you get the same skeleton (Figure 18.3). Note that "the same skeleton" means merely *the same bubbles are connected to the same bubbles.* It does *not* have anything to do with where those bubbles are positioned on the page.


**Figure 18.3:** The bad case: both causal diagrams have the *same* skeleton.

In this case, the only way to resolve which of the causal models is the true one is to investigate the phenomenon on the ground. We have to study the mechanisms – physical and societal – by means of which each of them might plausibly cause the other. Medical researchers could explore the effects of nicotine on the human brain, and determine whether there is a mechanism by which serotonin is reduced. Social psychologists could conduct surveys and focus groups and learn how often cigarettes are sought by victims of depression and why. But the data itself will not give a verdict.

## 18.2 The good case: different "skeletons"

Often, though, the situation isn't that dire. Consider the controversy raised in one of my recent freshman seminars. The class was discussing the invention of chopsticks, and the impact that may have had on eastern culture as well as culinary techniques. One student made a different kind of claim. He said, "this is why so many of the great video game players in the world are from Asian countries! When kids from those regions grow up using chopsticks, it demands more attention to fine motor skills than using a fork would. And when they develop this terrific finger-eye coordination at a young age, it leads to greater expertise with a controller or

keyboard. Thus they are better equipped to compete in high-level gaming."

Perhaps. But as I listened to this student, I couldn't help remembering what my own boys told me: that many of the Asian countries place a higher cultural value on video games than we do in the western world. Apparently, high-achieving video game players are afforded the same fame and fortune in South Korea or Japan that our NFL and NBA players are in the U.S. They are awarded lucrative contracts, perform paid testimonial advertising, give autographs to cheering throngs, and so forth. It stands to reason, then, that a culture which rewards excellent video game play would produce excellent video gamers *regardless* of whether those players used forks or chopsticks.

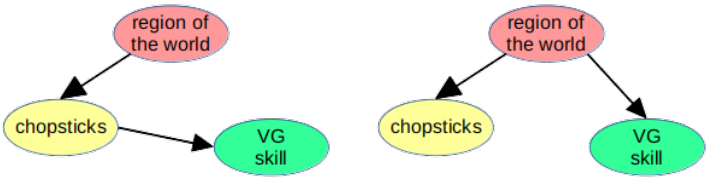



**Figure 18.4:** Two competing causal models about why many great video game players are from Asian countries.

These two competing hypotheses are illustrated in Figure 18.4. On the left is my student's model: the region of the world you're in (Asian or non-Asian) influences whether or not you primarily use chopsticks at your meals. With this much, I agree. But he then further claims that the use of chopsticks *causally influences* how good a video game player you are.

The right side of the diagram shows my own mental model: the region of the world you're in causally influences both chopstick usage *and* video game prowess. In my model, chopsticks and VG skill are *associated*, but not *causally* associated.

Now before we go on, consider the following exercise. Without even knowing the technical detail that comes next, can you figure out how to confirm or refute my student's (left-hand) causal model? What could you do with the data?

The solution is intuitive to many, but not to all. Simply put, you **condition on** the region of the world variable. This means you split the data into two groups: those from Asian countries and those from non-Asians countries. Think about it: if you *considered only Asians*, and discovered that chopstick-using Asians are better video gamers than non-chopstick-using Asians, then that would lend credence to the hypothesis that one causes the other. (And the same goes for considering only non-Asians.) But if you looked only at Asians (or only at non-Asians) and found that chopsticks and video game skill are *un*correlated, then that pretty much refutes the hypothesis. Everything in the coming sections is an elaboration of that principle.

## Comparing the skeletons

The reason this example turns out to be one of the "good news" cases is that the skeletons of the causal diagrams are different. Check out Figure 18.5. At first glance, you might assume that they are the same, just as in the smoking/depression example. After all, they're both chains-of-three nodes. But they're *not* the same. In one, chopsticks is the bubble with connections to the other two, and in the other it's region of the world. Just because they're the same shape doesn't mean they're the same skeleton: the same bubbles have to be connected to the same bubbles.


**Figure 18.5:** The good case: the causal diagrams have *different* skeletons.

And since the skeletons are different, the data can distinguish between the two, and tell us which causal model (or neither) is likely to be correct.

### Reasoning about independence

The reason we can use the data to render a verdict on our competing causal diagrams is that they embody different *independence assumptions*.

Look carefully at the left side of Figure 18.4 on p. 188. If that causal model were true, then chopsticks and VG skill would not be absolutely independent. Nor would region of the world and VG skill: after all, if you're from an Asian country, you're more likely to use chopsticks, and if you use chopsticks, you're more likely to be good at video games, so of course the region of the world and VG skill variables are correlated.

However, in that left-hand diagram, region of the world and VG skill will be *conditionally independent given chopsticks*. In symbols:

$$P(\text{VG} \mid \text{region}) \neq P(\text{VG})$$

*but*

$$P(\text{VG} \mid \text{region},\ \text{chopsticks}) = P(\text{VG} \mid \text{chopsticks})$$

Why is this? Because in the left-hand diagram, the only reason that knowing a person's region was of any use to predicting their VG skill was because it influenced how likely it was that they used chopsticks. If you actually *have* the information about chopsticks directly, well then you can toss region out the window. It's irrelevant at that point.

The right-hand side of Figure 18.4 is much different. Its independence assumptions are that VG skill and *chopsticks* are conditionally independent given *region*. Namely:

$$P(\text{VG} \mid \text{region}) \neq P(\text{VG}) \quad \text{(again)}$$

*but*

$$P(\text{VG} \mid \text{chopsticks},\ \text{region}) = P(\text{VG} \mid \text{region})$$

This is the flip side of the former case: now, although chopsticks can tell you something useful about VG skill in a pinch, the primary influencer of gaming skill is not chopsticks, but *region*. Once you tell me what region of the world somebody is from, I have much better information about their possible video game use, and knowing whether they use chopsticks is no longer of interest to me.

To sum up: both models agree that

$$P(\text{VG} \mid \text{region}) \neq P(\text{VG}).$$

But the left one (my student's hypothesis) asserts:

$$P(\text{VG} \mid \text{region},\ \text{chopsticks}) = P(\text{VG} \mid \text{chopsticks})$$
$$P(\text{VG} \mid \text{chopsticks},\ \text{region}) \neq P(\text{VG} \mid \text{region}),$$

while the right one (my own hypothesis) asserts:

$$P(\text{VG} \mid \text{region},\ \text{chopsticks}) \neq P(\text{VG} \mid \text{chopsticks})$$
$$P(\text{VG} \mid \text{chopsticks},\ \text{region}) = P(\text{VG} \mid \text{region}).$$

(Note carefully the "=" vs. "≠" signs in those equations, because they're the only difference!)

Armed with this insight, we realize that judging between our alternate causal models boils down to analyzing the data to see which conditional independence assumptions actually hold. Let's see how to do that.

## 18.3 Confirming or denying causal hypotheses

### Testing the data for absolute independence

We already know how to test for *absolute* independence: just see whether an association exists between the two variables. For two

categorical variables, it's $\chi^2$; for two numeric variables, it's a Pearson's correlation; and for one of each, it's a $t$-test (or, if you have more than two values for the categorical variable, an $F$-test.

Let's synthesize some data. For this example, we'll make it easy and say that our three variables of interest – region, chopsticks, and VG – are all categorical, and furthermore are all "binary" (only two values each). Suppose for a moment that both of the above hypotheses were wrong, and actually there was *no* association between *any* of the variables. To make a data set reflecting this (certainly wrong) reality, we could write code like this:

```
region = np.random.choice(['Asian','non-Asian'],
    p=[.4,.6],size=10000)
chopsticks = np.random.choice(['yes','no'],
    p=[.3,.7],size=10000)
VG = np.random.choice(['good','bad'],p=[.2,.8],size=10000)

data = pd.DataFrame({'region':region,
    'chopsticks':chopsticks,'VG':VG})
```

```
          region chopsticks    VG
0          Asian         no   bad
1      non-Asian        yes  good
2      non-Asian        yes   bad
3          Asian         no  good
4      non-Asian        yes   bad
                .   .   .
```

If this were the case, we'd run our $\chi^2$ test and get our expected negative result:

```
scipy.stats.chi2_contingency(
    pd.crosstab(data.chopsticks, data.VG))[1]
```

```
0.5055960853810801
```

Here, the right thing to do is throw out both my student's hypothesis and my own. Both of them predict that chopsticks and VG would be associated, and since they're not, both causal models are probably bogus.

## Testing the data for conditional independence

Okay. That's old stuff. Now let's talk about testing for *conditional* independence. This involves *three* variables: the two you're checking for independence, and the one you're conditioning on.

Now it turns out this is a hard problem when the variable you're conditioning on is numeric, but not so hard when it's categorical. In our case, of course, it's categorical, since that's the only kind of data we have.

### "chopsticks cause videogame prowess?"

Suppose for the moment that my student was correct. How could we generate a synthetic data set reflecting his view of the world? How about:

```
region = np.random.choice(['Asian','non-Asian'],p=[.4,.6],
    size=10000)
chopsticks = np.where(region=='Asian',
    np.random.choice(['yes','no'],p=[.8,.2],size=10000),
    np.random.choice(['yes','no'],p=[.1,.9],size=10000))
VG = np.where(chopsticks=='yes',
    np.random.choice(['good','bad'],p=[.5,.5],size=10000),
    np.random.choice(['good','bad'],p=[.1,.9],size=10000))
```

I'm guessing at the numbers, of course. But compare this code with the left-side causal model in Figure 18.4 (p. 188) and see if you agree that they coincide. First, we generate `region` independently. Then, we give `Asian`s a much higher likelihood of being chopstick users (80% as opposed to a mere 10% of non-Asians). Then, we make many more of the chopstick users good video game players (50% of them) than we do non-chopstick users (only 10%).

Testing for conditional independence is just a matter of conditioning; *i.e.* treating the two conditioned groups separately.

My student predicted these two things, remember:

$$P(\text{VG} \mid \text{region},\ \text{chopsticks}) = P(\text{VG} \mid \text{chopsticks}) \quad \textit{prediction \#1}$$
$$P(\text{VG} \mid \text{chopsticks},\ \text{region}) \neq P(\text{VG} \mid \text{region}) \quad \textit{prediction \#2}$$

Let's see if they're true (with the synthetic data set that we know should have made them true). The first one claims that VG and region are conditionally independent given chopsticks. If this is true, then $\chi^2$ tests on VG and region – if taken among only the chopstick users, or among only the non-chopstick users – should give us *negative* results. Do they?

```
choppers = data[data.chopsticks == "yes"]
nonChoppers = data[data.chopsticks != "yes"]

scipy.stats.chi2_contingency(pd.crosstab(choppers.region,
    choppers.VG))[1]
scipy.stats.chi2_contingency(pd.crosstab(nonChoppers.region,
    nonChoppers.VG))[1]
```

```
0.41149872565464615
0.3220502005397185
```

As expected, **yes**. The $p$-values are well above .05, which tells us that region and VG are *not* correlated – at least when we only look at chopstick users, and when we only look at non-chopstick users.

Look at that code carefully. We first made two different data frames – `choppers` and `nonChoppers` – by taking a subset of the original data frame. Then, we subjected each one to a $\chi^2$ test of the relevant variables. Both $p$-values came back greater than $\alpha$, confirming that these conditional independencies exist.

To test prediction #2, we split into groups a different way: Asians and non-Asians. Then, we check whether `chopsticks` and `VG` are independent. To wit:

```
asians = data[data.region == "Asian"]
nonAsians = data[data.region != "Asian"]

scipy.stats.chi2_contingency(pd.crosstab(asians.chopsticks,
    asians.VG))[1]
scipy.stats.chi2_contingency(pd.crosstab(nonAsians.chopsticks,
    nonAsians.VG))[1]
```

```
1.4977381776979758e-33
3.1074726542441227e-71
```

As expected, they are correlated, and therefore *not* independent. There is clearly an association between chopstick usage and video game skill, even when controlling for region of the world.

**"culture causes videogame prowess?"**

Okay, now let's suppose the $I$ was correct in saying that chopstick usage itself has negligible impact on video game skill: the real effect is that certain parts of the world have cultures conducive to video games. To generate a synthetic data set reflecting *this* view of the world, we'd do something like this:

```
region = np.random.choice(['Asian','non-Asian'],p=[.4,.6],
    size=10000)
chopsticks = np.where(region=='Asian',
    np.random.choice(['yes','no'],p=[.8,.2],size=10000),
    np.random.choice(['yes','no'],p=[.1,.9],size=10000))
VG = np.where(region=='Asian',
    np.random.choice(['good','bad'],p=[.4,.6],size=10000),
    np.random.choice(['good','bad'],p=[.15,.85],size=10000))
```

It looks similar at a glance to what we had before, but notice carefully that both `chopsticks` *and* `VG` are now being influenced by `region`. Good video game players will still be more likely to use chopsticks, but not *because* they use chopsticks. Instead, it's because they're often from Asian countries. Compare this code with

the right-side causal model in Figure 18.4 (p. 188) and see if you agree.

What did my causal model predict? These two things:

$$P(\text{VG} \mid \text{region},\ \text{chopsticks}) \neq P(\text{VG} \mid \text{chopsticks}) \quad \textit{prediction \#1}$$
$$P(\text{VG} \mid \text{chopsticks},\ \text{region}) = P(\text{VG} \mid \text{region}) \quad \textit{prediction \#2}$$

We test these just as before, though looking for the opposite results. If we condition on chopsticks, we should see that region and VG are *still correlated*:

```
choppers = data[data.chopsticks == "yes"]
nonChoppers = data[data.chopsticks != "yes"]

scipy.stats.chi2_contingency(pd.crosstab(choppers.region,
    choppers.VG))[1]
scipy.stats.chi2_contingency(pd.crosstab(nonChoppers.region,
    nonChoppers.VG))[1]
```

```
2.888410498627128e-34
9.646356783989529e-68
```

These low $p$-values confirm just what we thought: using chopsticks has nothing to do with it, man: even factoring that out, video game skill still goes with region of the world.

And for prediction #2:

```
asians = data[data.region == "Asian"]
nonAsians = data[data.region != "Asian"]

scipy.stats.chi2_contingency(pd.crosstab(asians.chopsticks,
    asians.VG))[1]
scipy.stats.chi2_contingency(pd.crosstab(nonAsians.chopsticks,
    nonAsians.VG))[1]
```

```
0.9962429463855988
0.4256313356217548
```

we find that as expected, once you control for country, chopstick usage and video game skill have nothing much to do with each other.

## 18.4 Taking a breath

Whew. That was a lot of number crunching, and subtle reasoning. It's easy to get lost in the numbers and say, "wait...did I just confirm that? Or deny it? Which hypothesis was I testing? Was my $p$-value too low? too high? Aggh!"

When you step back and take a breath, you'll see the pattern. In both of these cases, we stacked the deck, of course. We deliberately generated an artificial data set to confirm the student's hypothesis, and then generated one to confirm mine. Who knows what the real answer is? I don't actually have any data on video game competitions nor chopstick usage.

The important thing to see is that if the skeletons of two different causal theories are different, then you don't have to throw up your hands and say "correlation doesn't equal causation! So I guess I know nothing!" The data often has a lot to say, and even in observational studies, a careful analysis can reveal deep truths.

# Chapter 19

## ML classifiers: Naïve Bayes (1 of 3)

For some folks, the coolest and most exciting parts of Data Science are the **machine learning (ML)** algorithms. These are the under-the-hood techniques for doing prediction and analytics. We'll look at a few of them briefly in this class, and you'll delve into them more fully in later courses.

Recall that a **classifier** is an algorithm/program to predict which of several **labels** (or **classes**) to assign to a data point. Perhaps we're trying to predict what political party someone is affiliated with, and our labels are "Democrat," "Republican," and "Green." Perhaps we're trying to predict whether someone will default on a loan, and the labels are "safe" and "high-risk."

There are many different algorithms for classification, but they all use a set of **labeled examples** as "**training data**." The idea is that by scrutinizing a bunch of examples for which we *know* the label, we can intelligently figure out what label to assign to new, **unlabeled examples**.

The attributes of our training data (and new data) that we'll use for prediction are sometimes called **features**. If our training data is in a DataFrame, the features are essentially all the relevant columns except for one, which is the **target**. Our goal, given a new data point that has values for all the features, is to label its target with the label it's most likely to have, assuming the training data are representative examples.

A classifier's **performance** can be measured in several ways, but the most straightforward is to score how many unlabeled examples it gives the correct label to. This of course begs the question: if the example is *un*labeled, how can we know whether or not the classifier's label was correct? What we have to do in practice is set aside some of our (precious) labeled data as a set of **test data**. We sort of pretend we don't know the answers for the test data, feed them to the algorithm which has been trained on the *training* points, and then score how well it did.

One of the simplest (and quickest) classifiers around is called the **Naïve Bayes classifier**, for reasons which will become apparent. In some ways, it's the rock-bottom, no-frills default algorithm for classification. One reason it's important is that it's simple and actually works surprisingly (even embarrassingly) well in many cases. Another reason is that even when it doesn't turn out to have the best performance, it's still a **baseline** which other algorithms' performance can be compared to. A researcher might report: "our whiz-bang algorithm X got 89.4% of examples correct on this test set, compared with 83.7% for straightforward Naïve Bayes."

## 19.1 The Naïve Bayes algorithm

Suppose we're designing a security system for a Galactic Cruiser. One thing we need to do is identify possible evildoers on our security cameras. Given what we can observe about them, can we tell good guys from bad guys?

| face | height | demeanor | lightsaber | type |
|---|---|---|---|---|
| clean | short | menacing | green | Sith |
| beard | medium | calm | green | Jedi |
| clean | tall | menacing | red | Sith |
| beard | medium | calm | blue | Jedi |
| beard | medium | calm | blue | Jedi |
| clean | medium | calm | blue | Sith |
| clean | tall | menacing | red | Jedi |
| clean | medium | menacing | red | Sith |
| clean | short | calm | blue | Jedi |
| | | . . . | | |

The training data above, in a `DataFrame` called "`t`" (for "training"), has four features: whether the `face` of the person in question has a `beard` or is `clean`-shaven, what their `height` is (clustered in three broad ranges), whether their `demeanor` is `menacing` or `calm`, and what color `lightsaber` they wield. The final column is our label: this person is known to be a `Jedi` (good guy) or a `Sith` (bad guy).

A test point that we might want to evaluate looks like this:

```
  face  height  demeanor lightsaber  type
beard   short  menacing        red   ??
```

In other words, a short, menacing, bearded person with a red lightsaber has just showed up on security camera #305. Should we sound the alarm? That, of course, depends upon their (as yet unknown) `type`. We want to predict this based on our past examples.

The **Naïve Bayes** classification algorithm applies conditional probability to this question. Really, what we're asking is: "which of the following two quantities is greater:

1. P(Jedi | beard,short,menacing,red), or
2. P(Sith | beard,short,menacing,red)?"

Note that we're combining joint and conditional probabilities here. Given that we have the *joint* event "bearded, short, menacing, and red," what's the *conditional* probability of them being a Jedi (or Sith)? If we estimate the first as .8 and the second as .2, for instance, we won't sound the alarm.

## 19.2 Using Bayes' rule

With Bayes' rule, we can rewrite these as:

(1) Estimated Jedi probability:

$$\text{P(Jedi | beard,sh,menace,red)} = \frac{\text{P(beard,sh,menace,red | Jedi)} \cdot \text{P(Jedi)}}{\text{P(beard,sh,menace,red)}}$$

and

(2) Estimated Sith probability:

$$\text{P(Sith} \mid \text{beard,short,menace,red)} = \frac{\text{P(beard,short,menace,red} \mid \text{Sith)} \cdot \text{P(Sith)}}{\text{P(beard,short,menace,red)}}$$

Note that the two equations are identical except for the words "Jedi" and "Sith," which are interchanged. Let's focus on equation (1) first.

Bayes' Rule has allowed us to turn things on their head. In essence, instead of asking "if they have these physical features, would they likely be a Jedi?" we're asking "if they're a Jedi, would they be likely to have these physical features?"

The right-hand side of equation (1) has three parts: two in the numerator, and one in the denominator. Ignore the denominator for a moment. The second part of the numerator, P(Jedi), is our **prior** probability. That's easy to estimate from the training data: we just count up what percentage of our samples are Jedi overall.

The first half of the numerator needs more work. It reads:

$$P(\text{beard}, \text{short}, \text{menacing}, \text{red} \mid \text{Jedi})$$

Now ***if*** it just so happened that those four features were *independent* of one another, this would actually be super easy to compute. We could just do this:

$$P(\text{beard} \mid \text{Jedi}) \cdot P(\text{short} \mid \text{Jedi}) \cdot P(\text{menacing} \mid \text{Jedi}) \cdot P(\text{red} \mid \text{Jedi})$$

Under this outrageous assumption, we've split the expression into *each feature individually.* This is called **the Naïve Bayes assumption**. Of course it's probably *not* true that beardedness, height, demeanor, and lightsaber color are all independent of each other; for one thing, if some or all of these features are indicative of Jedi-ness (which we hope), then they certainly *will* vary together! But the Naïve Bayes classifier says "aw heck, let's just throw caution to the wind and see how things work out."

All these components are now trivially obtainable from the training data. For example, what's a good estimate of P(beard | Jedi)? Simple: look at *only the Jedi* in the training data, and count up how many "`beard`s" and "`clean`s" there are. The fraction that are `beard`s is our estimate of P(beard | Jedi).[1]

To make it concrete, in our training data on p. 200, there are a total of six Jedi (count them!), of whom four have beards (count them!). Therefore, our estimate for P(beard | Jedi) is $\frac{4}{6} = \frac{2}{3}$. In other words, based on this training data, we guesstimate that if you're a Jedi, it's about 67% likely that you're bearded.

## 19.3 A numerical example

Let's work out the numerical answer (numerator only) for the training data listed earlier. First, considering *only* the five `Jedi` rows gives us our Jedi numerator:

$$\begin{array}{cccccccccccc} P(\text{beard}|\text{Jedi}) & \cdot & P(\text{short}|\text{Jedi}) & \cdot & P(\text{menace}|\text{Jedi}) & \cdot & P(\text{red}|\text{Jedi}) & \cdot & P(\text{Jedi}) & = \\ \frac{4}{6} & \cdot & \frac{1}{6} & \cdot & \frac{2}{6} & \cdot & \frac{1}{6} & \cdot & \frac{6}{11} & = .0034 \end{array}$$

Now let's do the same thing for the five `Sith` rows to get the Sith numerator:

$$\begin{array}{cccccccccccc} P(\text{beard}|\text{Sith}) & \cdot & P(\text{short}|\text{Sith}) & \cdot & P(\text{menace}|\text{Sith}) & \cdot & P(\text{red}|\text{Sith}) & \cdot & P(\text{Sith}) & = \\ \frac{1}{5} & \cdot & \frac{1}{5} & \cdot & \frac{4}{5} & \cdot & \frac{2}{5} & \cdot & \frac{5}{11} & = .0058 \end{array}$$

Look very very carefully at the training data on p. 200 and confirm that you agree with the above numbers. Using a pencil to write marks on the training data often helps you to keep everything straight.

### Throw away the denominator

Okay, those are the two numerators. To get true probabilities, we have to divide by the denominators, of course. But the nice

[1] If you have trouble seeing this, go back to the definition of conditional probability on p. 178. We're really calculating $\frac{P(\text{beard}, \text{Jedi})}{P(\text{Jedi})}$ here, which is "the number of bearded Jedi divided by the number of total Jedi."

thing is: *the denominators are the same in the two cases!* For both expressions, we would need to divide by P(beard, short, menacing, red) (in words, "what's the probability that any random person would be a bearded, short, menacing person with a red lightsaber?") This of course has the same value even if we compute it twice. For this reason, we *throw away the denominator* since in the end all we really care about is "which is higher, P(Jedi | *stuff*) or P(Sith | *stuff*)?"

In this case, P(Sith | *stuff*) is the higher of the two quantities (.0058 vs. .0034) and so we boldly predict: "this person looks like a Sith! Sound the alarm."

All that counting and dividing, of course, is a pain. So we'll get Python to automate it for us. That's the subject of the next chapter.

# Chapter 20

## ML classifiers: Naïve Bayes (2 of 3)

How can we automate the calculations of the previous chapter in Python? Let's assume that our data is in a Pandas `DataFrame` called "`t`" (for "training") as it was in the last chapter (p. 200). Now imagine writing this function:

```
def predict(face, height, demeanor, lightsaber):
    ...
```

This function takes as input a new (unlabeled) data point and returns a prediction for it: either the word "`Jedi`" or the word "`Sith`."

We'll do most of the work outside the function, actually. We'll read in the file and then pre-compute all the probabilities that we'll need for our calculations. This is effectively the training stage: we're "training" our classifier function on the data.

If you think it through, the calculations from Chapter 19 imply the need for the following probabilities:

- $P(label)$ for every one of the target labels (these are the "priors")
- $P(value \mid label)$ for every value in a column and every target label (the conditionals)

In our case, this amounts to:

- Priors:
  - $P$(Jedi)
  - $P$(Sith)
- Conditionals:
  - $P$(clean | Jedi) and $P$(clean | Sith)
  - $P$(beard | Jedi) and $P$(beard | Sith)
  - $P$(tall | Jedi) and $P$(tall | Sith)
  - $P$(medium | Jedi) and $P$(medium | Sith)
  - $P$(short | Jedi) and $P$(short | Sith)
  - $P$(menacing | Jedi) and $P$(menacing | Sith)
  - $P$(calm | Jedi) and $P$(calm | Sith)
  - $P$(red | Jedi) and $P$(red | Sith)
  - $P$(green | Jedi) and $P$(green | Sith)
  - $P$(blue | Jedi) and $P$(blue | Sith)

These are all straightforward to compute with Pandas. I find it convenient to create a dictionary, called something like "`probs`," to store all the probabilities. To compute the priors, all we have to do is figure out what fraction of the rows go with each label:

```
probs = {}
probs['Jedi'] = len(t[t.type=='Jedi'])/len(t)
probs['Sith'] = len(t[t.type=='Sith'])/len(t)
```

For the conditionals like "$P$(calm | Sith)", we ask: *considering only the rows that have `Sith` labels*, what fraction also have `calm` labels? That boils down to this:

```
probs['calm|Sith'] = (
    len(t[(t.type=='Sith') & (t.demeanor=='calm')]) /
    len(t[(t.type=='Sith')]))
```

The other 19 conditionals follow exactly the same pattern. (It may strike you that we're repeating a lot of very similar code here, and making slight edits to each one, and that there's a better, more general way. You're right. Stay tuned for Section 20.2.)

Now for the actual `predict()` function. All we have to do is multiply everything out per the above equations and see which of the two numerators is greater. The result is in Figure 20.1. Stare carefully at it and convince yourself that it does precisely the same calculations we did in Section 19.3 (p. 203). Note that we don't use the `t` variable inside this function at all. We've already computed all the `probs`, and once we've done that, the `DataFrame` and the data itself ceases to matter. We run the function just by passing it the values derived from our spycam:

```
print(predict("beard","tall","calm","blue"))
print(predict("clean","tall","menacing","red"))
```

```
'Jedi'
'Sith'
```

```
def predict(face, height, demeanor, lightsaber):
    jediness = (probs[face+"|Jedi"] *
                probs[height+"|Jedi"] *
                probs[demeanor+"|Jedi"] *
                probs[lightsaber+"|Jedi"] *
                probs["Jedi"])
    sithness = (probs[face+"|Sith"] *
                probs[height+"|Sith"] *
                probs[demeanor+"|Sith"] *
                probs[lightsaber+"|Sith"] *
                probs["Sith"])
    if jediness > sithness:
        return "Jedi"
    else:
        return "Sith"
```

**Figure 20.1:** Our Naïve Bayes ML `predict()` function.

## 20.1 Estimating confidence

Our `predict()` function, as written, just gives a binary answer: either `Sith` or `Jedi`. It may be useful to know *how confident* it is in its prediction for any given input. All we need to do is compute the correct ratio. Remember that `jediness` and `sithness` are just the *numerators* of probabilities, and that those probabilities have the same denominator. Therefore, in order to compute the true $P(\text{Jedi} \mid e)$, where $e$ is all our evidence (calm, beard, and so forth), we just need to compute:

$$P(\text{Jedi} \mid e) = \frac{\text{jediness}}{\text{jediness} + \text{sithness}}$$

and similarly,

$$P(\text{Sith} \mid e) = \frac{\text{sithness}}{\text{jediness} + \text{sithness}}$$

The denominator drops out when we divide the quantities anyway.

So let's enhance our `predict()` function to return a list of *two* values: the prediction, and the confidence level (on a scale of .5 to 1, meaning "only 50% confident in our prediction" all the way to "absolutely 100% confident in our prediction." To wit:

```
def predict(face, height, demeanor, lightsaber):
    ...
    if jediness > sithness:
        return ["Jedi", jediness/(jediness+sithness)]
    else:
        return ["Sith", sithness/(jediness+sithness)]
```

(We're returning a list here, of the two values.) Taking it for a spin:

```
predict("clean","tall","menacing","red")
predict("beard","tall","menacing","blue")
```

```
['Sith', 0.9760957241941071]
['Jedi', 0.7298292697172792]
```

So we're incredibly confident that our clean-shaven, tall, menacing, red-wielder is a Sith, but not nearly so confident that our bearded, tall, menacing blue-wielder is a Jedi.

## 20.2 Coding it more generally

The above calculation of the probabilities left something to be desired, since it was hardcoded and repetitive. We can improve on this by writing our code in a more general way, rather than explicitly referring to problem-specific names like "`Jedi`" and "`demeanor`" and "`blue`." Here's one way to do all the training calculations:

```
t = pd.read_csv("...")

probs = {}
features = t.columns[0:len(t.columns)-1]
target = t.columns[len(t.columns)-1]

for label in t[target].drop_duplicates():

    # Calculate priors.
    probs[label] = len(t[t[target] == label])/len(t)

    # Calculate conditionals.
    for feature in features:
        for value in t[feature].drop_duplicates():
            probs[value+"|"+label] = (
                len(t[(t[target] == label) &
                                (t[feature] == value)]) /
                    len(t[t[target] == label]))
```

Lots going on here. First, after reading the data, we set `features` to be the names of all the columns except the last one, and `target` to be the name of the last one.

Then we loop through all the different target labels (*e.g.*, "`Jedi`" and "`Sith`"), calculating both priors and conditionals. The priors are straightforward: they're just the fraction of rows that match the label, like we did in the top box on p. 206.

We're making an assumption when calculating conditionals: that all the values in the columns are unique (*i.e.*, that we won't have, for example, an "`out-of-state`" column with some "`beard`" values and also have a "`married`" column with "`beard`" values.) As long as this is true, we know we have a unique string to use as a key (like "`medium|Sith`") and it won't have a name collision with any other conditional.

The `predict()` method itself will be generalized as follows: instead of taking exactly four parameters named "`face`", "`demeanor`", *etc.*, it will take a *list* of parameter values, so that it can be called like this:

```
predict(['beard','tall','menacing','blue'])
```

The code is in Figure 20.2 (p. 211). We use the variable `scores` to keep a list of the numerators for each target label: this is only necessary to compute the confidence level in the result. We go through all the possible target labels, computing our score for each, and adding it to `scores`. Along the way, each time we encounter a label who has a higher score than any previous label, we remember it (and its score) in the variables `top_label` and `top_score`. That way, at the end of the loop, we can return our list of two elements: the predicted label, and our confidence in it.

## 20.3 Measuring performance

Okay, so how well does this classifier work? This depends on how we measure its "goodness." You may remember from Chapter 29 of the first volume of this series that this is sometimes a nuanced decision. For the spaceship case, perhaps it's more important to nail every potential Sith, even at the risk of unnecessarily investigating and detaining some Jedi. If we wanted to do this, we would need our

```
def predict(values):

   # Compute one score for each target label.
   scores = []

   # Keep track of the highest score, and its label, as we go.
   top_score = 0
   top_label = ""

   for label in t[target].drop_duplicates():

       # Start with the prior
       score = probs[label]

       # Multiply in the conditionals
       for value in values:
           score *= probs[value+"|"+label]
       scores.append(score)

       # If the score we just computed is the highest so far,
       # we have a new most-likely label.
       if score > top_score:
           top_score = score
           top_label = label

   return [ top_label, top_score / sum(scores) ]
```

**Figure 20.2:** The `predict()` function, written more generally.

measure of `performance` to penalize false negatives more than it does false positives.

Most commonly, we'll simply ask, "what percentage of the time is it right?" In other words, we'll count errors the same in either direction (predicting `Sith` for someone who is actually a Jedi is just as "bad" as predicting `Jedi` for an actual Sith). That's what we'll do first.

Now as we know, we can't test a classifier's performance on the data it's trained on and expect to get anything accurate. So we'll need to split our data into a training set and a test set. This can be done easily in Pandas with:

```
complete_data_set = pd.read_csv("security_cam.csv")
train = complete_data_set.sample(frac=.7)
test = complete_data_set.drop(train.index)
t = train
```

This call to `.sample()` randomly[1] chooses 70% of the original data set's rows and copies them to a new `DataFrame` called "`train`". Then the next line makes "`test`" a `DataFrame` of all the others (the remaining 30%). For convenience, we then copy `train` into the `t` variable so that none of our previous code has to change.

All our probabilities are thus computed based *only* on the training data (the random 70% of the data set). We can then use the `test` set to compute our accuracy. All we need to do is iterate through the `test` set, passing each row to `predict()` and seeing whether we get the correct answer:

```
num_correct = 0
for i in range(len(test)):
    row = test.iloc[i]
    p = predict([row['face'],row['height'],
        row['demeanor'],row['lightsaber']])
    if p[0] == row['type']:
        num_correct += 1

print("We got {}% correct on the test data.".format(
    num_correct/len(test)*100))
```

[1] You might ask, "why not just take the *first* 70% of the rows as the training data, and the last 30% as the test data? Why choose randomly?" The answer is that it's probably okay to do that, but sometimes there is meaning to the order of the rows in the data set and we want to avoid biasing the training vs. test rows one way or another. For example, if our `security_cam.csv` was arranged chronologically, then the first 70% of the spycam measurements would all have been taken *earlier* than the ones we'd test our performance on. A big deal? Possibly not...but on the other hand, perhaps the makeup of our spaceship clientele has changed over time, and thus not shuffling the rows would lead to inaccuracies.

We get a different answer every time we run our program, since it will choose a different training/test split in each case.

```
We got 82.63% correct on the test data.
```

If we did want to err on the side of caution, and penalize false-Jedi predictions more than false-Sith predictions, we could do that as follows:

```
num_missed_jedi = 0
num_missed_siths = 0
for i in range(len(test)):
    row = test.iloc[i]
    p = predict([row['face'],row['height'],
        row['demeanor'],row['lightsaber']])
    if p[0] != row['type']:
        if p[0] == 'Jedi':
            num_missed_siths += 1
        if p[0] == 'Sith':
            num_missed_jedi += 1

penalty = num_missed_jedi + num_missed_siths * 2
our_score = (1 - penalty/len(test)) * 100
```

```
Our score on the test data was 66.33.
```

Here we're penalizing actual-Siths-that-we-predicted-were-Jedi *twice* as much as actual-Jedi-that-we-predicted-were-Sith. Our score is no longer a "percentage," really; it's just a number – kinda sorta between 0 and 100 (although it could be lower if we misidentified enough Siths) – which we can use to compare with other classifiers.

# Chapter 21

# ML classifiers: Naïve Bayes (3 of 3)

## 21.1 Numeric variables

In all the examples above, we had categorical features. Computing something like "$P$(calm | Jedi)" is thus just a matter of counting the `Jedi` rows which (exactly) match the value `calm`. But what if we have a numeric feature, like a person's age or salary?

One quick-and-dirty way to deal with numeric features is to "bin" them, kind of like a histogram. Note that this is actually what we already did with the "`height`" column in the Jedi example: instead of heights like 4'9" and 6'6", we had values like `short` and `tall`.

This has obvious drawbacks. For one, we're throwing away all the detail present in the measurement and treating different values exactly alike. For another, it's up to us to somewhat arbitrarily choose how many bins to use and where the demarcation lines are. This has an *ad hoc* feel to it.

### Gaussian Naïve Bayes

Better is to treat the continuous variable as what it really is: a number. **Gaussian Naïve Bayes** is probably the most common way to deal with this in a principled fashion: we make the assumption that the numeric feature is distributed **normally** ("normal"=="Gaussian"), and estimate its mean and standard deviation from the training data. Then, to estimate $P$(value | target_label)

for any particular test data point's value, we choose the estimated value of its **probability density** (p. 31) and use that.

Remember from Section 5.2 (p. 36) that if a variable is "distributed normally" it means that its values are "bell-curvy." There's some average value which occurs a lot, and values farther and farther from that average are less and less likely to occur.

Now suppose we had a numeric `height` feature (measured in inches) instead of a categorical one. Our training data (in the "`t`" `DataFrame`) might look like this:

```
    face  height  demeanor lightsaber  type
   clean    62.5  menacing      green  Sith
  beard    68.3      calm      green  Jedi
   clean    78.1  menacing        red  Sith
  beard    63.9      calm       blue  Jedi
  beard    61.9      calm       blue  Jedi
   clean    68.2      calm       blue  Sith
   clean    80.1  menacing        red  Jedi
   clean    33.5      calm      green  Jedi
                . . .
```

Our Gaussian Naïve Bayes assumption will be that *for each class, the* ***`height`*** *feature is distributed normally.* Given this assumption, we can characterize its normal distribution with just two parameters: its estimated mean and standard deviation. So we take all the `Jedi` rows, and calculate their `height`s' mean and standard deviation:

```
t[t.type=='Jedi'].height.mean()
t[t.type=='Jedi'].height.std()
```

```
64.0571
9.6619
```

Performing the same calculation for the `Sith` rows gives us:

```
t[t.type=='Sith'].height.mean()
t[t.type=='Sith'].height.std()
```

```
68.3902
9.3197
```

Interesting. Looks like Sith Lords are a bit taller than Jedi in general, and slightly less variable.

Now let's say we're doing a Jedi-vs.-Sith prediction for a person whose height (according to our security camera) is 69 inches. We'll need to know the value of the density at $x$=69 for both our estimated Jedi and estimated Sith distributions. Using the SciPy library, we can get "frozen" distributions for each:

```
import scipy.stats
jedi_height = scipy.stats.norm(64.0571, 9.6619)
sith_height = scipy.stats.norm(68.3902, 9.3197)
```

Think of a frozen distribution as just a variable on which we can call a `.pdf()` method to find the height of its distribution at a particular value. Let's see how high the estimated Jedi and Sith densities are for a height of 69 inches:

```
jedi_height.pdf(69)
sith_height.pdf(69)
```

```
0.036230663486274517
0.042717943988373371
```

Not surprisingly, the Sith number comes out a fair bit higher, since according to our estimated density, the average Sith's height is taller than the average Jedi's.

Keep in mind that the ".0362" and ".0427" numbers here are a bit hard to interpret. They are *not* "the probability that a Jedi/Sith is exactly 69 inches tall" – that probability, as with all continuous random variables, is *zero*. Instead, it's "the value of the density at $x$=69" which isn't really in any units that make sense. It's okay, though, since we are throwing away out denominator and doing relative comparisons anyway.

By the way, there are also other useful things you can call on a frozen SciPy distribution, including `.cdf()` to get the value of the cumulative density function at any point, `.ppf()` to get a quantile, `.rvs()` to generate random values from it, ordinary statistical things like `.median()`, `.mean()`, `.std()`, and other more exotic statistical things like moments, confidence intervals, differential entropy, survival functions, *etc.* See the documentation for details.

### Incorporating into the classifier

Let's add this feature to our classifier. First, the training code for the not-so-generally-coded version (p. 206), which had lines like this:

```
probs['tall|Sith'] = (
    len(t[(t.type=='Sith') & (t.demeanor=='tall')]) /
    len(t[(t.type=='Sith')]))
```

Since `height` is now numeric, we need to replace all those height-related lines with code like this:

```
sith_heights = t[t.type == 'Sith'].height
sith_height = scipy.stats.norm(sith_heights.mean(),
    sith_heights.std())
jedi_heights = t[t.type == 'Jedi'].height
jedi_height = scipy.stats.norm(jedi_heights.mean(),
    jedi_heights.std())
```

The "`sith_height`" and "`jedi_height`" variables are now our frozen distribution functions. In `predict()`, then, we simply use the appropriate one as another multiplier:

```
def predict(face, height, demeanor, lightsaber):
    jediness = (probs[face+"|Jedi"] *
                jedi_height.pdf(height) *     <-- CHANGED
                probs[demeanor+"|Jedi"] *
                probs[lightsaber+"|Jedi"] *
                probs["Jedi"])
    sithness = (probs[face+"|Sith"] *
                sith_height.pdf(height) *     <-- CHANGED
                probs[demeanor+"|Sith"] *
                probs[lightsaber+"|Sith"] *
                probs["Sith"])
    if jediness > sithness:
        return "Jedi"
    else:
        return "Sith"
```

Squint at that code and notice the changed lines from Figure 20.1 (on p. 207). We've removed the "`probs[height+"|Jedi"]`" lines, since they're no longer applicable: `height` is numeric now. Instead, we multiply our `jediness`/`sithness` by the value of the corresponding class's estimated density at that point.

To incorporate this numeric variable into the more general version of the code (p.209), we need to intelligently distinguish between numeric and categorical columns. This can be done via the `.dtype` accessor on a `DataFrame` column:

```
print(t.lightsaber.dtype)
print(t.height.dtype)
```

```
dtype('O')
dtype('float64')
```

(The "`O`" stands for "object," which is Pandas' non-intuitive way of telling you that the column is something non-numeric, like a string.) You can directly compare the result to "`np.dtype("float64")`", but the safer and preferred way is to use NumPy's `issubdtype()` function which more intelligently detects any numeric type (`int`s, `float`s, *etc.*, no matter the precision).

Our new generic implementation begins with:

```
probs = {}
densities = {}
target = t.columns[len(t.columns)-1]
num_fs= [ c for c in t.columns[:-1]
    if np.issubdtype(t[c].dtype,np.number) ]
cat_fs = [ c for c in t.columns[:-1]
    if not np.issubdtype(t[c].dtype,np.number) ]
```

We're creating a `densities` dictionary, somewhat similar to our `probs` dictionary, to store feature-specific information for our numeric variables (`probs` will continue to store information for categorical variables). Instead of simple numeric values, `densities` will store frozen distribution functions. Additionally, instead of a single `features` list like we had on p. 209, we now have two lists – `num_fs` and `cat_fs` – for the names of the numeric and categorical features, respectively.

Something else in that code might be new to you: we're using something called a **list comprehension**, which is just a sleek way of creating a list without the need for a `for` loop. Notice the boxies after the equals signs for `num_fs` and `cat_fs`, and the `if` clauses. This code says "if column `c` is a numeric variable, put it in `num_fs`, otherwise put it in `cat_fs`."

All right, now we can populate `densities` (and `probs`):

```
for label in df[target].drop_duplicates():
    rows_with_this_label = df[df[target] == label]
    probs[label] = len(rows_with_this_label)/len(df)
    for feature in numeric_features:
        density = scipy.stats.norm(
            rows_with_this_label[feature].mean(),
            rows_with_this_label[feature].std())
        densities[feature+"|"+label] = density
    for feature in categorical_features:
        for value in df[feature].drop_duplicates():
            probs[value+"|"+label] = (
                len(df[(df[target] == label) &
                                (df[feature] == value)]) /
                    len(df[df[target] == label]))
```

Our generic `predict()` function from (p.210) needs to be adjusted somewhat, since if we just pass a list of values, we can't tell *which* feature a numeric value is supposed to go with. There are various ways to solve this, but we'll choose to pass a key/value pair string in this case (like `"height=69.3"`). Flip to p. 222 for the complete code (Figure 21.1). We call the function like this:

```
predict(['beard','height=65','menacing','blue'])
predict(['beard','height=85','menacing','blue'])
```

```
['Jedi', 0.85863336769968801]
['Jedi', 0.72742228657164021]
```

And how does this thing do?

```
We got 82.33% correct on the test data.
```

Not too shabby.

```
def predict(values):

    scores = []
    top_prob = 0
    top_answer = ""

    for label in df[target].drop_duplicates():

        prob = probs[label]    # Start with the prior

        for value in values:
            if "=" in value:
                # Numeric feature.
                num_feature, num_value = value.split("=")
                num_value = float(num_value)
                prob *= densities[num_feature+"|"+label].pdf(
                    num_value)
            else:
                # Categorical feature.
                prob *= probs[value+"|"+label]

        scores.append(prob)

        if prob > top_prob:
            top_prob = prob
            top_answer = label

    return [ top_answer, top_prob / sum(scores) ]
```

**Figure 21.1:** A general Naïve Bayes `predict()` function, enhanced to allow numeric features (which are passed as key/value strings like `"height=51.5"`).

# Chapter 22

# APIs

Back in Chapter 15, I called the screen-scraping scenario "the worst of all possible worlds." Using an **API**, the subject of this lesson, is sort of the best. I say "sort of" because it's certainly not the *easiest*. The easiest is when you have a ready-made CSV file with exactly the data you want, and you suck it into a `DataFrame`, done. The thing is, much of the data you'll be interested in analyzing as a Data Scientist wasn't put together like that for you. Instead, it exists as part of a vast database somewhere, and you need flexibility and power to extract on demand exactly the parts you want. This is what a good API lets you do.

API actually stands for "Application Programming Interface," which is a pretty uninformative acronym. What it really means is "a set of functions someone has provided for you to call in order to access their data, together with clean documentation telling you precisely what each of those functions do." As you'll see with experience, some APIs are better designed than others, and make it easier to get what you want. In this chapter we'll look at two examples and generalize some common principles from them.

## 22.1 REST APIs

Another strange pseudo-acronym you'll encounter is "**REST**"[1], which is a *style* of API. REST APIs have the following characteristics:

- They're designed to be used over the Web. (Although "over the Web" may not mean what you think it means; for one, it *doesn't* mean "using a browser." Instead, it means "accessing the data using HTTP requests in the form of structured URLs/hyperlinks." We'll be writing *Python code* to retrieve what appear to be pseudo-Web-pages outside our browser.)
- They're simple and elegant. Unlike their predecessor (and competitor) protocols SOAP and RPC, REST was designed and promoted by people[2] who didn't like clutter and who wanted communication to be streamlined and compactly specified. REST APIs are typically nice to use.
- They're based directly on the **HTTP** protocol itself, and under the hood make use of the HTTP operations like `GET`, `HEAD`, `POST`, `DELETE`, `PUT`, *etc.* Because of this, different REST APIs tend to be pretty uniform in how they work.
- They're "**stateless**," as HTTP is itself. This means the server retains no *memory* of the past requests from a client. ("**Server**" is a word meaning "a machine on the Internet that you want to access," and "**client**" here essentially means "your own computer, which makes requests of the server.") This has some limitations, but makes APIs quick and simple to use.
- The data they provide can come in a variety of formats, typically JSON or XML.

### Other terms

APIs that conform to Roy Fielding's original spec are known colloquially as – I kid you not – "**RESTful**."

[1] This sort of stands for "REpresentational State Transfer," another utterly unhelpful phrase.

[2] Originally Roy Fielding in his 2000 Ph.D. dissertation from UC-Irvine.

You'll also sometimes hear the buzzwords "**Web services**" or "**SOA**" (Service-oriented Architecture). Although these terms are a bit broader and communicate something subtly different than just "the use of Web-based APIs" (REST or otherwise), in practice you will see terms like this used jointly to refer to the same technologies. If you hear someone talking about "a Web services approach," your ears should perk up and you should anticipate being able to apply at least some of the lessons in this module.

Finally, the term **endpoint** refers to a particular, addressable part of an API that is normally defined by a base URL. For instance, the standard Twitter search API is at `https://api.twitter.com/1.1/search/tweets.json` and the endpoint for getting full information about specific tweets is `https://api.twitter.com/1.1/statuses/lookup.json`. In general, an API will have many different endpoints, each of which defines its own parameters and is used for a particular type of information request.

## 22.2 RESTful APIs and the `requests` package

Python's `requests` package is an easy way to make a call to an external API and get the results. It basically encapsulates the under-the-hood stuff that formulates, sends, and parses the results of an HTTP request.

HTTP defines various operations to communicate with a server such as `GET`, `POST`, and `HEAD`. The `requests` package bundles these up in functions like: `requests.get()`, `requests.post()`, *etc.* The most common method we'll use in API access is the `.get()` command. It can actually be used to retrieve *any* Web-accessible page on the network:

```
import requests
class_home_page = requests.get(
    "http://stephendavies.org/data219")
print(class_home_page.content.decode('utf-8'))
```

That "`.content.decode('utf-8')`" thing is kind of a pain. The first part (`.content`) gives you the actual HTML code of the page itself (rather than a variable representing the entire request/response sequence). The second part says to take that big string and interpret it as a format that can represent all **Unicode** characters. Unicode and other character encodings are an interesting subject in their own right, but for now, just get in the habit of calling the `.content.decode('utf-8')` method on every packet of data you get from an API.

Anyway, if you run the above code, you'll see the (gnarly) HTML code for the entire course web page on your screen as one big string. Seeing this emphasizes that *when we execute RESTful API requests, we're really not doing much more than accessing "web pages," where "web page" here means a set of results that the server puts together for us.* This similarity to how browsers work is what makes RESTful APIs so simple and powerful.

## 22.3 The Star Wars API

Most of the time we won't get HTML back, but rather a data format such as XML or JSON. Predictably, I'll start with a Star Wars example. The SWAPI (Star Wars API) is a neat little database that returns JSON data about entities in the Star Wars universe. Let's ask it for "person with ID 13" (whoever that turns out to be):

```
response = requests.get("https://swapi.co/api/people/13")
print(response.content.decode('utf-8'))
```

```
{'name':'Chewbacca', 'height':'228', 'mass':'112', 'hair_color':'brown',
'skin_color':'unknown', 'eye_color':'blue', 'birth_year':'200BBY',
'gender':'male', 'homeworld':'https://swapi.co/api/planets/14/', 'films':
['https://swapi.co/api/films/2/', 'https://swapi.co/api/films/6/',
'https://swapi.co/api/films/3/', 'https://swapi.co/api/films/1/',
'https://swapi.co/api/films/7/'],
'species':['https://swapi.co/api/species/3/'],
'vehicles':['https://swapi.co/api/vehicles/19/'], 'starships':
['https://swapi.co/api/starships/10/',
'https://swapi.co/api/starships/22/'], 'created':'2014-12-10T16:42:45',
'edited':'2014-12-20T21:17:50', 'url':'https://swapi.co/api/people/13/'}
```

Looks like we got Han Solo's wingman Chewbacca. That output is a little hard on the eyes, though. Let's call `json.loads()` on that string (see p. 71) to get a Python dictionary with all Chewie's info, and then pretty-print it:

```
from pprint import pprint
import json
chewie = json.loads(response.content.decode('utf-8'))
pprint(chewie)
```

```
{'birth_year': '200BBY',
 'created': '2014-12-10T16:42:45.066000Z',
 'edited': '2014-12-20T21:17:50.332000Z',
 'eye_color': 'blue',
 'films': ['https://swapi.co/api/films/2/',
           'https://swapi.co/api/films/6/',
           'https://swapi.co/api/films/3/',
           'https://swapi.co/api/films/1/',
           'https://swapi.co/api/films/7/'],
 'gender': 'male',
 'hair_color': 'brown',
 'height': '228',
 'homeworld': 'https://swapi.co/api/planets/14/',
 'mass': '112',
 'name': 'Chewbacca',
 'skin_color': 'unknown',
 'species': ['https://swapi.co/api/species/3/'],
 'starships': ['https://swapi.co/api/starships/10/',
               'https://swapi.co/api/starships/22/'],
 'url': 'https://swapi.co/api/people/13/',
 'vehicles': ['https://swapi.co/api/vehicles/19/']}
```

Better. You can see that the API gave us a well-structured chunk of data, in a dictionary, which we can explore and manipulate in all the usual ways. Notice Note that some of the data consists of *other REST URLs*, which we could then choose to further query. This is a sign of a well-written API.

Let's use the URL we got for Chewie's home world and make another API call to retrieve that:

```
chewie = json.load(response.content.decode('utf-8'))
pprint(json.loads(requests.get(
    chewie['homeworld']).content.decode('utf-8')))
```

```
{'climate': 'tropical',
 'created': '2014-12-10T13:32:00.124000Z',
 'diameter': '12765',
 'edited': '2014-12-20T20:58:18.442000Z',
 'films': ['https://swapi.co/api/films/6/'],
 'gravity': '1 standard',
 'name': 'Kashyyyk',
 'orbital_period': '381',
 'population': '45000000',
 'residents': ['https://swapi.co/api/people/13/',
               'https://swapi.co/api/people/80/'],
 'rotation_period': '26',
 'surface_water': '60',
 'terrain': 'jungle, forests, lakes, rivers',
 'url': 'https://swapi.co/api/planets/14/'}
```

Cool: now we have information on the planet Kashyyyk, which we could then further explore aspects of. We could geek out all day with this.

## 22.4 The Twitter API

Twitter's API uses the same principle, although it's of course larger and more complicated. In addition, there's the hurdle of *authenticating* your Python program with the API so you can access the data.

### Authentication

Many APIs require some form of **authentication**, which essentially means you need to provide some personal information to identify you to the site. Since we'll be dealing only with open APIs, this isn't a security thing as much as it's a "control of information" thing. By

forcing you to register with the site and provide some contact info, the organization retains a measure of control and knowledge over how its information is used. Also, many sites impose **rate limits** which constrain how much information an account can suck from the site every hour.

Every site has a different procedure for this, and the documentation varies considerably in helpfulness. It's usually a matter of finding and connecting the dots. Twitter, like many sites, uses the **OAuth** authentication protocol (see `oauth.net`), an open standard that allows users to grant one website permission to access data from another. (You've probably used this without realizing it if you've ever enabled some third-party app which then caused a confirmation dialog box to pop up saying, "application so-and-so is requesting access to the following information of yours...do you approve?")

For Twitter, here's the procedure that works as of this writing:

1. If you're not actually a Twitter user, create a Twitter account.
2. Sign on to `dev.twitter.com`.
3. Go to `apps.twitter.com` and create an "application." For our purposes, an application is sort of like a project, of which you can have several. It's mainly an organizational thing.
4. Navigate to your application and choose "Keys and Access Tokens." Create an Access Token.

You will now see, on the "Keys and Access Tokens" page, *four* strings of gobbledygook, all four of which you'll need:

- A "consumer key." Mine is `9dFucBtR1P58pJICXGV2gaKhj`.
- A "consumer secret." (I'll keep mine secret.)
- An "access token." Mine is `1019144197-5dhD0p1VbE80kPnzZrhjq43G08iMbguggkn67q1`.
- An "access token secret." (I'll keep mine secret.)

What do all these different things mean? Honestly, you don't need to know. Just realize they're all necessary components of the way Twitter authenticates, and if you just use them all in the right places, you'll be able to get to any Twitter data you want, programmatically.

(Btw, the second and fourth of those items – the "secrets" – are not supposed to be shared with anyone, nor to appear in human-readable form in your source code. For one-off data analysis projects, I confess I don't think this is super important.)

### Authenticating with the `requests_oauthlib` package

To authenticate with OAuth, we'll use Python's `requests_oauthlib` package. You may have to install it first, by typing "`conda install requests-oauthlib`" at your operating system's command line. Then, this code should work:

```
from requests_oauthlib import OAuth1
cons_key = "(your key)"
cons_secret = "(your consumer secret)"
access_token = "(your access token)"
access_secret = "(your access secret)"
oauth = OAuth1(cons_key, cons_secret, access_token,
    access_secret)
```

We now have a variable called `oauth` which can be passed to functions in the `requests` package to get data.

### HTTP GET parameters

The Twitter API is documented at `https://dev.twitter.com/docs`, a page well worth perusing in detail. You'll see numerous endpoints documented there, each of which has its parameters listed when you click through.

Conceptually, making an API request is like making a function call: you're triggering some operation, passing parameters, and getting a return value. The syntax is a bit different though. In Python, you're used to making a function call like this:

```
get_user_timeline('katyperry',4)     <-- (not real; I'm making this up)
```

to indicate something like "get the latest four tweets from user `@katyperry`." Now in order to "call" a "function" from the *API* and "pass" these "parameters," you code up a URL with syntax like this:

(all one string:)

```
https://api.twitter.com/1.1/statuses/user_timeline.json?scre
en_name=katyperry&count=4
```

Stare at all that nonsense. Note that our "parameters" are expressed as key/value pairs, with no spaces, at the end of the URL: after a "`?`", and each separated by "`&`" signs. The following code, then:

```
four_from_katy = json.loads(requests.get(
   "https://api.twitter.com/1.1/statuses/" +
      "user_timeline.json?screen_name=katyperry&count=4",
         auth=oauth).content.decode('utf-8'))

for tweet in four_from_katy:
   print(tweet.text)
```

produces this result (as of today):

```
Sending <3 out to all of you on this #ShoesdayTuesday! I will be
donating 10% from the sale of every shoe and handb...
https://t.co/TsyHuFquc6

this is how you wash with styyylesss https://t.co/C7rlCUGv9Y

OMGEE We're leaving it to you, America! We couldn't choose between
@GraceLeermusic & @LaurenMascitti so we're leavi...
https://t.co/OH2X3o9XAV

It's the end of the #AmericanIdol journey for #DemiRae - but the
beginning of a new journey for her. Keep being the...
https://t.co/P5Fqx2Q7l5
```

## 22.5 URL encoding

Sometimes the parameters you want to put into a URL contain spaces or punctuation characters. You'll need to encode those properly in order for the URL to be valid and for the API to not get confused.

If a value you want to pass contains a space, you'll need to convert that space to a plus sign ("+"). The search endpoint for Twitter is `https://api.twitter.com/1.1/search/tweets.json`, for example, and requires a "`q`" parameter with your query string. I could search for Star Wars toys with:

```
toys = json.loads(requests.get(
   "https://api.twitter.com/1.1/search/tweets.json?q=" +
      "star+wars+toys&count=5",auth=oauth).content.decode(
          'utf-8'))
```

Note how instead of putting "`star wars toys`" in the URL, I put "`star+wars+toys`". In case you're in a shopping mood, btw, this endpoint returns a dictionary of information:

```
print(toys.keys())
```

```
['statuses', 'search_metadata']
```

It looks like the tweets themselves ("statuses") are in the `statuses` key, so:

```
for tweet in toys['statuses']:
    print(tweet['text'])
```

```
The #StarWars portfolio of #toys is about to get bigger. #Hasbro
announced it's going to make #JabbatheHutt's sail...
https://t.co/FYC1DLftXX

RT @hottoysofficial: #HotToys 1/6th scale #ObiWanKenobi (Regular
& Deluxe Version) collectible figures from #StarWars EP3 are
available for...

HotToys Old Luke Skywalker Star Wars Movie Series 12'' Man Figure
Collection https://t.co/NbHgtpnDwi #Toys https://t.co/ejrGXjVT3F

Star Wars Black Series  6" Rey (JEDI TRAINING )Toys R Us
Exclusive https://t.co/ArxT9kPjZt https://t.co/lcLbp7pwjG
```

If you have weird characters other than spaces, you have to convert them to a "percent syntax" in which you encode each weird character as a percent sign followed by the proper two hexadecimal digits. This is a pain to do by hand, but don't worry: the `quote_plus()` function from the `urllib.parse` package makes things easy:

```
import urllib.parse
print(urllib.parse.quote_plus(
    "http://cs.umw.edu/star wars toys! 20% off"))
```

```
'http%3A%2F%2Fcs.umw.edu%2Fstar+wars+toys%21+20%25+off'
```

Now, instead of using the original URL that had the illegal characters (like "`!`" and space and "`%`"), we can just use the `quote_plus()`'d version in its place when we call the API.

## 22.6 Specialized packages

For many popular APIs, including Twitter, you may find Python packages written to streamline and hide some of the protocol idiosyncrasies. These may be easier to use, depending on how well written and maintained they are. For Twitter, there are numerous ones: `python-twitter`, `TwitterAPI`, `tweepy`, `TweetPony`, `twython`, and more. This is a testimony to how powerful (and common) it is to be able to access data through external APIs.

# Chapter 23

## ML classifiers: kNN (1 of 2)

Let's return to the ML classification problem, for which Naïve Bayes and Friends from Chapters 19–21 – and the Decision Trees from Volume One – are so far our only solution.

In some ways the technique in this lesson is at the opposite extreme from Naïve Bayes. Instead of very generally assuming that each of the features is an independent and separate indicator of a data point's class (as the "Naïve Bayes assumption" did) the **kNN** (for **"*k*-nearest neighbors"**) algorithm assumes that a point's features are very much bound together. In order to classify a point, a kNN classifier finds the *closest* training points to it, and predicts the label that those points suggest (majority rules).

The parameter $k$ in kNN is simply the number of "closest training points" we'll consider. It is nearly always an odd number, so that in the two-class case there are no ties. Suppose we have a 7-NN classifier, and we're asked to classify a particular person as either `Jedi` or `Sith`. If we find the seven most similar training points to our person, and discover that four of them are `Jedi` and the other three are `Sith`, we'll predict "`Jedi`." The basic idea is that simple.

Figure 23.1 shows a visual example. Here we have training data that a bank uses to decide whether to extend home loans to applicants. The bank keeps track of two features: how many years the potential customer has been at his/her current job, and the total amount of credit card debt he/she is carrying. The training points are shown

on the plot as either red X's (these customers defaulted on their loans in the past) or green +'s (they repaid their loans).

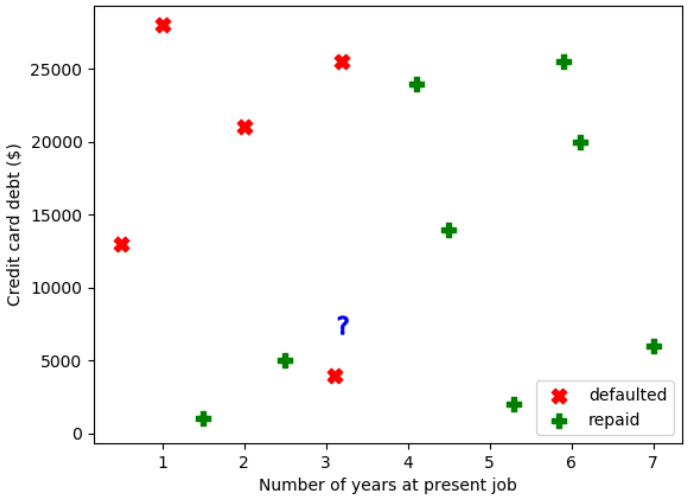



**Figure 23.1:** Training data for a bank's home mortgage operations.

Now suppose Mr. Blue Question Mark walks in. Should we approve his loan application? A 1-NN classifier would say *no*, since the closest data point to the blue question mark is a red X. A 3-NN classifier, on the other hand, would say *yes*, since if we take the three nearest neighbors of the question mark, we get two greens and one red. (See Figure 23.2.)

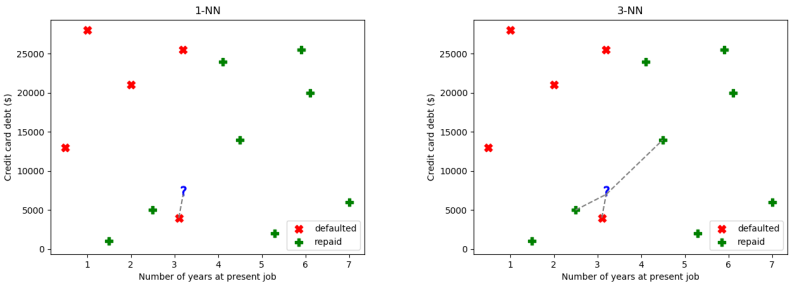



**Figure 23.2:** The 1, and 3, "closest" points to our mystery man.

## 23.1 Distance measures

Much hinges on the question of *closeness*. What do we mean when we say two data points are "close" together? There are some options here, many of which are common sense. The approach we used above was to take the ordinary *Euclidean distance*, also called the "straight-line distance" (or "crow-flies distance") between the data points. We just use the Pythagorean Theorem where each feature is plotted on an axis. And in fact this is the most common choice.

You probably remember the formula for the distance between two points in a plane. Less well known is that the Pythagorean formula works *in any number of dimensions*. In other words, if I have one $n$-dimensional data point whose values are $(x_1, x_2, x_3, ..., x_n)$ and another whose are $(y_1, y_2, y_3, ..., y_n)$, the distance between them is:

$$d = \sqrt{(x_1 - y_1)^2 + (x_2 - y_2)^2 + (x_3 - y_3)^2 + \cdots + (x_n - y_n)^2}$$

You can't visualize more than three dimensions (and most people can do only two), but you can compute it, and you get a perfectly sensible number.

This isn't the only approach people use. In general, we can use any **distance measure** (or "distance function," or "distance metric") that assigns a numerical "distance" value to any two points. To be valid, a distance measure must simply satisfy certain common sense rules.[1] Another common choice is the **Manhattan distance** (or "taxicab distance") which is essentially the shortest path between the two points that doesn't travel diagonally (*i.e.*, the path only travels along axes.)

## 23.2 Feature standardization

Now I actually did something sneaky to you with the bank example. When I showed you the plots, I calculated the crow-flies distances

[1] Including: the distance between two points must always be greater than or equal to 0; the distance from $x$ to $y$ must be the same as the distance from $y$ to $x$; and the distance from $x$ to $z$ must not be any greater than the distance from $x$ to $y$ to $z$ (the "triangle inequality.")

to Mr. Blue Question Mark *as they appeared on the page.* But if you look at the scales of those axes, you'll realize I didn't compute them right! These variables are on vastly different scales. In terms of absolute differences, the amount of credit card debt, measured in the tens of thousands, completely overwhelms the work history, which is at most a few decades. Taking the straightforward Euclidean distance between two people, then, would actually be quite a blunder: clearly a difference of $50 of credit card debt isn't nearly as significant as a difference of 50 years in seniority!

The underlying data for Figures 23.1 and 23.2 is here:

```
print(bank)
```

```
    num_yrs  cc_debt  default
0       1.0    28000      yes
1       0.5    13000      yes
2       1.5     1000       no
3       2.0    21000      yes
4       2.5     5000       no
5       3.1     4000      yes
6       3.2    25500      yes
7       4.1    24000       no
8       4.5    14000       no
9       5.3     2000       no
10      5.9    25500       no
11      6.1    20000       no
12      7.0     6000       no
13      3.2     7500    maybe
```

Let's compute the Euclidean distance from each of the points to Mr. Blue Question Mark (row #13), and sort by that new column (remember that in Python, `**` is used for "to-the-power-of"):

```
pts_dist = np.array([])
for row in bank.itertuples():
   pts_dist = np.append(pts_dist,
      np.sqrt((row.cc_debt - 7500)**2 + (row.num_yrs - 3.2)**2))
bank['dist'] = pts_dist
print(bank.sort_values('dist'))
```

| | num_yrs | cc_debt | default | dist |
|---|---|---|---|---|
| 13 | 3.2 | 7500 | maybe | 0.000000 |
| 12 | 7.0 | 6000 | no | 1500.004813 |
| 4 | 2.5 | 5000 | no | 2500.000098 |
| 5 | 3.1 | 4000 | yes | 3500.000001 |
| 9 | 5.3 | 2000 | no | 5500.000401 |
| 1 | 0.5 | 13000 | yes | 5500.000663 |
| 8 | 4.5 | 14000 | no | 6500.000130 |
| 2 | 1.5 | 1000 | no | 6500.000222 |
| 11 | 6.1 | 20000 | no | 12500.000336 |
| 3 | 2.0 | 21000 | yes | 13500.000053 |
| 7 | 4.1 | 24000 | no | 16500.000025 |
| 6 | 3.2 | 25500 | yes | 18000.000000 |
| 10 | 5.9 | 25500 | no | 18000.000202 |
| 0 | 1.0 | 28000 | yes | 20500.000118 |

It's madness. The "closest" point to Mr. Blue is the one with a `num_yrs` of 7 and a `cc_debt` of 6000...the green point that's pegged all the way to the right side of the plot! (See Figure 23.1.)

If you think it through, you'll realize why. Moving left-or-right on this plot is cheap; it's differences in *vertical* position that generate large distances. The far-right green plus really *is* very close to Mr. Blue, because her credit card debt is very close to his ($6,000 vs. $7,500). Her 7 years of consecutive work history compared to his 3.2 just isn't a factor, because it's measured in single digits.

This is a very common issue with data sets, and fortunately, there's an easy way around it. Instead of using the absolute numbers in our Pythagorean formula calculation (or Manhattan distance calculation, or whatever), we first **transform** our features so they are all **standardized** (or "**Z-score normalized**[2]") All we have to do is take each feature, and:

1. subtract its mean from each point, then
2. divide each point by its standard deviation.

This puts all features on the same level playing field, so to speak. If you remember from your stats class, what we've done is compute

[2]This definition of the term "normalized" has nothing to do with the normalization of data sets we learned about in Sections 10.5 and 11.3, btw.

the **Z-score** for each data point: the number of standard deviations above (or below) the mean it is. Now no feature gets an advantage in the distance calculation over any other feature, even if they're on wildly different scales: 2.5 standard deviations is 2.5 standard deviations, no matter what the underlying units.

Here's code to do that with the bank example:

```
def zscores(arr):
    return (arr - arr.mean()) / arr.std()

bank.cc_debt = zscores(bank.cc_debt)
bank.num_yrs = zscores(bank.num_yrs)
```

Now, if we compute distances with these Z-scores, instead of the raw values, we get something that looks much more reasonable:

```
zscore_dist = np.array([])
for row in bank.itertuples():
   zscore_dist = np.append(zscore_dist,
      np.sqrt((row.cc_debt - bank.iloc[len(bank)-1].cc_debt)**2 +
         (row.num_yrs - bank.iloc[len(bank)-1].num_yrs)**2))
bank['dist'] = zscore_dist
print(bank.sort_values('dist'))
```

```
      num_yrs    cc_debt  default      dist
13 -0.181877  -0.667388    maybe  0.000000
5  -0.231804  -1.024786      yes  0.360869
4  -0.531366  -0.922673       no  0.432797
8   0.467174  -0.003647       no  0.928342
2  -1.030636  -1.331128       no  1.077471
9   0.866590  -1.229014       no  1.189415
1  -1.529906  -0.105761      yes  1.460345
3  -0.781001   0.711151      yes  1.503103
7   0.267466   1.017493       no  1.743769
6  -0.181877   1.170664      yes  1.838051
12  1.715350  -0.820559       no  1.903400
11  1.266006   0.609037       no  1.930188
10  1.166152   1.170664       no  2.279389
0  -1.280271   1.425948      yes  2.364006
```

The data is plotted on Z-score normalized axes in Figure 23.3. As you can see, the nearest neighbor to Mr. Blue is the point .023 standard deviations lower than the mean job seniority, and 1.02 standard deviations lower than the mean credit card debt, which is precisely the red X nearest to the question mark.

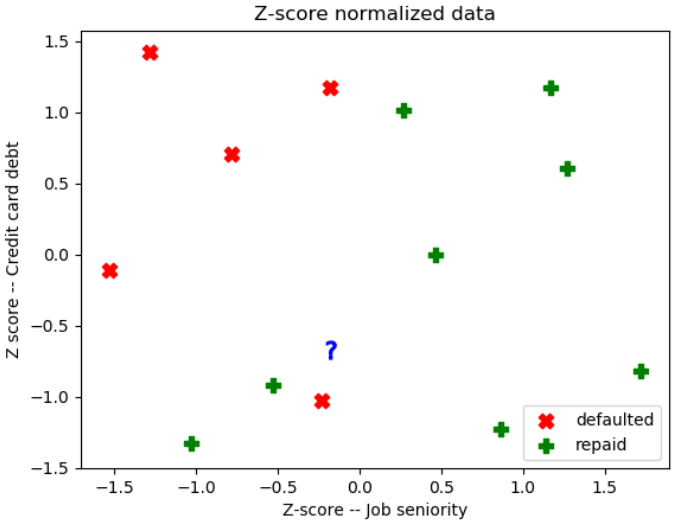



**Figure 23.3:** Both variables have been Z-score normalized (note the axis scales)!

## 23.3 Categorical features

Now what do we do if our features are categorical? We can just make them numerical, but in a principled way. If we have a binary feature, with only two possible values – `public`/`private`, `collegeGraduate`/`notACollegeGraduate` – it's easy: we just assign one number (say, "1") to one value and another ("2") to the other one. Now we've turned a categorical column of `employed`-or-`unemployed`'s into a numeric column of 1-or-2's, which lets us compute Z-scores and distance measures as we did above.

With more than two possible values, though, you have to be careful. Consider a feature whose three values are "`baseball`," "`football`,"

and "`lacrosse`." Many people might unsuspectingly assign the numbers 1, 2, and 3 to these values and then treat the feature as a numeric one. But you can't do this. Here's why: assuming the original values were on a categorical/nominal scale (recall the "Scales of Measure" chapter from Volume I of this series), converting them to numbers in a simpleminded fashion like this *imposes an interval scale where none exists.*

Think about it. A person whose favorite sport is baseball isn't any *more* like a football fan than she is like a lacrosse fan. Yet if we turn `baseball` into 1, `football` into 2, and `lacrosse` into 3, that's exactly what our kNN classifier is going to think. It will view baseball fans and lacrosse fans as "further apart" because after all, 3 minus 1 is 2.

In order to avoid biasing the classifier with this non-information, we use a technique called **one-hot encoding**. We turn each categorical feature into a whole *set* of binary features, one for each value. So instead of a `sport` feature with values `baseball`, `football`, and `lacrosse`, we use *three* features – called `baseball`, `football`, and `lacrosse` – each with values of 0 or 1. Example:

| age | edLevel | sport |
|---|---|---|
| 37 | HS | football |
| 41 | college | baseball |
| 19 | college | football |
| 22 | college | lacrosse |

$\Rightarrow$

| age | HS | college | football | baseball | lacrosse |
|---|---|---|---|---|---|
| 37 | 1 | 0 | 1 | 0 | 0 |
| 41 | 0 | 1 | 0 | 1 | 0 |
| 19 | 0 | 1 | 1 | 0 | 0 |
| 22 | 0 | 1 | 0 | 0 | 1 |

Perhaps you can see why it's called "one-hot" encoding: each row has exactly one "hot" (*i.e.*, 1) entry for each of the one-hotted features. Specifically, every row has either a 0 for `HS` and a 1 for `college`, or vice versa; and every row has a 1 for exactly *one* of `football`, `baseball`, and `lacrosse`, and 0 for the other two. This

is sort of like going from **long form** to **wide form** data, if you think about it.

You can use `np.where()` function to create one-hot features, or the `scikit-learn` package's `OneHotEncoder.fit_transform()` function. It's a little weird; when you create your `OneHotEncoder`, you have to pass it an argument of "`sparse=False`" if you want it to work the way you expect.

```
from sklearn.preprocessing import OneHotEncoder

ohe = OneHotEncoder(sparse=False)
onehot_features = ohe.fit_transform(df[['edLevel','sport']])
```

Careful: although this function takes a `DataFrame` as input, it returns a `NumPy` array as output:

```
print(df[['edLevel','sport']])
```

```
    edLevel     sport
0        HS  football
1   college  baseball
2   college  football
3   college  lacrosse
3     lacrosse
Name: sport, dtype: object
```

```
print(onehot_features)
```

```
[[1. 0. 0. 1. 0.]
 [0. 1. 1. 0. 0.]
 [0. 1. 0. 1. 0.]
 [0. 1. 0. 0. 1.]]
```

If you want these columns back in your `DataFrame`, you'll have to stick them back in there:

```
df['HS'] = onehot_features[:,0]
df['college'] = onehot_features[:,1]
df['baseball'] = onehot_features[:,2]
df['football'] = onehot_features[:,3]
df['lacrosse'] = onehot_features[:,4]
df = df.drop(['edLevel','sport'],axis=1)

print(df)
```

```
    age   HS  college  baseball  football  lacrosse
0    37  1.0      0.0       0.0       1.0       0.0
1    41  0.0      1.0       1.0       0.0       0.0
2    19  0.0      1.0       0.0       1.0       0.0
3    22  0.0      1.0       0.0       0.0       1.0
```

But as we'll see in the next chapter, the array itself is ready-made for `scikit-learn`'s powerful classifier implementations. Stay tuned.

# Chapter 24

## ML classifiers: kNN (2 of 2)

Last chapter gave the theory of kNN classifiers. Now how to code one in Python?

Conceptually it's pretty easy. We'll want to Z-score normalize everything first, of course. Then, for a new, unlabeled data point, we'll compute the "distance" (via whichever measure we choose) between it and every point in the training set. Then, we sort these points by distance, choose the $k$ with the smallest distance, and take a majority vote.

We'll use our bank loan example, but with a lot more rows. Let's synthesize a data set real quick:

```
NUM = 1000
default = np.random.choice(['yes','no'], p=[.3,.7], size=NUM)
cc_debt = np.where(default == 'yes',
   np.random.normal(12000,4000,NUM).clip(0,40000).astype(int),
   np.random.normal(7000,3000,NUM).clip(0,40000).astype(int))
num_yrs = np.where(default == 'yes',
   np.random.uniform(0,10,NUM).round(1),
   np.random.uniform(2,12,NUM).round(1))
bank = pd.DataFrame({'debt':cc_debt,'num_yrs':num_yrs,
   'default':default})[['debt','num_yrs','default']]
```

In our simplistic, synthesized world, we're assuming that 30% of our 1,000 people default on their loans, and that those who do tend

to have a bit more credit card debt and somewhat fewer years at their current job. The resulting `DataFrame` looks like this:

```
          debt  num_yrs default
0         7318      8.3     yes
1         2524      9.5      no
2        14866      5.1     yes
3        10611      5.4      no
4         9897      3.7      no
..         ...      ...     ...
995       5136      6.8      no
996       7594     11.4      no
997       7851      7.1      no
998          0      7.5      no
999      13697      7.0     yes
[1000 rows x 3 columns]
```

and we can plot it:

```
sns.pairplot(data=bank,x_vars=['num_yrs'],y_vars=['debt'],hue='default')
```

to get the grouped scatter plot in Figure 24.1.

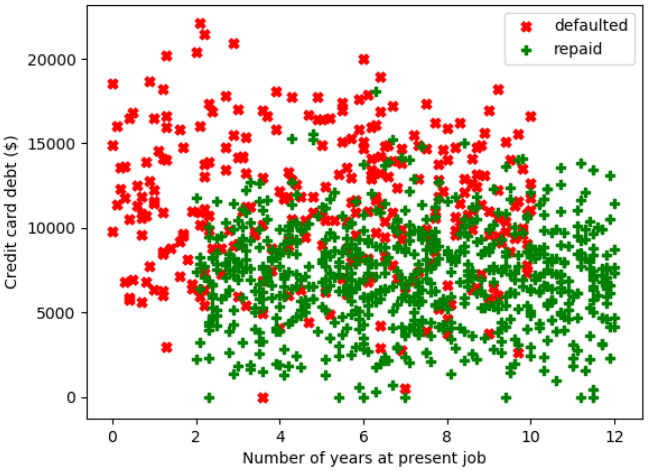



**Figure 24.1:** Synthesized bank data.

## 24.1 Coding kNN by hand

To use this as training data, we'll Z-score normalize the features. We'll also need to Z-score the *new* data points that come in to be classified, so we'd better remember the mean and standard deviation of each feature for later use.

```
def zscores(arr):
    return (arr - arr.mean()) / arr.std()

debt_mean = bank.debt.mean()
debt_std = bank.debt.std()
num_yrs_mean = bank.num_yrs.mean()
num_yrs_std = bank.num_yrs.std()

bank.debt = zscores(bank.debt)
bank.num_yrs = zscores(bank.num_yrs)
```

```
          debt   num_yrs default
0     1.321445  0.152280     yes
1     0.877662 -0.407452      no
2     0.150633 -1.000109     yes
3     2.152262 -1.790319     yes
4     0.927766  1.238819      no
..         ...       ...     ...
995 -1.450414 -0.670855      no
996 -0.777325  0.415683      no
997 -0.172235  0.942490      no
998  0.385818  0.316907     yes
999 -0.669958  1.600998      no
```

Now let's write a function called `predict()` (to match the name we used in Chapters 20 and 21) which will make a loan-default prediction for a new applicant. We'll also write a `dist()` (for "distance") function to help it do its job.

```
def dist(x,y):
    return np.sqrt((x[0]-y[0])**2 + (x[1]-y[1])**2)
```

As you can see, we're using Euclidean distance here (Pythagorean Theorem). Our `predict()` will call this `dist()` function for every point to determine that point's Euclidean distance from our test point. Then, it will sort those by distance, pick the top $k$, and choose the majority:

```
def predict(debt, num_yrs, k):
    bank['dists'] = dist([bank.debt, bank.num_yrs],
        [(debt - debt_mean) / debt_std,
        (num_yrs - num_yrs_mean) / num_yrs_std])
    k_closest_pts = bank.sort_values('dists').iloc[0:k]
    return k_closest_pts.default.value_counts().index[0]
```

Can you understand what this function is doing?

First, notice that because of the magic of Pandas vectorized operations, we don't even need a loop. The first line of the function calls `dist()` a grand total of once, giving it a list of the entire training data's x-values and y-values as the first argument, and then the new point's x-value and y-value (both Z-score normalized) as the second argument. Pretty slick!

Then walk through how the majority rule is applied. Suppose `predict()` is passed a value of 7 for `k` (to do 7-NN). The variable "`k_closest_pts`," after the next line, will be a `DataFrame` that looks like so:

```
          debt   num_yrs default     dists
651 -0.058795 -0.720668     yes  0.101662
254 -0.010493 -0.720668     yes  0.105948
515  0.057728 -0.854746      no  0.106971
384  0.076899 -0.821226      no  0.120755
418 -0.147929 -0.754187     yes  0.123796
873  0.087356 -0.821226     yes  0.131212
672 -0.061782 -0.955304      no  0.135271
```

Notice how the rows are ordered in decreasing distance from our new data point. In the final line of the function, we take the

`.value_counts()` of this `DataFrame`'s `default` column. This produces an intermediate value like:

```
yes    4
no     3
Name: default, dtype: int64
```

and when we take `.index[0]` of that, we get the label with the highest value count. In this case, it's "`yes`," soooo...let's not give a loan to that guy.

### Evaluating the hand-coded version

We can measure how well this classifier performs using essentially the same code we wrote back on p. 212:

```
num_correct = 0
for i in range(len(test)):
    row = test.iloc[i]
    p = predict(row['debt'], row['num_yrs'], 3)
    if p == row['default']:
        num_correct += 1
print("We got {}% correct.".format(
    num_correct/len(test)*100))
```

```
We got 73.667% correct.
```

Not all that great, but looking again at Figure 24.1 (p. 246) you can see why! There's a huge region in that space where defaulters and non-defaulters have about the same prominence. For new points that fall in the midst of that morass, we're only guessing. In a region like that, no classifier is going to have much of a chance.

## 24.2 The `scikit-learn` library

As I alluded to in the last chapter, there's a great Python package called `scikit-learn` that implements many machine learning algorithms, including kNN (and Naïve Bayes). Let's see how to make

use of it, returning to the Jedi/Sith security camera example. Our original data set, which we'll randomly divide into training and test sets, looked like this:

```
s = pd.read_csv("security_cam.csv")
train = s.sample(frac=.7)
test = s.drop(train.index)
print(train)
```

```
      face  height  demeanor lightsaber  type
879  beard    tall      calm      green  Jedi
770  beard  medium      calm       blue  Jedi
49   clean   short      calm       blue  Sith
892  clean   short      calm        red  Sith
774  clean  medium  menacing       blue  Jedi
..     ...     ...       ...        ...   ...
```

Recall that the `OneHotEncoder`'s `.fit_transform()` method returns a NumPy array:

```
from sklearn.preprocessing import OneHotEncoder

ohe = OneHotEncoder(sparse=False)
one_hotted_features = ohe.fit_transform(
    train.drop(['type'], axis=1))
```

```
[[1. 0. 0. 0. 1. 1. 0. 0. 1. 0.]
 [1. 0. 1. 0. 0. 1. 0. 1. 0. 0.]
 [0. 1. 0. 1. 0. 1. 0. 1. 0. 0.]
 [0. 1. 0. 1. 0. 1. 0. 0. 0. 1.]
 [0. 1. 1. 0. 0. 0. 1. 1. 0. 0.]
              . . .
```

It'd be good practice to run your eyeballs over those five rows and compare them with the categorical data, to verify that they line up. The first row, which says "`1 0 0 0 1 1 0 0 1 0`," means: "yes, a

`beard`; no, not `clean`; not `medium` or `short`, but `tall`; yes `calm`, but no, not `menacing`; and a lightsaber that is *not* `blue`, *is* `green`, and is *not* `red`." (Remember, the `OneHotEncoder` puts the feature values in alphabetical order.)

Now to actually perform kNN, we create a `KNeighborsClassifier` variable, telling it the value of `k` we want.

```
from sklearn.neighbors import KNeighborsClassifier

knn = KNeighborsClassifier(n_neighbors=5)
```

Here, we're doing 5-NN. In `scikit-learn`, we "**fit**" a classifier to training data by calling the `.fit()` method. It takes two arguments: the feature columns, and the target column:

```
knn.fit(one_hotted_features, train.type)
```

Finally, we call `.predict()` on the classifier – passing it the features for our test points – and it gives us back a column of its predictions for each one.

```
knn_predictions = knn.predict(
    ohe.fit_transform(test.drop(['type'], axis=1)))
```

Comparing the true answers with the kNN predictions, side-by-side, lets us see how well we did:

```
results = pd.DataFrame({'true_answer':test.type,
    'prediction':knn_predictions})
print(results)
```

```
     true_answer prediction
1           Sith       Sith
4           Jedi       Sith
8           Jedi       Jedi
13          Jedi       Jedi
21          Sith       Sith
..           ...        ...
```

and we can sum up how many times they coincided to get a measure of accuracy:

```
(test.type == knn_predictions).sum() / len(test) * 100
```

```
85.667
```

So our 5-NN classifier was correct more than 85% of the time in its Jedi-vs-Sith calls. (That last line of code uses a convenient shortcut, by the way: when "`test.type == knn_predictions`" is evaluated, it gives an array of `True`s and `False`s, specifying whether each test point was classified correctly or incorrectly. Taking the `.sum()` of that array treats the `True`s as 1's and the `False`s as 0's, which is a nice and easy way to simply count the number of `True`s.)

### `scikit-learn` for Naïve Bayes

Let's use `scikit-learn` for Naïve Bayes too, and then compare the two.

Naïve Bayes doesn't treat its features as numerical, so we don't need to one-hot encode them. Oddly, though, `scikit-learn` requires us to convert them to numbers anyway, and for this it provides the very misleadingly named `OrdinalEncoder`:

```
from sklearn.preprocessing import OrdinalEncoder

oe = OrdinalEncoder()
converted_features = oe.fit_transform(
    train.drop(['type'], axis=1))
```

(Don't confuse this with the `OneHotEncoder` from the same package; they have a lot of letters in common!)

I say the name is misleading because the word "ordinal," as you remember from the "Scales of Measure" chapter in the first volume of this series, implies that there is a meaningful order to the possible values of a variable: "cool" is closer to "warm" than it is to "hot," for instance. But the Naïve Bayes classifier, as we've seen, makes no such interpretation. So "ordinally encoding" our categorical features so we can pass them to a `CategoricalNB` variable which will (properly) *not* interpret them on an ordinal scale seems like exactly the wrong verbiage. But they didn't ask me.

The result of this is an array of numbers:

```
       face  height  demeanor lightsaber
879  beard    tall      calm      green
770  beard  medium      calm       blue
49   clean   short      calm       blue
892  clean   short      calm        red
774  clean  medium  menacing       blue
..     ...     ...       ...        ...

[[0. 2. 0. 1.]
 [0. 0. 0. 0.]
 [1. 1. 0. 0.]
 [1. 1. 0. 2.]
 [1. 0. 1. 0.]
    . . .
```

You can see that for the `lightsaber` feature, the `OrdinalEncoder` used 0 for `blue`, 1 for `green`, and 2 for `red` (again in alphabetical order).

Similarly to kNN, we create a `CategoricalNB` variable, `.fit()`, it to the training data, and then call its `.predict()` method:

```
from sklearn.naive_bayes import CategoricalNB

naive_bayes = CategoricalNB()
naive_bayes.fit(converted_features, train.type)
nb_predictions = naive_bayes.predict(
    oe.fit_transform(test.drop(['type'], axis=1)))
(test.type == nb_predictions).sum() / len(test) * 100
```

```
81.0
```

Naïve Bayes was the loser with this training set: only 81% accuracy as opposed to 5-NN's 85+%. However, that turns out to be far from the whole story. The full story will require another chapter.

# Chapter 25

# Two key ML principles

## 25.1 "The bias-variance trade-off"

Earlier in the book (p. 94) I made a reference to something called "the bias-variance trade-off." This turns out to be one of the most important general principles in all of ML, and it's now time to look at it in detail.

The **bias-variance trade-off** is a manifestation of the "no free lunch" principle. Classifiers that possess one advantage inherently have a counteracting disadvantage. Here are the two key terms:

- **bias**[1] – the degree to which a model is expected to misclassify items, even those in its own training set, because it just can't "bend" enough to catch every data point.
- **variance** – the degree to which a model will differ based on the particular training set that is chosen, because it "bends" too much to try and catch every data point.

[1] Tip: when thinking about this topic, try to erase your previous definitions for the word "*bias*" that you have running around in your brain. They probably don't apply. The normal meaning of the word "bias" implies a systematic propensity to err *in a particular direction.* Like, "you're biased towards thinking people are shorter than they are, because you're tall." But in this chapter, *bias* just means "being 'off' in general, in whatever direction, and probably not the same direction each time."

The basic theory is as follows. Suppose you have a very simple classifier that takes 714 training points from a security camera and tries to identify a single, smooth, perfectly straight line roughly separating Jedi from Sith. Maybe our model says "just use the `lightsaber` feature by itself, and call '`Jedi`' or '`Sith`' based on whether the test point's lightsaber value is more typical of the `Jedi` Knights or the `Sith` Lords in the training set."

This simple classifier can be said to have **low variance**. Why? Because if, instead of those particular 714 training points chosen from the population, I had sampled a different 714 training points, *the classification decisions I would make on new data would be about the same.* To see why this is the case, consider how different the training sets would have to be in order for me to make any *different* decisions. Let's say the lightsaber colors for my original 714 training points were:

| | Jedi | Sith |
|---|---|---|
| red | 17 | 85 |
| blue | 283 | 28 |
| green | 299 | 2 |

Clearly, my very simple classifier is going to predict `Sith` for `red`-lightsaber wielders and `Jedi` for anyone else. Now if I had collected a different training set, the numbers above would be different, but they would have to be a *lot* different to change any of my future predictions. I'd have to have an additional 68 `red Jedi`, for instance, or 255 additional `blue Sith`, or a whopping 297 additional `green Sith`. Not likely.

That's the bright side. On the dark side, by classifying points in this way, this simple model is going to get a lot of data points wrong: $17 + 28 + 2 = 47$ points incorrect *in its own training set*, in fact. This mean it's a pretty **high bias** classifier.

It's a tradeoff. In exchange for being virtually immune to the idiosyncrasies in the training sample, we've sacrificed some precision.

The other extreme can be seen by visualizing a 1-NN classifier. When given a new data point, 1-NN will find the *single* nearest neighbor to it in the training set, and call `Jedi` or `Sith` accordingly. This is very **low bias** – heck, we're guaranteed to get every training point correct! [2] But it is also very **high variance**: swap out the training set for another, and you'll get many, many different classifications. Our classifier has essentially memorized a zillion individual examples, and will regurgitate all that intricate detail on command. But had we gotten a different random sample, the "single nearest neighbor" to a test point would have been totally different, and might result in a different classification.

### "Overfitting"

Another very important term to learn here is the word "**overfitting**." That's what our 1-NN classifier is doing. When a model is overfitting, it means that it is allowing itself to be "too flexible" in its quest to bend exactly to its training points. It thus gets hyper-calibrated to a particular training set. Instead of locking on to the true, general, repeatable patterns of the underlying data-generating process, it's locking on to whatever idiosyncrasies were present in the particular data points it was given. And this will almost always lead to bad performance on new data.

There are formulas you can use to work out quantitatively what the estimated bias and variance are for a classifier. But I think this dichotomy is more important from a conceptual perspective. The main lesson is: the more your classifier "bends" (*i.e.*, has a very wiggly and flexible boundary between its ranges of predicted values) the more precise it potentially is in selectively labeling data points. However, this also means that a lot of its decisions are going to hinge on the particular data sample it was trained on, which means it will probably be overfitting: picking up noise in addition to signal.

[2] Think about it: if we go through the training points one by one, and treat them as new points, the "nearest neighbor" to each one will be itself! (Unless there are data points with identical feature values but different labels, in which case whatcha gonna do.)

### kNN vs. Naïve Bayes

Let's compare how 3-NN and Naïve Bayes perform on these two dimensions. Figure 25.3 at the end of the chapter (p. 262) defines two functions. One runs a Naïve Bayes classifier on a security camera data set, using a random sample of 70% for training, and returns the percentage accuract on the test set. The other does the same for a kNN classifier (its second parameter is the value of `k`.)

We can then run the following code to test each classifier on 200 different random training sets:

```
nb_performances = np.empty(200)
for i in range(200):
    nb_performances[i] = naive_bayes(s)

knn_performances = np.empty(200)
for i in range(200):
    knn_performances[i] = kNN(s, 3)

results = pd.DataFrame({'Naive Bayes':nb_performances,
    '3-NN':knn_performances})
results_l = pd.melt(results, [], var_name='classifier',
    value_name='accuracy')
facet = sns.FacetGrid(results_l, col='classifier')
facet.map(plt.hist, 'accuracy', bins=20)
```

The result is shown in Figure 25.1. It is very revealing. First, notice that on average, the 3-NN classifier beats Naïve Bayes. The mean accuracies are:

```
print("NB: mean accuracy {:.2f}%.".format(nb_performances.mean()))
print("3-NN: mean accuracy {:.2f}%.".format(knn_performances.mean()))
```

```
NB: mean accuracy 80.47%.
3-NN: mean accuracy 86.81%.
```

This tells us that 3-NN has **lower bias**, which is a good thing: good enough for another 6%-ish prediction accuracy, in fact.

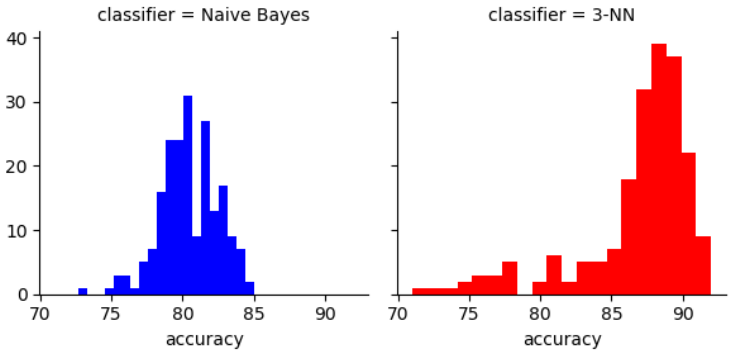



**Figure 25.1:** The accuracies of Naïve Bayes and 3-NN classifiers, on 200 different training sets.

The second thing to notice, though, is that the performance of 3-NN is more variable. Its range is from 70-92, as opposed to Naïve Bayes' 73-85. This means that on some training sets, its performance is actually lower than the worst of any of the Naïve Bayes runs. The standard deviation bears this out:

```
print("NB: std dev {:.2f}.".format(nb_performances.std()))
print("3-NN: std dev {:.2f}.".format(knn_performances.std()))
```

```
NB: std dev 2.04.
3-NN: std dev 4.07.
```

So 3-NN has **higher variance**, which is a bad thing. If we get unlucky with our training set, we're going to have an inaccurate classifier. As I said, there's no free lunch.

It's tempting to think that high variance isn't as bad as high bias. After all, even though we might get unlucky, shouldn't we still choose the option with the higher mean?

But the problem is that in real life, our training set and our new data are almost never measured at the same time, and in exactly the same circumstances. We collected data at some point in the

past, train our classifier on it in the present, and will run it to classify new data in the future. If the patterns in the data fluctuate at all between past and future (as they invariably do), then a high-variance classifier will "lock on" to those (obsolete) patterns in the past and try to apply them to the future data. A low-variance classifier won't make that mistake, since it's not as ambitious: it's settling for less precise, but more generally applicable trends.

### Varying $k$

Restricting our focus for the moment to just kNN classifiers, the question arises as to the optimal value of $k$. It may or may not surprise you to learn that there's no easy answer to this, and that it varies widely by data set and in fact even by the training set chosen.

Here's some code to try all (odd) values of $k$ between 1 and 29. For each value, it runs ten different trials and averages their performance, so that we can smooth out the differences from particularly lucky or unlucky training sets:

```
ks = np.array([])
performances = np.array([])

for k in range(1,30,2):
    for trial in range(10):
        ks = np.append(ks, k)
        performances = np.append(performances, kNN(s, k))

results = pd.DataFrame({'k':ks, 'performance':performances})
agg_results = results.groupby('k').performance.mean()
agg_results.plot(kind='line', color='red',ylim=(70,100))
```

The resulting plot is in Figure 25.2. This Sith/Jedi data set is simple enough that there aren't many really noticeable trends. Basically, as long as $k$ is above 5 or so, we max out the performance. Only when $k = 1$ or $k = 3$ do we see the too-high-variance problem come into play.

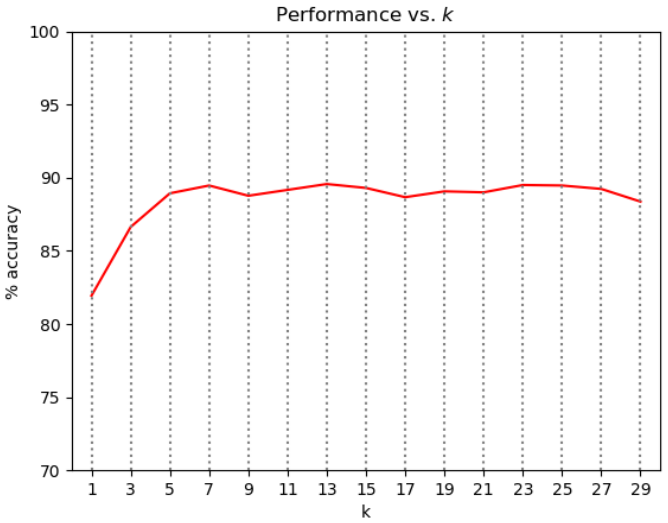



**Figure 25.2:** The accuracy of a kNN classifier on the Sith/Jedi data, as we fiddle with the number of nearest neighbors used.

Real-life data sets normally have more variation than this. Often, there's an optimal range for $k$ that's quite a bit better than values outside that range, and there's no surefire way to predict what that range will be until you try it.

In general, though, the big picture is that *as $k$ increases, the classifier becomes lower-variance and higher-bias.* Can you see why? For low values of $k$, we're picking the one (or three, or five, or ...) training points that just happen to be nearest to our new data point. That's going to be a lot different depending on which points happen to be in the training set. But if $k$ is, say, 99, then no matter what training set we get, we're going to classify most points the same. Like the simple "just go based on lightsaber color" classifier described on p. 256, too many different things would have to simultaneously change between training sets in order for any different result.

```
# Run Naive Bayes, and return the accuracy as a percentage.
def naive_bayes(s):
    train = s.sample(frac=.7)
    test = s.drop(train.index)

    oe = OrdinalEncoder()
    converted_features = oe.fit_transform(
        train.drop(['type'], axis=1))

    naive_bayes = CategoricalNB()
    naive_bayes.fit(converted_features, train.type)
    nb_predictions = naive_bayes.predict(
        oe.fit_transform(test.drop(['type'], axis=1)))
    return (nb_predictions==test.type).sum() / len(test) * 100


## Run kNN, and return the accuracy as a percentage.
def kNN(s, k):
    train = s.sample(frac=.7)
    test = s.drop(train.index)

    ohe = OneHotEncoder()
    one_hotted_features = ohe.fit_transform(
        train.drop(['type'], axis=1))

    knn = KNeighborsClassifier(n_neighbors=k)
    knn.fit(one_hotted_features, train.type)
    knn_predictions = knn.predict(
        ohe.fit_transform(test.drop(['type'], axis=1)))
    return (knn_predictions==test.type).sum() / len(test) * 100
```

**Figure 25.3:** Two functions, each of which chooses a random 70% of a data set's rows for training, runs a classifier on the remaining rows, and returns its percent accuracy. Note that every time either of these functions is called, a different answer will be returned, since a new training set will be chosen at random.

## 25.2 "The curse of dimensionality"

A second key ML principle goes by the humorous name "**the curse of dimensionality**." It goes something like this. Suppose that in addition to `height`, `demeanor`, `lightsaber`, and `face`, we also have at our disposal many other features about Jedi & Sith: their ages, salaries, home planets, personality profiles, number of traffic tickets, *etc.* This is good news, right? It gives us more and more data to sift through statistically and discover potential correlations with, right? What's not to like?

Yes, but there's a catch. It turns out that as we increase the number of features more and more (or, put another way, as we increase the "dimensionality" of the problem from our original four dimensions to 5, 6, 7, ..., and up into the hundreds) we have a **data sparsity** problem. This means there aren't enough training points to adequately cover all of this ground.

In terms of kNN classifiers, you can think of it this way: effectively, *all* the points become far apart. We want to find the 3 (or 15, or 77) "nearest neighbors," but when we have so many features (many of which will turn out to be irrelevant for the problem), we find that *any* two data points will differ on a large number of them. Essentially, our noise swamps our signal.

When we have tons of features, we need an enormous number of training samples in order to guarantee that we have several samples with each combination of values (or their ranges). In our original problem, we didn't need too much data to ensure that we'd have at least a few `tall`, `green`-lightsabered, `menacing` individuals with a `clean` face. But how many training points will we need before we have several `tall`, `green`-lightsabered, `menacing`, 38-year-old, extroverted, abstract-thinking individuals from Tatooine with 4 traffic tickets and a beard who earn 6,000 Galactic credits annually? Answer: a lot. And if we don't have that many, a kNN classifier trained on all those features is going to struggle trying to find "people like this one" in order to make a prediction.

The moral to the story is that we will often need to trim our set of features, sometimes aggressively, if we have too many. It feels

wasteful – all this great data on all these people, and we're throwing it away! – but it's the right thing to do. This process is called **feature selection**, and we'll cover it more fully in the next chapter.

In the meantime, here are three useful principles for avoiding the curse:

1. By far the most important thing to recognize is that if you have additional features that are *truly* correlated with the target – and don't simply repeat information contained in the features you already have – it's okay to include them. Adding more stuff that actually contains useful information for prediction isn't generally a problem. The problem is when you add features that are largely *noise*, since they will overwhelm the truly significant features if there are too many of them.

2. A common rule of thumb is to make sure you have at least *five* training points for each combination of feature values. (In our Jedi example, with three `height`s and three `lightsaber` values and two values for the other features, this would imply a training set of at least $(3\times3\times2\times2)\times5 = 180$ training points.)

3. When the size of the training set becomes too small, use **parametric** methods (like Naïve Bayes or linear regression) rather than instance-based methods (like kNN) because they suffer less from the curse.

# Chapter 26

# Feature selection

The "curse of dimensionality" (p. 263) makes us inclined to actually use fewer features in our classifier than we have at our disposal. This is for two reasons:

- Many of the available features are likely to be "noisy," meaning they are only loosely correlated with the target feature, if at all. Including noisy features will make it more difficult for any classifier to separate the wheat from the chaff: the features which truly are predictive will get drowned out by those that merely clutter the picture.
- Even for those features which do contain substantive, reliable information about the target, it's not likely that they're all *independent* of each other. If (say) five of our twenty features each furnished some unique and meaningful information about what the target label is likely to be, that sounds great...but it's more likely that some (or even all) of these five are correlated with each other, and hence contain overlapping information. We'll get a better-performing classifier if we avoid giving it redundant features that contain pesky noise to boot.

So how do we reduce the feature space? There are essentially three approaches:

1. **Subset selection**. We'll simply choose a subset of the original features and use those "as is" (after normalizing them or one-hot-encoding them, of course).
2. **Shrinkage** (a.k.a. "**regularization**"). Especially popular with linear models, we can essentially "tone down" some of the less important features by shrinking their coefficients towards zero.
3. **Transforming the feature space**. In this case, we actually don't use the *original* features at all; instead, we form a set of new features out of parts of the original features. This may sound weird – especially since our new features don't have any obvious "meaning"; they're just combinations of some of the original ones – but it can be very powerful and informationally efficient.

I'll say much more about the first of these, since the latter two require some advanced math.

## 26.1 Subset selection

Let's say we have four features in our original data set (call them $F_0, F_1, F_2, \text{and} F_3$, to stick with Python's numbering convention.) As stated above, we may not want to actually use all four. So which ones could we use?

It turns out we have $2^4$ (which is 16) choices of different feature sets to use. They are:

- all four of them
- just $F_0, F_1$ and $F_2$
- just $F_0, F_1$ and $F_3$
- just $F_0$ and $F_1$
- just $F_0, F_2$ and $F_3$
- just $F_0$ and $F_2$
- just $F_0$ and $F_3$
- just $F_0$
- just $F_1, F_2$ and $F_3$

- just $F_1$ and $F_3$
- just $F_1$ and $F_2$
- just $F_1$
- just $F_2$ and $F_3$
- just $F_2$
- just $F_3$
- none of them (just use the prior)

The way we get the number "$2^4$" is to reason as follows: "each feature can either be included, or excluded, in any feature set we choose. So for each of the four features, there are two independent choices (either take it or leave it) which leaves us with $2 \times 2 \times 2 \times 2$ different possible sets of features."

The one using all of the features is most likely to overfit, and the one using none of them is most likely to underfit. Often the best-fitting classifier (on new data! not the original training data) will be one of the intermediate ones.

So...how do we find that best-fitting classifier then?

### Consider all subsets

The obvious solution is to say "we've identified all possible subsets of features, let's try 'em!" And indeed we can do this if the number of features is modest. Train a classifier (whether Naïve Bayes, kNN, or anything else) using only the features in a given subset, compute the error rate, and then choose the subset with the lowest error rate.

Figure 26.1 (p. 269) contains some code that does just that (for Naïve Bayes)[1] The `security_cam2.csv` file we're using here is the one from Chapter 20, with both categorical and numerical features in it.

The output I got when I ran this was:

[1]Notes: the `is_numeric_dtype()` function distinguishes between numeric and categorical variables, so we can normalize one and one-hot the other. Also, on some versions of Pandas, you may have to call "`.reshape(-1,1)`" on the value of "`df[feature].values`" in the `else` branch of the `prepare_this_puppy()` method.

```
beard,height,lightsaber: 93.87
beard,demeanor,height,lightsaber: 93.40
beard,demeanor,lightsaber: 93.20
beard,lightsaber: 90.00
demeanor,height,lightsaber: 90.00
height,lightsaber: 90.00
demeanor,lightsaber: 90.00
lightsaber: 90.00
beard,demeanor,height: 85.80
beard,height: 85.60
```

By a hair, the feature set that excludes `demeanor` but includes everything else did the best, with 93.87% accuracy. Right behind it was the full feature set. (If we ran this multiple times, with different training set choices, our results would vary somewhat.) This isn't too surprising, since in this artificial data set, all of the features *were* pretty indicative of Jediness/Sithness, and they all *were* fairly independent of each other.

### Sadly...

Now here's the deal. Although we might think we could declare victory with this "consider all the possible subsets and choose the best" technique, it turns out that except in very small cases, *it's absolutely impossible.* Consider: what if instead of four features, we had forty? (Certainly not a large number of features by *any* means.) We would have had:

$$2^{40} = 1,099,511,627,776$$

or over a trillion different possible sets of features. Even if we could train a *thousand* different classifiers on our training data *every second*, here's how long it would take:

$$1,099,511,627,776 \times \frac{1 \text{ second}}{1000 \text{ classifiers}} \times \frac{1 \text{ minute}}{60 \text{ seconds}} \times \frac{1 \text{ hour}}{60 \text{ minutes}} \times \frac{1 \text{ day}}{24 \text{ hours}} \times \frac{1 \text{ year}}{365 \text{ days}}$$
$$= \mathbf{34.9 \text{ years}} !$$

```
from sklearn.preprocessing import OneHotEncoder
from sklearn.naive_bayes import CategoricalNB
from pandas.api.types import is_numeric_dtype

w = pd.read_csv("security_cam2.csv")
train = w.sample(frac=.7)
test = w.drop(train.index)

# Given a DataFrame and a set of column headings to include, return a
# NumPy matrix with all these features prepared and concatenated.
# "Prepared" means: (1) for categorical variables, one-hot them, and
# (2) for numeric variables, compute their Z-scores.
def prepare_this_puppy(df, include):
   ohe = OneHotEncoder(sparse=False)
   prepared_features = []
   for feature in include:
      if is_numeric_dtype(df[feature].dtype):
         thing = df[feature]-df[feature].mean()/df[feature].std()
         prepared_features.append(np.array([thing.values]).transpose())
      else:
         prepared_features.append(ohe.fit_transform(
             df[feature].values.reshape(-1,1)))
   return np.concatenate(prepared_features, axis=1)

feature_sets = [ 'lightsaber,face,height,demeanor',
                 'lightsaber,face,height',
                 'lightsaber,face,demeanor',
                 'lightsaber,face',
                 'lightsaber,height,demeanor',
                 'lightsaber,height',
                 'lightsaber,demeanor',
                 'lightsaber',
                 'face,height,demeanor',
                 'face,height',
                 'face,demeanor',
                 'face',
                 'height,demeanor',
                 'height',
                 'demeanor' ]
scores = pd.Series()

for feature_set in feature_sets:
   train_features = prepare_this_puppy(train,feature_set.split(","))
   test_features = prepare_this_puppy(test,feature_set.split(","))
   naive_bayes = CategoricalNB()
   naive_bayes.fit(train_features,train.type.values)
   nb_predictions = naive_bayes.predict(test_features)
   scores[feature_set] = round(
      sum(nb_predictions == test.type)/len(test)*100,2)

scores = scores.sort_values(ascending=False)[:10]
for feature_set, score in scores.items():
   print("{}: {:.2f}".format(feature_set,score))
```

**Figure 26.1:** Trying *all* possible feature subsets with Naïve Bayes.

Ouch. You probably haven't even been alive for that long. And obviously the situation gets worse the greater the number of features. If we had merely 100 features (also not an unreasonably large number at all), the universe will have long since died of heat death by the time we're finished considering subsets, even if we had every computer that had ever been made working non-stop on the problem.

## 26.2 "Greedy" approaches

So we have to find a way to choose a subset of features without considering every different possibility. The most common way to do this is to use a **greedy algorithm**. (You may remember this term from the first volume of this series, when we talked about the "greedy" decision tree induction algorithm.) A greedy algorithm is a procedure that finishes computing quickly because it repeatedly takes shortcuts. More precisely, a greedy algorithm always chooses *the immediately best-looking option* and goes with it, ignoring the fact that if it took more time and considered further ahead, it might have made an ultimately better choice.

(To further illustrate a greedy algorithm: imagine a chess program that always tried to take a piece if one was open to capture. It figures, "hey, taking the opponent's pieces is a good thing, and there's a piece sitting there unprotected: why not take it?" Obviously such an algorithm might play well against a newbie, but against even a modestly sophisticated player it would suck, since it would be easily lured into traps. Without being able to consider the longer-term consequences of what it's doing, it would make many decisions that looked good in the near-term but which would soon be revealed as dumb.)

### Forward selection

The most common greedy algorithm used for feature selection is called **forward selection**:

**Forward selection algorithm**

1. Train $p$ different one-feature classifiers, where $p$ is the number of features, and see how each one does. Choose as the winner the feature that works the best in isolation.
2. Now, for each of the $p-1$ remaining features, train a classifier with your original winner *plus* the new one. Choose as the winner the "best"[2] *two*-feature classifier.
3. Repeat this for each of the $p-2, p-3, p-4, \ldots$ remaining features, finding the "best" three-feature, four-feature, five-feature, ... classifier.
4. Your final answer is the best of the "best." Out of the "best" one-feature, two-feature, *etc.* classifiers, choose the one with the best performance. This is the feature set you'll declare the winner.

Two things are important to see here. First, you're training and considering a *vastly* smaller number of classifiers than you are in the "best subset" approach we did previously. For the forty feature case, you'll be considering:

$$\text{forward selection} : 40 + 39 + 38 + \cdots + 1 = 780 \text{ classifiers}$$
$$\text{best subset} : 2^{40} = 1,099,511,627,776 \text{ classifiers}$$

So the time it will take to do this has gone from 35 *years* to .78 *seconds*. Not bad.

The other thing to recognize is that we are *not* by any means guaranteed to get the best possible set of features this way. In fact, we almost certainly won't. To see this, you have to realize that the feature that looks the best of all in isolation might *not* be one of the *pair* of features that works best as a pair. And this phenomenon continues every iteration of our forward selection loop.

This can seem weird at first: if feature $F_{26}$ gives us the best one-feature classifier of all forty, shouldn't feature $F_{26}$ plus another one be the best *two*-feature classifier? The answer is not necessarily.

[2] I put "best" in quotes here because it may well not actually be the best two-feature classifier out of all possible two-feature classifiers, as we'll see.

Much of the reason why has to do with the overlap between features – recall that they will almost certainly contain redundant information among them, and so if you knew from the outset that you wanted a two-feature classifier, you might well choose $F_4$ and $F_{39}$ instead of $F_{26}$, which was a great solo artist but didn't pair up as well with anyone else.

## Backward selection

As you might have guessed, you can do this entire process "in reverse," which is appropriately called **backward selection**:

**Backward selection algorithm**

1. Start by including *every* feature (instead of none of them).
2. Train $p$ different $p-1$-feature classifiers, each of which *leaves out* one feature. Choose as the winner the one with the best performance.
3. Now, repeatedly leave out another feature, and choose as a winner the best $p-2$-feature, $p-3$-feature, $p-4$-feature, ... classifier.
4. Your final answer is the best of the "best." Out of the "best" $p-1$-feature, $p-2$-feature, *etc.* classifiers, choose the one with the best performance. This is the feature set you'll declare the winner.

Backward selection has the same advantages and disadvantages as forward selection. Unsurprisingly, it will ordinarily *not* produce the same "best" feature set that forward selection does (nor that best-subset does). Often data scientists perform both forward and backward selection and then spend some time scrutinizing the feature sets each came up with to decide on their final, best feature set.

## Evaluating classifier "goodness"

By the way, I repeatedly referred to "best performance" in the description above. What does this mean in practice?

From the bias-variance trade-off, we know that more complex ("wiggly") classifiers will tend to overfit a data set. Hence we can't blindly

use performance on a training set to choose between a four-feature classifier and a five-feature classifier, because the five-feature one will *almost certainly win for the wrong reasons.* If it has more features to work with, it has more flexibility, and hence will surely "wiggle" closer to the points it trains on. This could be a blessing but also a curse, depending on whether it's really picking up signal or locking on to noise.

There are two different ways of dealing with this problem in order to "fairly" compare classifiers of different complexities. I think of them as the math-oriented and the computer-science-oriented ways:

- **The "math-oriented" way.** If you use the entire data set to train on, you can still adjust for the complexity factor by *penalizing* more complex models in a principled way. The details are outside the scope of this class, but I'll throw the following buzzterms at you so that if you see them you'll know what category to file them under: **"Mallows' $C_p$"**, **AIC**, **BIC**, and **adjusted** $R^2$. All of these are ways of taking a model's error rate and adjusting it in light of how complex that model is, and therefore how likely it is to overfit.
- **The "computer-science-oriented" way.** Just use a separate training set and test set, drrr. Any overfitting that a complex model might do will automatically be penalized since it will perform poorly on the data it was not trained on.

## 26.3 Shrinkage

For completeness, I briefly mention two other common methods of dealing with the too-many-features problem. The first, most commonly used in linear regression/classification, goes by the general term "**shrinkage**," and its two most common variants are called **ridge regression** and **lasso regression**. These can both be thought of as ways of "partially including" features. Each of them has a parameter you can dial to control how aggressively they will "shrink" coefficients to zero. This helps when some of your features are correlated with others, since dialing down their influence will prevent them from jointly dominating the prediction. The math-

ematics are subtle, although one point worth mentioning is that with lasso, feature coefficients can actually be reduced all the way to *zero*, which effectively eliminates them and performs a kind of feature selection as in the previous section. (Ridge regression does not have this property.)

## 26.4 Transforming the feature space

Finally, one of the coolest approaches to reducing the feature space is to *transform it into a different set of dimensions*. This may sound heady, and it is: it involves some linear algebra which you may know or learn someday. But the basic idea is that the raw features themselves, as given in the data set, may not be the most useful measurements of the data: perhaps some *combinations* of the features can give us more mileage. Instead of height, age, salary, and work experience, perhaps we can take some mathematical function of height-and-age, and another mathematical function of salary-and-work-experience, and work with those two combined features instead. (Often, the combined features will involve components of *all* the original features, not just in pairs as in this example.) The general term **dimensionality reduction** is what to look for in this area, together with specific techniques like **principal components analysis** (PCA) and **singular value decomposition** (SVD).

# Chapter 27

# Association Analysis

Classification isn't the only machine learning task. Another one is called **association analysis**, in which the goal isn't to predict the class of new data items, but rather to determine which features of a data set have "interesting" relationships. Usually, "interesting" means "correlated in a way that can be taken advantage of."

The principles of association analysis are used in fields as diverse as bioinformatics, recommender systems, and cybersecurity intrusion detection. Another common application is **market basket analysis**, in which it can be employed to detect which sets of products tend to be bought together. This information is useful, for instance, to retailers who seek optimal product placement and effective marketing campaigns.

## 27.1 Market basket analysis

All competitive grocery stores today keep track of their customers' purchases as they check out. Even if they don't have a rewards program to lure customers into getting a store-specific "VIP card," they still know which sets of products were bought together in a single trip to the store. Each such trip, consisting of multiple products being purchased, is called a **transaction**.

This type of association analysis relies on a huge table (`DataFrame`) of 1's and 0's. Each row is a transaction, and each column is a

product the store sells. A "1" in an entry indicates that *at least one* of that product was bought in that transaction. (Interestingly, quantities typically aren't stored; just binary information about "did this purchase contain at least one of that item or not?") Here's one such data set:

| diet_soda | apples | beer | chips_ahoy | diapers | cat_food |
|---|---|---|---|---|---|
| 0 | 1 | 0 | 0 | 0 | 0 |
| 1 | 1 | 0 | 0 | 0 | 1 |
| 1 | 1 | 1 | 0 | 1 | 0 |
| 0 | 0 | 1 | 1 | 1 | 0 |
| 1 | 1 | 0 | 1 | 1 | 0 |
| 1 | 1 | 1 | 1 | 1 | 1 |
| 0 | 0 | 0 | 0 | 0 | 1 |
| . | . | . | . | . | . |

The first customer in this set apparently just ran into the store to grab a bag of apples, while the second one bought some Diet Coke, an apple, and a couple bags of cat food, *etc.*

Now, some terms:

- **itemset**: An itemset is a group of one or more items. For instance, "{apples,beer,cat_food,chips_ahoy}" is an itemset, as is "{diet_soda}".
- **support count**: The support count for a given itemset is *the fraction of transactions in the entire data set that contain that itemset.* In the sample data above, the support count for "{diet_soda}" is $\frac{4}{7}$ = .571, since four out of the seven transactions contained diet soda. The support count for "{apples,chips_ahoy,diapers}" is just $\frac{2}{7}$ = .286.
- **association rule**: An association rule is a statement of a relationship between two itemsets. It looks like this: "{A,B} $\Rightarrow$ {C}," which means "people who buy A and B tend to also buy C." The itemset before the arrow is called the **antecedent** and the one after it is called the **consequent**. Association rules are general correlations, not hard-and-fast mandates. Their reliability can be measured with the metrics below:

- **support**: An association rule's "support[1]" is the fraction of transactions in the data set that contain *both* its antecedent *and* its consequent. It's a measure of how widespread and applicable it is. The rule "{diet_soda, apples} ⇒ {beer}" has a support of just $\frac{2}{7}$ = .286 in the data set above. A rule's support is always between 0 and 1.
- **confidence**: An association rule's "confidence," on the other hand, is a measure of its reliability. It's *the fraction of the times that it could apply where it's actually correct.* In terms of support, it's $\frac{\text{support(whole rule)}}{\text{support\_count(antecedent)}}$ The rule "{diet_soda,apples} ⇒ {beer}" has a support of $\frac{2}{4}$ = .5 in the data set above, since out of the four times that diet soda and apples were purchased together, beer was also purchased in two of them. A rule's confidence is always between 0 and 1.
- **lift**: Finally, an association rule's "lift" is a numerical measure of how much predictive power it has. The key concept is that we want to know how likely the consequent is to be satisfied when the antecedent is satisfied *relative to how likely the consequent is to be satisfied anyway.* Quantitatively, it's $\frac{\text{confidence(whole rule)}}{\text{support\_count(consequent)}}$. A rule's lift is always *between 1 and* $\infty$. A lift of 1 means it's essentially useless: knowing the antecedent is true doesn't really make the consequent any more likely.

If we crunch all the numbers, we want to look for association rules with high support, high confidence, and high lift. Which of those three end up being the greatest priority depends somewhat on the application. If a rule doesn't have high support, it doesn't come up much, so it may not be very useful. If it doesn't have high confidence, then the trend it signifies isn't super reliable, and we need to be aware of that. And if it doesn't have high lift, then its antecedent doesn't tell us a whole lot that we didn't already know.

[1]Note that the term **support** properly applies to a rule, whereas the term **support *count*** applies to an itemset. The `mlxtend` package calls them both "support," though.

## 27.2 Implementation: the `mlxtend` library

Surprisingly, `scikit-learn` doesn't seem to have an association analysis implementation out of the box. (At least, Stephen couldn't find one.) There is one in the open source `mlxtend` library, though, by Sebastian Raschka & friends. You may need to run "`conda install mlxtend`" at the command line for Spyder to access it.

Let's take it for a spin. First, we'll generate a synthetic data set with a known association. We'll stock five items for sale in our pretend store, each of which will have a different prior probability of being purchased (about 60% of all transactions will have bananas, 80% will have pizza, *etc.*) However, we'll ensure that in addition to 2,000 purely random ones, we'll have a solid *thousand* transactions with both bacon and eggs. This should guarantee that "{bacon} ⇒ {eggs}" comes out to be a meaningful association.[2] Figure 27.1 (p. 279) gives some code to synthesize such a data set.

Okay, let's analyze. First, let's shuffle the `DataFrame`'s rows so they're in a random order (not strictly necessary, but just on principle) and then let `mlxtend` do its work:

```
transactions = transactions.sample(frac=1)

from mlxtend.frequent_patterns import apriori
from mlxtend.frequent_patterns import association_rules

itemsets = apriori(transactions, min_support=0.1,
    use_colnames=True)
```

(Note that passing `frac=1` to the `.sample()` method says "give me *all* the rows, please; but in a shuffled order.)

[2] "...and {eggs} ⇒ {bacon} too, right?" you ask. Well, not necessarily, or at least not as strong: since 70% of the random transactions have eggs anyway, and only 10% of them have bacon, we're going to get a lot of bacon-less egg-full transactions, which will dial down the confidence of that association. But let's wait and see what `mlxtend` says.

```
eggs = []
bacon = []
bananas = []
pizza = []
coffee = []

for i in range(2000):
    eggs.append(np.random.choice([1,0],p=[.7,.3]))
    bacon.append(np.random.choice([1,0],p=[.1,.9]))
    bananas.append(np.random.choice([1,0],p=[.6,.4]))
    pizza.append(np.random.choice([1,0],p=[.8,.2]))
    coffee.append(np.random.choice([1,0],p=[.3,.7]))

for i in range(1000):
    eggs.append(1)
    bacon.append(1)
    bananas.append(np.random.choice([1,0],p=[.6,.4]))
    pizza.append(np.random.choice([1,0],p=[.8,.2]))
    coffee.append(np.random.choice([1,0],p=[.3,.7]))

transactions = pd.DataFrame({ 'eggs':eggs, 'bacon':bacon,
    'bananas':bananas, 'pizza':pizza, 'coffee':coffee})
```

**Figure 27.1:** Synthesizing a grocery shopping cart data set.

This code uses the so-called **apriori algorithm**. It computes the support count *only* for those itemsets that have a certain minimum support level (in this case, `min_support=0.1`). This is for simple combinatorics reasons: if you think about it, the number of possible itemsets is rather large if we have many columns. In fact, if we have $N$ columns, there are $2^N$ different itemsets![3] The apriori algorithm is smart about not evaluating them all, because it uses an easy trick: in order for an itemset to have greater than (say) .1 support count, *all of its subsets* must also have at least that much support. This lets apriori whittle down greatly the number of itemsets it needs to consider.

[3]Sample numbers: if we have 100 different items for sale in our store – certainly not a very large number at all – we'll have 1,267,650,600,228,229,401,496,703,205,376 different itemsets to consider. This is far, far more than the number of atoms in the universe.

Let's print out the ten itemsets with the greatest support count:

```
itemsets.sort_values('support',ascending=False).head(10)
```

| support | itemsets |
|---|---|
| 0.816000 | [eggs] |
| 0.801667 | [pizza] |
| 0.650667 | [eggs, pizza] |
| 0.593333 | [bananas] |
| 0.486000 | [bananas, eggs] |
| 0.475333 | [bananas, pizza] |
| 0.401667 | [bacon] |
| 0.387667 | [bananas, eggs, pizza] |
| 0.380667 | [bacon, eggs] |
| 0.316000 | [bacon, pizza] |

Not surprisingly, the one-item itemsets feature prominently in the list, with eggs on the very top since not only did all of our second batch of 1000 transactions have eggs, but about 70% of the others did as well.

Now, let's generate (and compute stats on) all possible association rules involving those item sets:

```
rules = association_rules(itemsets)
print(rules.sort_values('confidence',ascending=False).head(10))
```

| antecedents | consequents | support | confidence | lift |
|---|---|---|---|---|
| (bacon, coffee) | (eggs) | 0.11900 | 0.95454 | 1.18626 |
| (bacon, pizza) | (eggs) | 0.29966 | 0.94631 | 1.17603 |
| (bacon) | (eggs) | 0.38100 | 0.94619 | 1.17588 |
| (bacon, bananas) | (eggs) | 0.22500 | 0.94537 | 1.17486 |
| (bacon, bananas, pizza) | (eggs) | 0.17566 | 0.94275 | 1.17160 |
| (bacon, coffee) | (pizza) | 0.10133 | 0.81283 | 1.02760 |
| (coffee) | (pizza) | 0.24933 | 0.80777 | 1.02120 |
| (eggs, coffee) | (pizza) | 0.20000 | 0.80645 | 1.01953 |
| (pizza) | (eggs) | 0.63633 | 0.80446 | 0.99975 |
| (coffee) | (eggs) | 0.24800 | 0.80345 | 0.99849 |

As expected, "{bacon} ⇒ {eggs}" has a very high confidence (and support, and lift), as do rules of the form "{bacon + various other stuff} ⇒ {eggs}." Even in this synthetic case, however, the lift values aren't all that high numerically, so don't expect them to be.

## 27.3 Applying the knowledge

This is the point where the ML ends and the domain application begins. What should a store do if armed with these statistics? In this case, we've learned that {bacon} ⇒ {eggs} is a good bet. So we might ask ourselves: what product(s) that we're currently not selling very frequently (at least to bacon & egg lovers) would we like to sell more of? That choice of product will have lots to do with inventory levels, the amount of markup we have on the product (*i.e.*, how much profit we make on it), and so forth.

Let's say we've identified a target product to market to these bacon & egg lovers: a new brand of bagels that's targeted specifically to big breakfast eaters. It might make sense to position this item in our store somewhere *between* the aisles that bacon and eggs are sold on, so that every person buying both bacon and eggs will have to walk past it. This is just one simple example, but profit margins in grocery stores are so small that the difference between booming and going out of business can rely precisely on many micro-decisions like this, each inspired by a micro-insight from the data.

# Chapter 28

# "Special" data types

I'll end this book by alluding to a number of "special" types of data that require somewhat different techniques to analyze that what we've learned so far.

One example is **time series** data, where observations are made at regular, fixed points in time and one might be interested in identifying overall trends ("stays at our hotel are going up!"), seasonal contributions within those trends ("summers have more customers in general than winters do"), and noise components that may obscure both effects ("we simply had a bad year last year.") A whole body of literature has arisen to treat time series with specialized techniques.

Another example is **free-text** data (a.k.a. **free-form text**, a.k.a. **natural language data**) where the "data" is comprised of actual written sentences in a language like English. This very unstructured stream can be analyzed using a bevy of specialized techniques, from simple word counts to sequences of words ("*n-grams*") to full parsing of sentences. Often, techniques like **stemming** algorithms are used to recognize that words like "jump," "jumped," and "jumping" all represent the same basic concept. As with time series, the methods for working with natural language are well studied, numerous, and form an entire subfield on their own.

Yet another example is **geographic data** (a.k.a. **geospatial data**, a.k.a. **geodata**) used to represent points or areas on Earth. Lon-

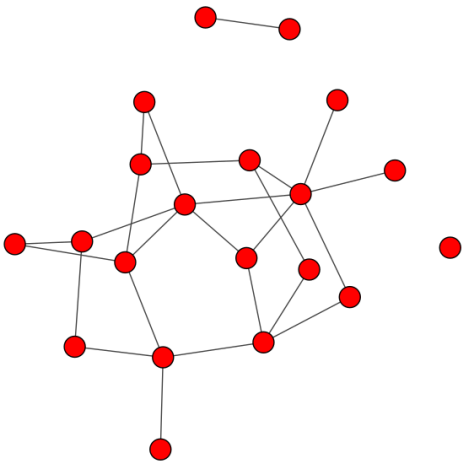
gitude and latitude, along with a set of transformational functions, can be used to annotate data about events and perform computations to learn from them.

All of these topics (and others) each deserve their own course(s), and can only be hinted at here.

## 28.1 Graph-based data

One other special data type which we'll spend some time on in this concluding chapter is **graph-based** (or **network-based**) data. It is rapidly becoming one of the most important types of data in the world, especially in view of the rise of our highly interconnected world (socially, culturally, economically, *etc.*) This type of data also a relatively "new kid on the block," which means that humankind is just now starting to get a handle on how to analyze it. It's an exciting area to learn about because there's so much (even relatively basic stuff) that's unknown and waiting to be discovered.

I'm using the word "**graph**" in a specialized sense here. It has nothing to do with the x-y plot that word usually invokes in one's mind. It is instead a special kind of data structure, or paradigm for organizing data. Rather than rows in a table, a graph, or **network**, consists of **vertices** (singular: **vertex**) connected by **edges**:



The circles are the vertices (also sometimes called **nodes**) and the lines are the edges (sometimes called **links** or **arcs**). This basic structure can be used to describe innumerable kinds of things:

- People and the social ties between them.
- Computers on a network and the connections that join them.
- International banks and the transactions they've performed with one another.
- Physical locations and the routes/roads that connect them.
- The pages on a particular website, and which ones link to which others.
- Scholarly research papers and the citations they make of one another.
- *Etc.*

Part of what makes graph-based data so important and powerful is this plethora of different applications. Aristotle, in fact, thought that this vertex-and-edge thing was so universal that essentially all the information we might want to conceive could be reduced to, and represent with, this structure.

### Graph terms

A whole specialized vocabulary has sprung up for talking about graphs and their properties. Here are just a few common terms and their meanings:

- **order** and **size** – Colloquially, researchers sometimes refer to the number of vertices in a graph as its **order**, and the number of its edges as its **size**. (The ratio of these quantities becomes a subject of interest as well.)
- **to traverse** – We use the verb "**traverse**" to mean "follow a link from one node to another." This often comes up in the context of searching for data in the graph, or finding a path through the graph with certain features.
- **directed/undirected** – In the graph above, vertices are connected by simple lines. This is called an **undirected** graph, and means that there is no intrinsic directionality to the edges:

a pair of vertices simply either is, or is not, joined by an edge. Sometimes, we care about which "way" the edge goes – for instance, if we represented a family tree, and the edges indicated parent/child relationships. Saying "Sam is the daughter of Betty Lou" is very different than saying "Betty Lou is the daughter of Sam." For this kind of graph, we will add arrowheads to the edges to show this. We typically say that one can only traverse directed links in the forwards direction (*i.e.*, in the direction of the arrow).

- a **simple graph** vs. a **multigraph** – With most graphs, there is at most one edge between any two pairs of vertices. (Either the locations have a road between them or not, either the two people are friends or they're not, *etc.*) In some cases, though, we may allow *multiple* edges per vertex pair. Perhaps in our application we need to know how *many* roads connect two locations, or how many communications were sent from person A to person B. Graphs that allow this are called **multigraphs**. Multigraphs are also typically allowed to have **self-loops** (an edge from a vertex to itself) which is not allowed in a simple graph.

- **attributes** – Both vertices and edges can be annotated with special pieces of information called **attributes**. If vertices represent people, perhaps we want to attach age or gender information to each one. If edges represent communications between companies, maybe we want to attach a date to each edge indicating when that communication took place. We can depict attributes on the visual display (or not) through a variety of means: text annotations, color/shape/size of the vertex, the thickness of the line, and so on.

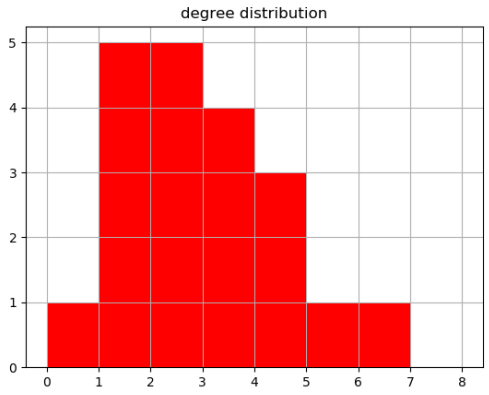
- **weighted** graphs – One particularly common type of **edge attribute** is a number called the **weight** of the edge. This is often depicted visually as the number positioned closely to the middle of the edge itself. Typically this weight represents some sort of "cost" of "using" that edge – for instance, the distance (in feet) of the network cable between the two computers, or the travel time (in minutes) of using the route from

one city to the other.

- the **degree** (of a vertex) – A vertex's "**degree**" is simply the number of connections it has. In the diagram above, the bottom-most node has degree 1, the one on the far right has degree 0, and the one at far left has degree 2. For directed graphs, this notion expands to that of "**in-degree**" and "**out-degree**," which give the number of incoming arrows and outgoing arrows, respectively.
- the **degree sequence** (of a graph) – If we take a census of the degrees of all the vertices in a graph, and list them in descending order, we get the **degree sequence** of the entire graph: The degree sequence of the red graph on p. 284, as you can tediously verify, is:

  6, 5, 4, 4, 4, 3, 3, 3, 3, 2, 2, 2, 2, 2, 1, 1, 1, 1, 1, 0

- the **degree distribution** (of a graph) – A graph's "**degree distribution**" can be thought of as a histogram of its degree sequence: how many nodes are there of degree 0? Of degree 5? Of degree 10? *Etc.* The degree distro can tell us a lot about the overall properties and structure of a large graph. Here's the one for our example:



- **dyads**, **triads**, and **cliques** – The word **dyad** is essentially just a synonym for **edge**. It means, "any pair of nodes that are completely connected together," where "completely connected" means "have an edge between them." This term may seem unnecessary until you consider the related terms **triad** and **clique**. A triad is a set of *three* nodes which are *completely* connected to each other – meaning, there is an edge between each pair of them. (Another way to think of a triad is as a triangle △.) "Clique" is the more general word for "some number of nodes, *all of which* have an edge to each of the others." We'll sometimes preface the word clique with a number, and say "this graph has a 5-clique" or "these eighteen vertices form an 18-clique." Note that a clique is a *very* strong binding between the vertices in a group – they're totally inbred. Our red example on p. 284, despite having a fair number of edges, has only a single triad (can you find it?) and no cliques of higher order.

- a **complete** graph – a (or "the") complete graph of a certain order is simply one that has every possible edge. A complete graph of order 4 will be of size 6, since there are 6 possible different pairs of vertices, and hence 6 possible edges.

- **subgraph** – a subgraph of a graph is simply one that has a subset of its vertices and a subset of its edges. A clique, then, is a *complete subgraph* of a certain order. Sometimes we refer to an **induced subgraph** of a graph: this is where we take (1) some subset of the original graph's vertices as the vertices of the induced subgraph, and then (2) all the edges in the original graph that connected vertices that we kept. In this way, specifying only the vertex subset completely defines what the induced subgraph will be.

- **connected** – a graph is **connected** (sometimes called "**fully connected**," which means the same thing) if every vertex is "reachable" from every other vertex by traversing its edges. The red example graph on p. 284 is not connected, because there's a pair of vertices at the top of the page that don't connect to anything else (and also one lonely guy at the far

right).

Now what does "connected" mean for a *directed* graph? There are two notions: "**strongly connected**" and "**weakly connected**." A directed graph is strongly connected only if you can reach every vertex from every other vertex only be traversing edges in the directions indicated. (No going backwards on a one-way street.) It's weakly connected, on the other hand, merely if it's connected once we *ignore* the directionality of the arrows.

- **component** – a **component** (also sometimes confusingly called a "**cluster**") of a graph is a connected subgraph. Very simple. Every graph will contain one or more components, each of which is a sort of island which can't be reached from the others. The red example on p. 284 has three components. A common term is "**giant component**" which is used to describe situations in which a graph is not fully connected...but almost is. The big mass of nodes which are all connected to each other is called the giant component to distinguish it from the onsie-twosie others that aren't connected. Our example graph is of just this type.

- **community** – in contrast to components, a **community** is a much vaguer, more nuanced concept. Unlike component-ness, which has a razor sharp criterion (all its nodes are reachable from each other, period) a *community* is an attempt to define a group of nodes that are "reasonably" connected to each other, at least when compared to their connections with those outside the community.

  Imagine a small social network for a high school class in which most girls were friends with most of the other girls, most boys were friends with most of the other boys, but there was also the occasional boy-girl friendship. We could identify the set of girl nodes, and the set of boy nodes, as "communities" because they are relatively cohesive internally and relatively decoupled from one another. Note that you can't ever really definitively declare: "such-and-such a set of nodes *is* a community, whereas this set definitely *isn't*." It's more subtle than

that. There's degrees of "community-hood" depending on how dense the connections are within and outside the community.

The subfield of **community detection** is devoted to algorithms that will identify such groups according to various criteria. It is a critical part of social network analysis.

- **cycle** – in a graph, a **cycle** is a group of nodes that are connected in a ring: you can start at one, traverse edges to the others, and then return to where you started.

### Special kinds of graphs

Certain patterns arise often enough to deserve their own names. Here are some special kinds of graphs:

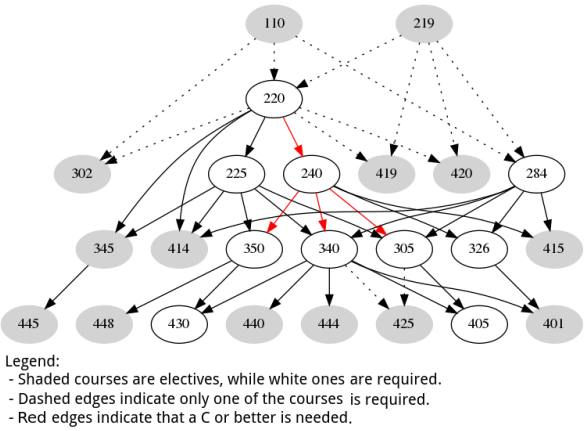
- **tree** – A tree is a directed, connected graph with no cycles. (A "family tree" for an asexually-reproducing organism is a good example of this, and often in fact we use the terms **parent** and **children** to refer to the node that points to a particular vertex, and the nodes that vertex points to, respectively.) You'll remember these from the **decision tree** chapters in the first volume of this series: a decision tree is in fact a tree.

  A tree has the interesting property that exactly one of its nodes will have no parent (we call it the "**root**" of the tree) and that there is exactly one traversable path from the root to any other node in the graph.

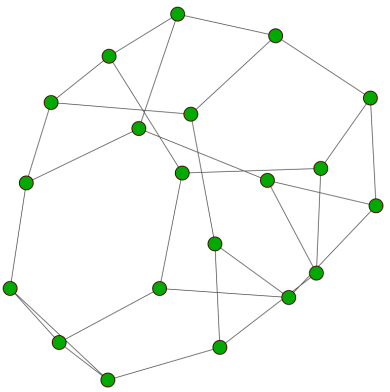
  Trees are used to represent a myriad of recursive hierarchical structures, such as organizational charts (The President supervises the VPs, each VP supervises Directors, each Director supervises Managers...), building assemblies (the engine is composed of a piston assembly, a crankshaft, and a cylinder head, which are each composed of...), information storage (the `C:\` drive contains `My Documents`, `My Computer`, and `My Pictures`; `My Documents` contains `DATA 101`, `DATA 219` and `love letters`,...) and countless more.

- **DAG** – Certain kinds of directed graphs, even if they're not trees, must inherently be cycle-free to even make sense. For

instance, the graph of CPSC course prerequisites at `http://ianfinlayson.net/misc/cpsc.png` (see below) must be cycle free because the edges indicate required prerequisites, and if there were a cycle in there...no one could ever graduate! These kinds of graphs are called **DAGs** ("directed, acyclic graphs") and are often used for managing workflows in projects.

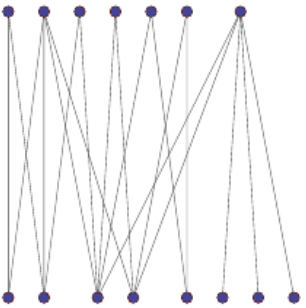



- **regular graph** – A graph is ***d*-regular** if all of its nodes have degree $d$. The graph below, for instance, is 3-regular (check it out!)



- **bipartite graph** – A graph is **bipartite** if its vertices can be split into two groups, and every edge *only* joins a vertex from one group with a vertex from the other. In a two-gender, completely heterosexual society, the graph of dating relationships would be bipartite. This kind of graph also comes up a lot in **recommender systems**: we have two types of vertices: users, and (say) books. An edge between a user and a book means that the user has purchased the book. (This is clearly bipartite, because users never purchase each other, and neither do books.)

  Bipartite graphs can be drawn with two rows of vertices, one of each type. All the edges run across the middle.

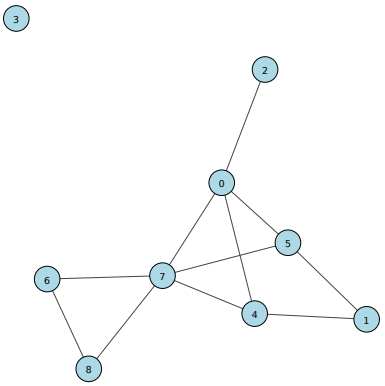


## Representations

When we use a graph package like `igraph`, by Gábor Csárdi, we can ignore details about *how* the graph we're working with is represented under the hood. (Hint: it's not a bunch of circles and lines.) However, there will be times when we need to retrieve, modify, or manipulate one or more of these representations, so let's learn what they are.

### Edge list

To a data scientist, perhaps the most straightforward way to represent a graph is via an **edge list**, which is very much like a CSV file or `DataFrame`. Each line gives two vertex names or IDs, which are connected by an edge.



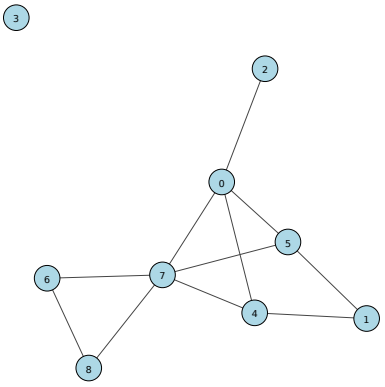

Edge list:

```
0,2
0,4
1,4
0,5
1,5
0,7
4,7
5,7
6,7
6,8
7,8
```

For a directed graph, the order of entries within a line would matter, of course, but for an undirected graph, it doesn't.

### Adjacency matrix

A graph's **adjacency matrix** is used in lots of different analysis techniques. It's simply a matrix (two-dimensional array) where every row (and column) corresponds to one vertex. A "1" in an entry $(i, j)$ means "yes, vertex $i$ and vertex $j$ are connected." Otherwise, they're not.




Adjacency matrix:

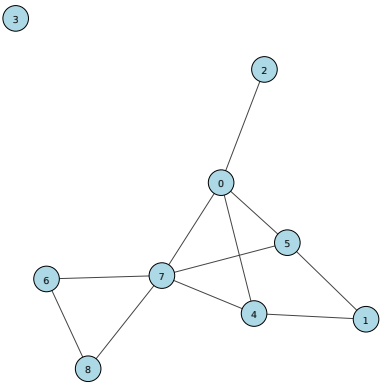
$$\begin{bmatrix} 0 & 0 & 1 & 0 & 1 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 \end{bmatrix}$$

Note how for an undirected graph (as we have here) the adjacency matrix will be **symmetric**, *i.e.*, a mirror image across the main

(upper-left-to-lower-right) diagonal. Note also that for a high-order but relatively low-size graph, the adjacency matrix will be *huge* (and "**sparse**": mostly zeros), much larger than it needs to be.

### Adjacency list

A much more compact version of the adjacency matrix is the **adjacency list**, which addresses the sparsity problem. Instead of a big $n \times n$ matrix with mostly zeroes, the adjacency list only gives us, for each vertex, *a list of the other vertices it connects to.* It looks like this:




Adjacency list:

```
0: [2, 4, 5, 7]
1: [4, 5]
2: [0]
3: []
4: [0, 1, 7]
5: [0, 1, 7]
6: [7, 8]
7: [0, 4, 5, 6, 8]
8: [6, 7]
```

## Descriptive measures

Graphs are extremely expressive, but for that reason they're hard to get your head around. If you look at a small graph (order 10, say), you can stare at it long enough to figure out what the structure is: who's connected to whom, where the cliques are, what the components are, and so on. But for anything bigger, it's a maze. Looking at a two-dimensional representation doesn't reveal much about the graph's inner properties. And it turns out that graphs have many interesting inner properties that help explain its behavior in the real world.

We've already seen one example of this, with the **degree distribution** (p. 287). This shows us, generally speaking, how many

high-connected and low-connected nodes we have, which may imply many things depending on the domain.

### Clustering coefficient

Another variable of interest is the **clustering coefficient**, also sometimes called the **transitivity**, of a graph. It measures how often it's true that friends-of-a-friend are also friends. If we define a "chevron" ($\wedge$) as two nodes sharing a neighbor (*i.e.*, vertex A is connected to B, and B is connected to C), the transitivity tells us what fraction of the time this is a complete triangle ($\triangle$) (*i.e.*, how likely it is that A is connected to C). This tells us something about how tightly clustered the graph is: are people wrapped up in tight-knit balls, or are their relationships more spread out throughout the society? (The transitivity of the light-blue graph on p.294 is .36, whereas the original red one on p.284 was only .2.)

### Centrality measures

A question that often arises in graphs is: which nodes are the most **central**? By "central" we don't mean "drawn near the center of the page," since that is solely dependent on the layout algorithm, not the graph structure. What, then, does "central" mean?

One measure is called **closeness centrality**. For a given node $x$, suppose we calculate *the sum of the length of the shortest paths between $x$ and every other node.* This is called the "**farness**," and will obviously be higher for nodes that are very far away from at least some others. It will presumably be the lowest for nodes that are most centrally located, since they are not hugely far from *any* of the other nodes.

If we take the reciprocal of the farness, we get the "**closeness**," and often we normalize this by multiplying by the order of the graph (so we can compare closeness values between graphs of different sizes.) The final formula for the closeness centrality of a node $x$, then, is:

$$c_{\text{closeness}}(x) = \frac{N}{\sum_{v \in V} \text{dist(v,x)}}$$

where $N$ is the order of the graph, $V$ are the vertices in the graph, and "dist$(a, b)$" is the shortest distance[1] between two nodes $a$ and $b$.

By this measure, the most central vertex in the light-blue graph is 7 (with a $c_{\text{closeness}}$ of .444), followed by 0, 5, and 4. The "least central" is node 3, with a measly .111.

A different way to think about centrality is in terms of information flow. Suppose these vertices are actors in a social network. Which ones are most crucial to a piece of news finding its way around to everyone?

One way to measure this is with **betweenness centrality**. For a given node $x$, we ask, "of all the pairs of vertices $a$ and $b$, how often is $x$ on the *shortest* path from $a$ to $b$?" If information is to travel from $a$ to $b$, it's probably most likely (though not certain) that it will travel along the shortest path between those two nodes. So if $x$ is on a lot of such paths, it means it will be a common conduit of information exchange between others. We define this mathematically as follows:

$$c_{\text{betweenness}}(x) = \sum_{a,b \in V} \frac{\sigma(a, b \mid x)}{\sigma(a, b)}$$

where the notation "$\sigma(a, b)$" means "the number of shortest paths from $a$ to $b$" (there could be more than one of these, in case of a tie), and where the notation "$\sigma(a, b \mid x)$" means "the number of shortest paths from $a$ to $b$ *which pass through* $x$."[2] The larger this number is, the greater the chance that $x$ will participate in an exchange of information between any two nodes.

Perhaps not surprisingly, for the light-blue case the same nodes are central by both these measures. Node 7 has a (normalized; see footnote) betweenness centrality of .184, followed by nodes 0, 5, and 4. One difference is between nodes 1 and 8: $c_{\text{closeness}}(8)$ is

[1] Also sometimes called the "**geodesic distance**" just to be confusing.

[2] Sometimes, we normalize this by dividing by $(N-1)(N-2)$, to get it to be a number between 0 and 1 like the closeness centrality is.

higher than $c_{\text{closeness}}(1)$ (.348 > .333), but $c_{\text{betweenness}}(1)$ is higher than $c_{\text{betweenness}}(8)$ (.333 > 0). This is because although 8 is a bit closer to the heart of the action, he's not on *anyone's* shortest path to anyone else. (There's nobody better than node 1, meanwhile, for getting info from 4 to 5.) Therefore, in terms of information passing purposes, he's kind of useless.

Finally, for those who have linear algebra in their arsenal, there are various ways of using **eigenvectors** of the adjacency matrix to measure centrality. One of these algorithms is called **PageRank**, which you may be familiar with since it made Google famous and the number one search engine in the world. The idea is that the more central *your neighbors* are, the more central you're likely to be. (In terms of playground drama: a popular person is not so much one with a lot of friends, but rather one with a lot of *popular* friends.)

The math involved is beyond the scope of this course, but if you've had some matrix algebra it's not too hard, and of course `igraph` can do the heavy lifting for us.

## 28.2 Conclusion

This has been nothing but a whirlwind tour to give you a taste of what graphs are and why they're important. As I mentioned, they're quite possibly the most important type of data in our new ultra-networked century, and currently they're not very well understood. They deserve an entire course (or two!) in their own right, and I hope to teach one someday!

# Index