Modeling and Simulation in Python

Version 1.2.4

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Green Tea Press

Needham, Massachusetts

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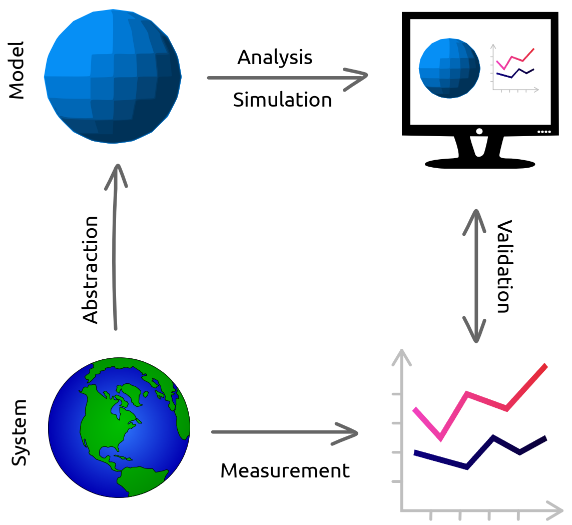
Preface

This book is about modeling and simulation of physical systems. The following diagram shows what I mean by "modeling":



Starting in the lower left, the **system** is something in the real world we are interested in. Often, it is something complicated, so we have to decide which details can be simplified or **abstracted** away.

The result of abstraction is a **model** that includes the features we think are essential. A model can be represented in the form of diagrams and equations, which can be used for mathematical **analysis**. It can also be implemented in the form of a computer program, which can run **simulations**.

The result of analysis and simulation can be a **prediction** about what the system will do, an **explanation** of why it behaves the way it does, or a **design** intended to achieve a purpose.

We can **validate** predictions and test designs by taking **measurements** from the real world and comparing the **data** we get with the results from analysis and simulation.

This process is almost always iterative: for any physical system, there are many possible models, each one including and excluding different features, or including different levels of detail. The goal of the modeling process is to find the model best suited to its purpose (prediction, explanation, or design).

Sometimes the best model is the most detailed. If we include more features, the model is more realistic, and we expect its predictions to be more accurate.

But often a simpler model is better. If we include only the essential features and leave out the rest, we get models that are easier to work with, and the explanations they provide can be clearer and more compelling.

As an example, suppose someone asked you why the orbit of the Earth is nearly elliptical. If you model the Earth and Sun as point masses (ignoring their actual size), compute the gravitational force between them using Newton's law of universal gravitation, and compute the resulting orbit using Newton's laws of motion, you can show that the result is an ellipse.

Of course, the actual orbit of Earth is not a perfect ellipse, because of the gravitational forces of the Moon, Jupiter, and other objects in the solar system, and because Newton's laws of motion are only approximately true (they don't take into account relativistic effects).

But adding these features to the model would not improve the explanation; more detail would only be a distraction from the fundamental cause. However, if the goal is to predict the position of the Earth with great precision, including more details might be necessary.

So choosing the best model depends on what the model is for. It is usually a good idea to start with a simple model, even if it is likely to be too simple, and test whether it is good enough for its purpose. Then you can add features gradually, starting with the ones you expect to be most essential.

Comparing the results of successive models provides a form of **internal validation**, so you can catch conceptual, mathematical, and software errors. And by adding and removing features, you can tell which ones have the biggest effect on the results, and which can be ignored.

0.1 Can modeling be taught?

These essential modeling skills — abstraction, analysis, simulation, and validation — are central in engineering, natural sciences, social sciences, medicine, and many other fields. Some students learn these skills implicitly, but in most schools they are not taught explicitly, and students get little practice. That's the problem this book is meant to address.

At Olin College, we use this book in a class called Modeling and Simulation, which all students take in their first semester. My colleagues, John Geddes and Mark Somerville, and I developed this class and taught it for the first time in 2009.

It is based on our belief that modeling should be taught explicitly, early, and throughout the curriculum. It is also based on our conviction that computation is an essential part of this process.

If students are limited to the mathematical analysis they can do by hand, they are restricted to a small number of simple physical systems, like a projectile moving in a vacuum or a block on a frictionless plane.

And they will only work with bad models; that is, models that are too simple for their purpose. In nearly every mechanical system, air resistance and friction are essential features; if we ignore them, our predictions will be wrong and our designs won't work.

In most freshman physics classes, students don't make modeling decisions; sometimes they are not even aware of the decisions that have been made for them. Our goal is to teach, and for students to practice, the entire modeling process.

0.2 How much programming do I need?

If you have never programmed before, you should be able to read this book, understand it, and do the exercises. I will do my best to explain everything you need to know; in particular, I have chosen carefully the vocabulary I introduce, and I try to define each term the first time it it used. If you find that I have used a term without defining it, let me know.

If you have programmed before, you will have an easier time getting started, but you might be uncomfortable in some places. I take an approach to programming you have probably not seen before.

Most programming classes[1] have two big problems:

1. They go "bottom up", starting with basic language features and gradually adding more powerful tools. As a result, it takes a long time before students can do anything more interesting than convert Fahrenheit to Celsius.

2. They have no context. Students learn to program with no particular goal in mind, so the exercises span an incoherent collection of topics, and the projects tend to be unmotivated.

In this book, you learn to program with an immediate goal in mind: writing simulations of physical systems. And we proceed "top down", by which I mean we use professional-strength data structures and language features right away. In particular, we use the following Python **libraries**:

- NumPy for basic numerical computation (see `http://www.numpy.org/`).
- SciPy for scientific computation (see `http://www.scipy.org/`).
- matplotlib for visualization (see `http://matplotlib.org/`).
- pandas for working with data (see `http://pandas.pydata.org/`).
- SymPy for symbolic computation, (see `http://www.sympy.org`).
- Pint for units like kilograms and meters (see `http://pint.readthedocs.io`).

[1]Including many I have taught.

- Jupyter for reading, running, and developing code (see http://jupyter.org).

These tools let you work on more interesting programs sooner, but there are some drawbacks: they can be hard to use, and it can be challenging to keep track of which library does what and how they interact.

I have tried to mitigate these problems by providing a library, called `modsim`, that makes it easier to get started with these tools, and provides some additional capabilities.

Some features in the `modsim` library are like training wheels; at some point you will probably stop using them and start working with the underlying libraries directly. Other features you might find useful the whole time you are working through the book, or even later.

I encourage you to read the the `modsim` library code. Most of it is not complicated, and I tried to make it readable. Particularly if you have some programming experience, you might learn something by reverse-engineering my designs.

0.3 How much math and science do I need?

I assume that you have studied calculus. You should know what derivatives and integrals are, but that's about all. In particular, you don't need to know (or remember) much about finding derivatives or integrals of functions analytically. If you know the derivative of x^2 and you can integrate $2x\ dx$, that will do it[2].

More importantly you should understand what those concepts *mean*; but if you don't, this book might help you figure it out.

You don't have to know anything about differential equations.

As for science, we will cover topics from a variety of fields, including demography, epidemiology, medicine, thermodynamics, and mechanics. For the most part, I don't assume you know anything about these topics. In fact, one of the

[2]And if you noticed that those two questions answer each other, even better.

skills you need to do modeling is the ability to learn enough about new fields to develop models and simulations.

When we get to mechanics, I assume you understand the relationship between position, velocity, and acceleration, and that you are familiar with Newton's laws of motion, especially the second law, which is often expressed as $F = ma$ (force equals mass times acceleration).

I think that's everything you need, but if you find that I left something out, please let me know.

0.4 Getting started

To run the examples and work on the exercises in this book, you will need to be able to:

1. Install Python on your computer, along with the libraries we will use.
2. Copy my files onto your computer.
3. Run Jupyter, which is a tool for running and writing programs, and load a **notebook**, which is a file that contains code and text.

The next three sections provide details for these steps. I wish there were an easier way to get started; it's regrettable that you have to do so much work before you write your first program. Be persistent!

0.5 Installing Python and the libraries

You might already have Python installed on your computer, but you might not have the latest version. To use the code in this book, you need Python 3.6, or later. Even if you have the latest version, you probably don't have all of the libraries we need.

You could update Python and install these libraries, but I strongly recommend that you don't go down that road. I think you will find it easier to use

Anaconda, which is a free Python distribution that includes all the libraries you need for this book (and lots more).

Anaconda is available for Linux, macOS, and Windows. By default, it puts all files in your home directory, so you don't need administrator (root) permission to install it, and if you have a version of Python already, Anaconda will not remove or modify it.

[Detailed instructions coming soon.]

0.6 Copying my files

The code for this book is available from https://github.com/AllenDowney/ModSimPy, which is a **Git repository**. Git is a software tool that helps you keep track of the programs and other files that make up a project. A collection of files under Git's control is called a repository[3]. GitHub is a hosting service that provides storage for Git repositories and a convenient web interface.

There are several ways you can copy the files from my repository to your computer.

If you don't want to use Git at all, you can download my files in a Zip archive from http://modsimpy.com/zip. Then you need a program like WinZip or gzip to unpack the Zip file.

To use Git, you need a **Git client**, which is a program that manages git repositories. If you have not used Git before, I recommend GitHub Desktop, which is a simple graphical Git client. You can download it from https://desktop.github.com. Currently, GitHub Desktop is not available for Linux. On Linux, I suggest using the Git command-line client. Installation instructions are at http://modsimpy.com/git.

Once you have a Git client, you can use it to copy files from my repository to your computer, which is called **cloning** in Git's vocabulary. If you are using a Command-line git client, type

```
git clone https://github.com/AllenDowney/ModSimPy
```

[3]The really cool kids call it a “repo”.

You don't need a GitHub account to do this, but you won't be able to write your changes back to GitHub.

If you want to use GitHub to keep track of the code you write while you are using this book, you can make of a copy of my repository on GitHub, which is called **forking**. If you don't already have a GitHub account, you'll need to create one.

Use a browser to view the homepage of my repository at https://github.com/AllenDowney/ModSimPy. You should see a gray button in the upper right that says Fork. If you press it, GitHub will create a copy of my repository that belongs to you. Then you can clone your repository like this:

```
git clone https://github.com/YourGitHubUserName/ModSimPy
```

Of course, you should replace `YourGitHubUserName` with your GitHub user name.

0.7 Running Jupyter

The code for each chapter, and starter code for the exercises, is in Jupyter notebooks. If you have not used Jupyter before, you can read about it at http://jupyter.org.

[Jupyter instructions coming soon.]

Contributor List

If you have a suggestion or correction, send it to `downey@allendowney.com`. Or if you are a Git user, send me a pull request!

If I make a change based on your feedback, I will add you to the contributor list, unless you ask to be omitted.

If you include at least part of the sentence the error appears in, that makes it easy for me to search. Page and section numbers are fine, too, but not as easy to work with. Thanks!

- I am grateful to John Geddes and Mark Somerville for their early collaboration with me to create Modeling at Simulation, the class at Olin College this book is based on.

- My early work on this book benefited from conversations with my amazing colleagues at Olin College, including John Geddes, Alison Wood, Chris Lee, and Jason Woodard.

- I am grateful to Lisa Downey and Jason Woodard for their thoughtful and careful copy editing.

Chapter 1

Modeling

The world is a complicated place. In order to make sense of it, we use **models**, which are generally smaller and simpler than the thing we want to study. The word "model" means different things in different contexts, so it is hard to define except by example.

Some models are actual objects, like a scale model of a car, which has the same shape as the car, but smaller. Scale models are often useful for testing properties of mechanical systems, like air resistance.

This book is about **mathematical models**, which are ideas, not objects. If you studied Newton's laws of motion, what you learned is a mathematical model of how objects move in space when forces are applied to them.

1.1 The falling penny myth

Let's see an example of how models are used. You might have heard that a penny dropped from the top of the Empire State Building would be going so fast when it hit the pavement that it would be embedded in the concrete; or if it hit a person, it would break their skull.

We can test this myth by making and analyzing a model. To get started, I'll assume that the effect of air resistance is small. This will turn out to be a bad assumption, but bear with me. If air resistance is negligible, the primary force acting on the penny is gravity, which causes the penny to accelerate downward.

If the initial velocity is 0, the velocity after t seconds is at, and the height the penny has dropped at t is

$$h = at^2/2$$

Using algebra, we can solve for t:

$$t = \sqrt{2h/a}$$

Plugging in the acceleration of gravity, $a = 9.8\,\mathrm{m/s^2}$ and the height of the Empire State Building, $h = 381\,\mathrm{m}$, we get $t = 8.8\,\mathrm{s}$. Then computing $v = at$ we get a velocity on impact of 86 m/s, which is about 190 miles per hour. That sounds like it could hurt.

Of course, these results are not exact because the model is based on simplifications. For example, we assume that gravity is constant. In fact, the force of gravity is different on different parts of the globe, and gets weaker as you move away from the surface. But these differences are small, so ignoring them is probably a good choice for this scenario.

On the other hand, ignoring air resistance is not a good choice. Once the penny gets to about 18 m/s, the upward force of air resistance equals the downward force of gravity, so the penny stops accelerating. After that, it doesn't matter how far the penny falls; it hits the sidewalk (or your head) at about 18 m/s, much less than 86 m/s, as the simple model predicts.

The statistician George Box famously said "All models are wrong, but some are useful." He was talking about statistical models, but his wise words apply to all kinds of models. Our first model, which ignores air resistance, is very wrong, and probably not useful. The second model is also wrong, but much better, and probably good enough to refute the myth.

The television show *Mythbusters* has tested the myth of the falling penny more carefully; you can view the results at `http://modsimpy.com/myth`. Their work is based on a mathematical model of motion, measurements to determine the force of air resistance on a penny, and a physical model of a human head.

1.2 Computation

There are (at least) two ways to work with mathematical models, **analysis** and **simulation**. Analysis often involves algebra and other kinds of symbolic manipulation. Simulation often involves computers.

In this book we do some analysis and a lot of simulation; along the way, I discuss the pros and cons of each. The primary tools we use for simulation are the Python programming language and Jupyter, which is an environment for writing and running programs.

As a first example, I'll show you how I computed the results from the previous section using Python. You can view this example at http://modsimpy.com/chap00. For instructions on downloading and running the code, see Section 0.4.

First I'll create a **variable** to represent acceleration.

```
a = 9.8 * meter / second**2
```

A variable is a name that corresponds to a value. In this example, the name is `a` and the value is the number `9.8` multiplied by the units `meter / second**2`. This example demonstrates some of the symbols Python uses to perform mathematical operations:

Operation	**Symbol**
Addition	`+`
Subtraction	`-`
Multiplication	`*`
Division	`/`
Exponentiation	`**`

Next, we can compute the time it takes for the penny to drop 381 m, the height of the Empire State Building.

```
h = 381 * meter
t = sqrt(2 * h / a)
```

These lines create two more variables: `h` gets the height of the building in meters; `t` gets the time, in seconds, for the penny to fall to the sidewalk. `sqrt` is a **function** that computes square roots. Python keeps track of units, so the result, `t`, has the correct units, seconds.

Finally, we can compute the velocity of the penny after t seconds:

```
v = a * t
```

The result is about 86 m/s, again with the correct units.

This example demonstrates analysis and computation using Python. Next we'll see an example of simulation.

1.3 Modeling a bike share system

You can view the code for the rest of this chapter at `http://modsimpy.com/chap01`. For instructions on downloading and running the code, see Section 0.4.

Imagine a bike share system for students traveling between Olin College and Wellesley College, which are about 3 miles apart in eastern Massachusetts.

This example demonstrates the features of Python we'll use to develop computational simulations of real-world systems. Along the way, I will make decisions about how to model the system. In the next chapter we'll review these decisions.

Suppose the system contains 12 bikes and two bike racks, one at Olin and one at Wellesley, each with the capacity to hold 12 bikes.

As students arrive, check out a bike, and ride to the other campus, the number of bikes in each location changes. In the simulation, we'll need to keep track of where the bikes are. To do that, I'll create a `System` object, which is defined in the `modsim` library.

Before we can use the library, we have to `import` it:

```
from modsim import *
```

This line of code is an **import statement** that tells Python to read the file `modsim.py` and make the functions it defines available.

Functions in the `modsim.py` library include `sqrt`, which we used in the previous section, and `System`, which we are using now. `System` creates a `System` object, which is a collection of **system variables**.

```
bikeshare = System(olin=10, wellesley=2)
```

In this example, the system variables are `olin` and `wellesley` and they represent the number of bikes at Olin and Wellesley. The initial values are 10 and 2, indicating that there are 10 bikes at Olin and 2 at Wellesley. The `System` object created by `System` is assigned to a new variable named `bikeshare`.

We can read the variables inside a `System` object using the **dot operator**, like this:

```
bikeshare.olin
```

The result is the value 10. Similarly, for:

```
bikeshare.wellesley
```

The result is 2. If you forget what variables a system object has, you can just type the name:

```
bikeshare
```

The result looks like a table with the variable names and their values:

	value
olin	10
wellesley	2

The system variables and their values make up the **state** of the system. We can update the state by assigning new values to the variables. For example, if a student moves a bike from Olin to Wellesley, we can figure out the new values and assign them:

```
bikeshare.olin = 9
bikeshare.wellesley = 3
```

Or we can use **update operators**, `-=` and `+=` to subtract 1 from `olin` and add 1 to `wellesley`:

```
bikeshare.olin -= 1
bikeshare.wellesley += 1
```

The result is the same either way.

1.4 Plotting

As the state of the system changes, it is often useful to plot the values of the variables over time. The `modsim` library provides a function that creates a new figure:

```
newfig()
```

In Jupyter, the behavior of this function depends on a command in the first cell:

- If you want the figures to appear in the notebook, use

  ```
  %matplotlib notebook
  ```

- If you want the figures to appear in separate windows, use

  ```
  %matplotlib qt
  ```

These commands are not actually Python; they are so-called "magic commands" that control the behavior of Jupyter.

The following lines plot the state of the system:

```
mark(bikeshare.olin, 'rs-')
mark(bikeshare.wellesley, 'bo-')
```

The `mark` function takes two values, called **arguments**:

- The first argument is the variable to plot. In this example, it's a number, but we'll see later that `mark` can handle other objects, too.
- The second argument is a "style string" that determines what the plot should look like. In general, a **string** is a sequence of letters, numbers, and punctuation that appear in quotation marks. The style string `'rs-'` means we want red squares with lines between them; `'bo-'` means we want blue circles with lines.

The plotting functions in the `modsim` library are based on Matplotlib, which is a Python **library** for generating figures. To learn more about these functions, you can read the Matplotlib documentation. For more about style strings, see http://modsimpy.com/plot.

1.5 Defining functions

So far we have used functions defined in `modsim` and other libraries. Now we're going to define our own functions.

When you are developing code in Jupyter, it is often efficient to write 1–2 lines in each cell, test them to confirm they do what you intend, and then use them to define a new function. For example, these lines move a bike from Olin to Wellesley:

```
bikeshare.olin -= 1
bikeshare.wellesley += 1
```

Rather than repeat them every time a bike moves, we can define a new function:

```
def bike_to_wellesley():
    bikeshare.olin -= 1
    bikeshare.wellesley += 1
```

`def` is a special word in Python that indicates we are defining a new function. The name of the function is `bike_to_wellesley`. The empty parentheses indicate that this function takes no arguments. The colon indicates the beginning of an indented **code block**.

The next two lines are the **body** of the function. They have to be indented; by convention, the indentation is 4 spaces.

When you define a function, it has no immediate effect. The body of the function doesn't run until you **call** the function. Here's how to call this function:

```
bike_to_wellesley()
```

When you call this function, it updates the variables of the `bikeshare` object; you can check by displaying or plotting the new state.

When you call a function that takes no arguments, you have to include the empty parentheses. If you leave them out, like this:

```
bike_to_wellesley
```

Python looks up the name of the function and displays:

```
<function __main__.bike_to_wellesley>
```

This result indicates that `bike_to_wellesley` is a function. You don't have to know what `__main__` means, but if you see something like this, it probably means that you looked up a function but you didn't actually run it. So don't forget the parentheses.

1.6 Parameters

Similarly, we can define a function that moves a bike from Wellesley to Olin:

```
def bike_to_olin():
    bikeshare.wellesley -= 1
    bikeshare.olin += 1
```

And run it like this:

```
bike_to_olin()
```

One benefit of defining functions is that you avoid repeating chunks of code, which makes programs smaller. Another benefit is that the name you give the function documents what it does, which makes programs more readable.

In this example, there is one other benefit that might be even more important. Putting these lines in a function makes the program more reliable because it guarantees that when we decrease the number of bikes at Olin, we increase the number of bikes at Wellesley. That way, we guarantee that the bikes in the model are neither created nor destroyed!

However, now we have two functions that are nearly identical except for a change of sign. Repeated code makes programs harder to work with, because if we make a change, we have to make it in several places.

We can avoid that by defining a more general function that moves any number of bikes in either direction:

```
def move_bike(n):
    bikeshare.olin -= n
    bikeshare.wellesley += n
```

The name in parentheses, `n`, is a **parameter** of the function. When we run the function, the argument we provide gets assigned to the parameter. So if we run `move_bike` like this:

```
move_bike(1)
```

It assigns the value of the argument, `1`, to the parameter, `n`, and then runs the body of the function. So the effect is the same as:

```
n = 1
bikeshare.olin -= n
bikeshare.wellesley += n
```

Which moves a bike from Olin to Wellesley. Similarly, if we call `move_bike` like this:

```
move_bike(-1)
```

The effect is the same as:

```
n = -1
bikeshare.olin -= n
bikeshare.wellesley += n
```

Which moves a bike from Wellesley to Olin. Now that we have `move_bike`, we can rewrite the other two functions to use it:

```
def bike_to_wellesley():
    move_bike(1)

def bike_to_olin():
    move_bike(-1)
```

If you define the same function name more than once, the new definition replaces the old one.

1.7 Print statements

As you write more complicated programs, it is easy to lose track of what is going on. One of the most useful tools for debugging is the **print statement**, which displays text in the Jupyter notebook.

Normally when Jupyter runs the code in a cell, it displays the value of the last line of code. For example, if you run:

```
bikeshare.olin
bikeshare.wellesley
```

Jupyter runs both lines of code, but it only displays the value of the second line. If you want to display more than one value, you can use print statements:

```
print(bikeshare.olin)
print(bikeshare.wellesley)
```

print is a function, so it takes an argument in parentheses. It can also take a sequence of arguments separated by commas, like this:

```
print(bikeshare.olin, bikeshare.wellesley)
```

In this example, the two values appear on the same line, separated by a space.

Print statements are also useful for debugging functions. For example, if you add a print statement to move_bike, like this:

```
def move_bike(n):
    print('Running move_bike with n =', n)
    bikeshare.olin -= n
    bikeshare.wellesley += n
```

The first argument of print is a string; the second is the value of n, which is a number. Each time you run move_bike, it displays a message and the value n.

1.8 If statements

The modsim library provides a function called flip that takes as an argument a probability between 0 and 1:

```
flip(0.7)
```

The result is one of two values: True with probability 0.7 or False with probability 0.3. If you run this function 100 times, you should to get True about 70 times and False about 30 times. But the results are random, so they might differ from these expectations.

True and False are special values defined by Python. Note that they are not strings. There is a difference between True, which is a special value, and 'True', which is a string.

True and False are called **boolean** values because they are related to Boolean algebra (http://modsimpy.com/boolean).

We can use boolean values to control the behavior of the program using an **if statement**:

```
if flip(0.5):
    print('heads')
```

If the result from `flip` is `True`, the program displays the string `'heads'`. Otherwise it does nothing.

The punctuation for if statements is similar to the punctuation for function definitions: the first line has to end with a colon, and the lines inside the if statement have to be indented.

Optionally, you can add an **else clause** to indicate what should happen if the result is `False`:

```
if flip(0.5):
    print('heads')
else:
    print('tails')
```

Now we can use `flip` to simulate the arrival of students who want to borrow a bike. Suppose we have data from previous observations about how many students arrive at a particular time of day. If students arrive every 2 minutes, on average, then during any one-minute period, there is a 50% chance a student will arrive:

```
if flip(0.5):
    bike_to_wellesley()
```

At the same time, there might be an equal probability that a student at Wellesley wants to ride to Olin:

```
if flip(0.5):
    bike_to_olin()
```

We can combine these snippets of code into a function that simulates a **time step**, which is an interval of time, like one minute:

```
def step():
    if flip(0.5):
        bike_to_wellesley()

    if flip(0.5):
        bike_to_olin()
```

Then we can run a time step, and update the plot, like this:

```
step()
plot_state()
```

In reality, the probability of an arrival will vary over the course of a day, and might be higher or lower, at any point in time, at Olin or Wellesley. So instead of putting the constant value 0.5 in `step` we can replace it with a parameter, like this:

```
def step(p1, p2):
    if flip(p1):
        bike_to_wellesley()

    if flip(p2):
        bike_to_olin()
```

Now when you call `step`, you have to provide two arguments:

```
step(0.4, 0.2)
```

The arguments you provide, `0.4` and `0.2`, get assigned to the parameters, `p1` and `p2`, in order. So running this function has the same effect as:

```
p1 = 0.4
p2 = 0.2

if flip(p1):
    bike_to_wellesley()

if flip(p2):
    bike_to_olin()
```

The advantage of using a function is that you can call the same function many times, providing different values for the parameters each time.

1.9 For loops

At some point you will get sick of running cells over and over. Fortunately, there is an easy way to repeat a chunk of code, the **for loop**. Here's an example:

```
for i in range(4):
    bike_to_wellesley()
    plot_state()
```

The punctuation here should look familiar; the first line ends with a colon, and the lines inside the for loop are indented. The other elements of the for loop are:

- The words `for` and `in` are special words we have to use in a for loop.
- `range` is a Python function we're using here to control the number of times the loop runs.
- `i` is a **loop variable** that gets created when the for loop runs. In this example we don't actually use `i`; we will see examples later where we use the loop variable inside the loop.

When this loop runs, it runs the statements inside the loop four times, which moves one bike at a time from Olin to Wellesley, and plots the updated state of the system after each move.

In the notebook for this chapter, you'll have a chance to run this code and work on some exercises.

1.10 Under the hood

Throughout this book, we'll use functions defined in `modsim.py`. You will learn how to use these functions, but you don't have to know how they work.

However, you might be curious about what's going on "under the hood". So at the end of some chapters I'll provide additional information. If you are an experienced programmer, you might be interested by the design decisions I made. If you are a beginner, and you feel like you have your hands full already, feel free to skip these sections.

Most of the functions in `modsim.py` are based on functions provided by other Python libraries; the libraries we have used so far include:

Pint , which provides units like meters and seconds, as we saw in Section 1.1.

NumPy , which provides mathematical operations like `sqrt`, which we saw in Section 1.2.

Pandas , which provides the `Series` object, which is the basis of the `System` object in Section 1.3.

Matplotlib , which provides plotting functions, as we saw in Section 1.4.

You don't really have to use the functions in `modsim.py`. You could use these libraries directly, and when you have more experience, you probably will. But the functions in `modsim.py` are meant to be easier to use; they provide some additional capabilities, including error checking; and by hiding details you don't need to know about, they let you focus on more important things.

However, there is one drawback: when something goes wrong, it can be hard to understand the error messages. I'll have more to say about this in later chapters, but for now I have a suggestion. When you are getting started, you should practice making errors.

Along with each chapter, I provide a Jupyter notebook that contains the code from the chapter, so you can run it, see how it works, and modify it, and see how it breaks.

For each new function you learn, you should make as many mistakes as you can, deliberately, so you can see what happens. When you see what the errors messages are, you will understand what they mean. And that should help later, when you make errors accidentally.

Chapter 2

Simulation

To paraphrase two Georges, "All models are wrong, but some models are more wrong than others." In this chapter, I demonstrate the process we use to make models less wrong.

As an example, we'll review the bikeshare model from the previous chapter, consider its strengths and weaknesses, and gradually improve it. We'll also see ways to use the model to understand the behavior of the system and evaluate designed intended to make it work better.

You can view the code for this chapter at `http://modsimpy.com/chap02`. For instructions on downloading and running the code, see Section 0.4.

2.1 Iterative modeling

The model we have so far is simple, but it is based on unrealistic assumptions. Before you go on, take a minute to review the code from the previous chapter, which you can view at `http://modsimpy.com/chap01`. This code represents a model of the bikeshare system. What assumptions is it based on? Make a list of ways this model might be unrealistic; that is, what are the differences between the model and the real world?

Here are some of the differences on my list:

- In the model, a student is equally likely to arrive during any one-minute period. In reality, this probability varies depending on time of day, day of the week, etc.
- The model does not account for travel time from one bike station to another.
- The model does not check whether a bike is available, so it's possible for the number of bikes to be negative (as you might have noticed in some of your simulations).

Some of these modeling decisions are better than others. For example, the first assumption might be reasonable if we simulate the system for a short period of time, like one hour.

The second assumption is not very realistic, but it might not affect the results very much, depending on what we use the model for.

On the other hand, the third assumption seems problematic, and it is relatively easy to fix. In Section 2.4, we will.

This process, starting with a simple model, identifying the most important problems, and making gradual improvements, is called **iterative modeling**.

For any physical system, there are many possible models, based on different assumptions and simplifications. It often takes several iterations to develop a model that is good enough for the intended purpose, but no more complicated than necessary.

2.2 More than one System object

Before we go on, I want to make a few changes to the code from the previous chapter. First I'll generalize the functions we wrote so they take a `System` object as a parameter. Then, I'll make the code more readable by adding documentation.

Here are two functions from the previous chapter, `move_bike` and `plot_state`:

```
def move_bike(n):
    bikeshare.olin -= n
    bikeshare.wellesley += n

def plot_state():
    mark(bikeshare.olin, 'rs-', label='Olin')
    mark(bikeshare.wellesley, 'bo-', label='Wellesley')
```

One problem with these functions is that they always use `bikeshare`, which is a `System` object. As long as there is only one `System` object, that's fine, but these functions would be more flexible if they took a `System` object as a parameter. Here's what that looks like:

```
def move_bike(system, n):
    system.olin -= n
    system.wellesley += n

def plot_state(system):
    mark(system.olin, 'rs-', label='Olin')
    mark(system.wellesley, 'bo-', label='Wellesley')
```

The name of the parameter is `system` rather than `bikeshare` as a reminder that the value of `system` could be any `System` object, not just `bikeshare`.

Now I can create as many `System` objects as I want:

```
bikeshare1 = System(olin=10, wellesley=2)
bikeshare2 = System(olin=2, wellesley=10)
```

And update them independently:

```
bike_to_olin(bikeshare1)
bike_to_wellesley(bikeshare2)
```

Changes in `bikeshare1` do not affect `bikeshare2`, and vice versa. This behavior will be useful later in the chapter when we create a series of `System` objects to simulate different scenarios.

2.3 Documentation

Another problem with the code we have so far is that it contains no **documentation**. Documentation is text we add to programs to help other programmers read and understand them. It has no effect on the program when it runs.

There are two forms of documentation, **docstrings** and **comments**. A docstring is a string in triple-quotes that appears at the beginning of a function, like this:

```
def run_steps(system, num_steps=1, p1=0.5, p2=0.5):
    """Simulate the given number of time steps.

    system: bikeshare System object
    num_steps: number of time steps
    p1: probability of an Olin->Wellesley customer arrival
    p2: probability of a Wellesley->Olin customer arrival
    """
    for i in range(num_steps):
        step(system, p1, p2)
        plot_state(system)
```

Docstrings follow a conventional format:

- The first line is a single sentence that describes what the function does.
- The following lines explain what each of the parameters are.

A function's docstring should include the information someone needs to know to *use* the function; it should not include details about how the function works. That's what comments are for.

A comment is a line of text that begins with a hash symbol, `#`. It usually appears inside a function to explain something that would not be obvious to someone reading the program.

For example, here is a version of `move_bike` with a docstring and a comment.

```
def move_bike(system, n):
    """Move a bike.

    system: bikeshare System object
    n: +1 to move from Olin to Wellesley or
       -1 to move from Wellesley to Olin
    """
    # Because we decrease one system variable by n
    # and increase the other by n, the total number
    # of bikes is unchanged.
    system.olin -= n
    system.wellesley += n
```

At this point we have more documentation than code, which is not unusual for short functions.

2.4 Negative bikes

The changes we've made so far improve the quality of the code, but we haven't done anything to improve the quality of the model yet. Let's do that now.

Currently the simulation does not check whether a bike is available when a customer arrives, so the number of bikes at a location can be negative. That's not very realistic. Here's an updated version of `move_bike` that fixes the problem:

```
def move_bike(system, n):
    # make sure the number of bikes won't go negative
    olin_temp = system.olin - n
    if olin_temp < 0:
        return

    wellesley_temp = system.wellesley + n
    if wellesley_temp < 0:
        return

    # update the system
    system.olin = olin_temp
    system.wellesley = wellesley_temp
```

The comments explain the two sections of the function: the first checks to make sure a bike is available; the second updates the state.

The first line creates a variable named `olin_temp` that gets the number of bikes that *would* be at Olin if `n` bikes were moved. I added the suffix `_temp` to the name to indicate that I am using it as a **temporary variable**.

`move_bike` uses the less-than operator, `<`, to compare `olin_temp` to `0`. The result of this operator is a boolean. If it's `True`, that means `olin_temp` is negative, which means that there are not enough bikes.

In that case I use a **return statement**, which causes the function to end immediately, without running the rest of the statements. So if there are not enough bikes at Olin, we "return" from `move_bike` without changing the state. We do the same if there are not enough bikes at Wellesley.

If both of these tests pass, we run the last two lines, which assigns the values from the temporary variables to the corresponding system variables.

Because `olin_temp` and `wellesley_temp` are created inside a function, they are **local variables**, which means they only exist inside the function. At the end of the function, they disappear, and you cannot read or write them from anywhere else in the program.

In contrast, the system variables `olin` and `wellesley` belong to `system`, the `System` object that was passed to this function as a parameter. When we change system variables inside a function, those changes are visible in other parts of the program.

This version of `move_bike` makes sure we never have negative bikes at either station. But what about `bike_to_wellesley` and `bike_to_olin`; do we have to update them, too? Here they are:

```
def bike_to_wellesley(system):
    move_bike(system, 1)

def bike_to_olin(system):
    move_bike(system, -1)
```

Because these functions use `move_bike`, they take advantage of the new feature automatically. We don't have to update them.

2.5 Comparison operators

In the previous section, we used the less-than operator to compare two values. For completeness, here are the other **comparison operators**:

Operation	**Symbol**
Less than	`<`
Greater than	`>`
Less than or equal	`<=`
Greater than or equal	`>=`
Equal	`==`
Not equal	`!=`

The equals operator, `==`, compares two values and returns `True` if they are equal and `False` otherwise. It is easy to confuse with the **assignment operator**, `=`, which assigns a value to a variable. For example, the following statement uses the assignment operator, which creates `x` if it doesn't already exist and gives it the value `5`

```
x = 5
```

On the other hand, the following statement checks whether `x` is `5` and returns `True` or `False`. It does not create `x` or change its value.

```
x == 5
```

You can use the equals operator in an if statement, like this:

```
if x == 5:
    print('yes, x is 5')
```

If you make a mistake and use `=` in the first line of an `if` statement, like this:

```
if x = 5:
    print('yes, x is 5')
```

That's a **syntax error**, which means that the structure of the program is invalid. Python will print an error message and the program won't run.

2.6 Metrics

Getting back to the bike share system, at this point we have the ability to simulate the behavior of the system. Since the arrival of customers is random, the state of the system is different each time we run a simulation. Models like this are called **stochastic**; models that do the same thing every time they run are **deterministic**.

Suppose we want to use our model to predict how well the bike share system will work, or to design a system that works better. First, we have to decide what we mean by "how well" and "better".

From the customer's point of view, we might like to know the probability of finding an available bike. From the system-owner's point of view, we might want to minimize the number of customers who don't get a bike when they want one, or maximize the number of bikes in use. Statistics like these that quantify how well the system works are called **metrics**.

As a simple example, let's measure the number of unhappy customers. Here's a version of `move_bike` that keeps track of the number of customers who arrive at a station with no bikes:

```python
def move_bike(system, n):
    olin_temp = system.olin - n
    if olin_temp < 0:
        system.olin_empty += 1
        return

    wellesley_temp = system.wellesley + n
    if wellesley_temp < 0:
        system.wellesley_empty += 1
        return

    system.olin = olin_temp
    system.wellesley = wellesley_temp
```

Inside `move_bike`, we update the values of `olin_empty`, which is the number of times a customer finds the Olin station empty, and `wellesley_empty`, which is the number of unhappy customers at Wellesley.

That will only work if we initialize `olin_empty` and `wellesley_empty` when we create the `System` object, like this:

```python
bikeshare = System(olin=10, wellesley=2,
                   olin_empty=0, wellesley_empty=0)
```

Now we can run a simulation like this:

```python
run_steps(bikeshare, 60, 0.4, 0.2)
```

And then check the metrics:

```python
print(bikeshare.olin_empty, bikeshare.wellesley_empty)
```

Because the simulation is stochastic, the results are different each time it runs.

2.7 Functions that return values

We have used several functions that return values; for example, when you run `sqrt`, it returns a number you can assign to a variable.

```
t = sqrt(2 * h / a)
```

When you run `System`, it returns a new `System` object:

```
bikeshare = System(olin=10, wellesley=2)
```

Not all functions have return values. For example, when you run `mark`, it adds a point to the current graph, but it doesn't return a value. The functions we wrote so far are like `mark`; they have an effect, like changing the state of the system, but they don't return values.

To write functions that return values, we can use a second form of the `return` statement, like this:

```
def add_five(x):
    return x + 5
```

`add_five` takes a parameter, `x`, which could be any number. It computes `x + 5` and returns the result. So if we run it like this, the result is `8`:

```
add_five(3)
```

As a more useful example, here's a new function that creates a `System` object, runs a simulation, and then returns the `System` object as a result:

```
def run_simulation():
    system = System(olin=10, wellesley=2,
                    olin_empty=0, wellesley_empty=0)
    run_steps(system, 60, 0.4, 0.2, plot=False)
    return system
```

If we call `run_simulation` like this:

```
system = run_simulation()
```

It assigns to `system` a new `System` object, which we can use to check the metrics we are interested in:

```
print(system.olin_empty, system.wellesley_empty)
```

2.8 Two kinds of parameters

This version of `run_simulation` always starts with the same initial condition, 10 bikes at Olin and 2 bikes at Wellesley, and the same values of `p1`, `p2`, and `num_steps`. Taken together, these five values are the **parameters of the model**, which are values that determine the behavior of the model.

It is easy to get the parameters of a model confused with the parameters of a function. They are closely related ideas; in fact, it is common for the parameters of the model to appear as parameters in functions. For example, we can write a more general version of `run_simulation` that takes `p1` and `p2` as function parameters:

```
def run_simulation(p1, p2):
    bikeshare = System(olin=10, wellesley=2,
                       olin_empty=0, wellesley_empty=0)
    run_steps(bikeshare, 60, p1, p2, plot=False)
    return bikeshare
```

Now we can run it with different arrival rates, like this:

```
system = run_simulation(0.6, 0.3)
```

In this example, `0.6` gets assigned to `p1` and `0.3` gets assigned to `p2`.

Now we can call `run_simulation` with different parameters and see how the metrics, like the number of unhappy customers, depend on the parameters. But before we do that, we need a new version of a for loop.

2.9 Loops and arrays

In Section 1.9, we saw a loop like this:

```
for i in range(4):
    bike_to_wellesley()
    plot_state()
```

The loop variable, `i`, gets created when the loop runs, but it is not used for anything. Now here's a loop that actually uses the loop variable:

```
p1_array = linspace(0, 1, 5)

for p1 in p1_array:
    print(p1)
```

`linspace` is a defined in the `modsim` library. It takes three arguments, `start`, `stop`, and `num`. In this example, it creates a sequence of `5` equally-spaced numbers, starting at `0` and ending at `1`.

The result is a NumPy **array**, which is a new kind of object we have not seen before. An array is a container for a sequence of numbers.

In the for loop, the values from the array are assigned to the loop variable one a time. When this loop runs, it

1. Gets the first value from the array and assigns it to `p1`.
2. Runs the body of the loop, which prints `p1`.
3. Gets the next value from the array and assigns it to `p1`.
4. Runs the body of the loop, which prints `p1`.

And so on, until it gets to the end of the range. The result is:

```
0.0
0.25
0.5
0.75
1.0
```

This will come in handy in the next section.

2.10 Sweeping parameters

If we know the actual values of parameters like p1 and p2, we can use them to make specific predictions, like how many bikes will be at Olin after one hour.

But prediction is not the only goal; models like this are also used to explain why systems behave as they do and to evaluate alternative designs. For example, if we observe the system and notice that we often run out of bikes at a particular time, we could use the model to figure out why that happens. And if we are considering adding more bikes, or another station, we could evaluate the effect of various "what if" scenarios.

As an example, suppose we have enough data to estimate that p2 is about 0.2, but we don't have any information about p1. We could run simulations with a range of values for p1 and see how the results vary. This process is called **sweeping** a parameter, in the sense that the value of the parameter "sweeps" through a range of possible values.

Now that we know about loops and arrays, we can use them like this:

```
p1_array = linspace(0, 1, 11)

for p1 in p1_array:
    system = run_simulation(p1, 0.2)
    print(p1, system.olin_empty)
```

Each time through the loop, we run a simulation with a the given value of p1 and the same value of p2, 0.2. Then we print p1 and the number of unhappy customers at Olin.

To visualize the results, we can run the same loop, replacing print with plot:

```
newfig()
for p1 in p1_array:
    system = run_simulation(p1, 0.2)
    mark(p1, system.olin_empty, 'rs', label='olin')
```

When you run the notebook for this chapter, you will see the results and have a chance to try additional experiments.

2.11 Incremental development

When you start writing programs that are more than a few lines, you might find yourself spending more and more time debugging. The more code you write before you start debugging, the harder it is to find the problem.

Incremental development is a way of programming that tries to minimize the pain of debugging. The fundamental steps are:

1. Always start with a working program. If you have an example from a book, or a program you wrote that is similar to what you are working on, start with that. Otherwise, start with something you *know* is correct, like `x=5`. Run the program and confirm that it does what you expect.

2. Make one small, testable change at a time. A "testable" change is one that displays something, or has some other effect, that you can check. Ideally, you should know what the correct answer is, or be able to check it by performing another computation.

3. Run the program and see if the change worked. If so, go back to Step 2. If not, you will have to do some debugging, but if the change you made was small, it shouldn't take long to find the problem.

When this process works, your changes usually work the first time, or if they don't, the problem is obvious. In practice, there are two problems with incremental development:

- Sometimes you have to write extra code to generate visible output that you can check. This extra code is called **scaffolding** because you use it to build the program and then remove it when you are done. That might seem like a waste, but time you spend on scaffolding is almost always time you save on debugging.

- When you are getting started, it might not be obvious how to choose the steps that get from `x=5` to the program you are trying to write. You will see more examples of this process as we go along, and you will get better with experience.

If you find yourself writing more than a few lines of code before you start testing, and you are spending a lot of time debugging, try incremental development.

Chapter 3

Explanation

In 1968 Paul Erlich published *The Population Bomb*, in which he predicted that world population would grow quickly during the 1970s, that agricultural production could not keep up, and that mass starvation in the next two decades was inevitable (see `http://modsimpy.com/popbomb`). As someone who grew up during those decades, I am happy to report that those predictions were wrong.

But world population growth is still a topic of concern, and it is an open question how many people the earth can sustain while maintaining and improving our quality of life.

In this chapter and the next, we use tools from the previous chapters to explain world population growth since 1950 and generate predictions for the next 50–100 years.

You can view the code for this chapter at `http://modsimpy.com/chap03`. For instructions on downloading and running the code, see Section 0.4.

3.1 World Population Data

The Wikipedia article `http://modsimpy.com/worldpop` contains tables with estimates of world population from prehistory to the present, and projections for the future.

To read this data, we will use Pandas, which is a library that provides functions for working with data. It also defines two objects we will use extensively, `Series` and `DataFrame`.

The function we'll use is `read_html`, which can read a web page and extract data from any tables it contains. Before we can use it, we have to import it. You have already seen this import statement:

```
from modsim import *
```

which imports all functions from the `modsim` library. To import `read_html`, the statement we need is:

```
from pandas import read_html
```

Now we can use it like this:

```
filename = 'data/World_population_estimates.html'
tables = read_html(filename,
                   header=0,
                   index_col=0,
                   decimal='M')
```

The arguments are:

- `filename`: The name of the file (including the directory it's in) as a string. This argument can also be a URL starting with `http`.
- `header`: Indicates which row of each table should be considered the header, that is, the row that contains the column headings. In this case it is the first row, which is numbered 0.
- `index_col`: Indicates which column of each table should be considered the **index**, that is, the labels that identify the rows. In this case it is the first column, which contains the years.
- `decimal`: Normally this argument is used to indicate which character should be considered a decimal point, since some conventions use a period and some use a comma. In this case I am abusing the feature by treating `M` as a decimal point, which allows some of the estimates, which are expressed in millions, to be read as numbers.

The result, which is assigned to `tables`, is a sequence that contains one `DataFrame` for each table. A `DataFrame` is an object that represents tabular data and provides functions for accessing and manipulating it.

To select one of the `DataFrames` in `tables`, we can use the bracket operator like this:

```
table2 = tables[2]
```

The number in brackets indicates which `DataFrame` we want, starting from 0. So this line selects the third table, which contains population estimates from 1950 to 2016.

We can display the first few lines like this:

```
table2.head()
```

The headings at the tops of the columns are long strings, which makes them hard to work with. We can replace them with shorter strings like this:

```
table2.columns = ['census', 'prb', 'un', 'maddison',
                  'hyde', 'tanton', 'biraben', 'mj',
                  'thomlinson', 'durand', 'clark']
```

Now we can select a column from the `DataFrame` using the dot operator, like selecting a system variable from a `System` object:

```
census = table2.census
```

The result is a `Series`, which is another object defined by the Pandas library. A `Series` is like a `DataFrame` with just one column. It contains two variables, `index` and `values`. In this example, `index` is the sequence of years from 1950 to 2016, and `values` is the sequence of corresponding populations.

In this chapter we'll use `DataFrame` and `Series` objects without knowing much about how they work. We'll see more details in Section **??**.

3.2 Plotting

`modsim.py` provides `plot`, which can plot arrays and `Series` objects, so we can plot the estimates like this:

```
def plot_estimates():
    un = table2.un / 1e9
    census = table2.census / 1e9

    plot(census, ':', color='darkblue', label='US Census')
    plot(un, '--', color='green', label='UN DESA')
```

The first two lines select the estimates generated by the United Nations Department of Economic and Social Affairs (UN DESA) and the United States Census Bureau.

At the same time we divide by one billion, in order to display the estimates in terms of billions. The number `1e9` is a shorter (and less error-prone) way to write `1000000000` or one billion. When we divide a `Series` by a number, it divides all of the elements of the `Series`.

The next two lines plot the `Series` objects. The style strings `':'` and `'--'` indicate dotted and dashed lines. The `color` argument can be any of the color strings described at `http://modsimpy.com/color`. The `label` argument provides the string that appears in the legend.

Figure 3.1 shows the result. The lines overlap almost completely; for most dates the difference between the two estimates is less than 1%.

3.3 Constant growth model

Suppose we want to predict world population growth over the next 50 or 100 years. We can do that by developing a model that describes how population grows, fitting the model to the data we have so far, and then using the model to generate predictions.

In the next few sections I demonstrate this process starting with simple models and gradually improving them.

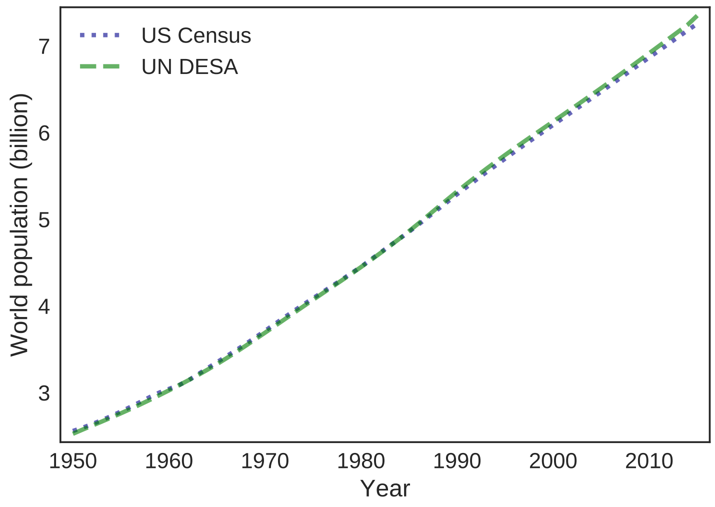


Figure 3.1: Estimates of world population, 1950–2015.

Although there is some curvature in the plotted estimates, it looks like world population growth has been close to linear since 1960 or so. As a starting place, we'll build a model with constant growth.

To fit the model to the data, we'll compute the average annual growth from 1950 to 2015. Since the UN and Census data are so close, I'll use the Census data, again in terms of billions:

```
census = table2.census / 1e9
```

We can select a value from a `Series` using the bracket operator:

```
census[1950]
```

So we can get the total growth during the interval like this:

```
total_growth = census[2015] - census[1950]
```

The numbers in brackets are called **labels**, because they label the rows of the `Series` (not to be confused with the labels we saw in the previous section, which label lines in a graph).

In this example, the labels 2015 and 1950 are part of the data, so it would be better not to make them part of the program. Putting values like these in the program is called **hard coding**; it is considered bad practice because if the data changes in the future, we have to modify the program (see http://modsimpy.com/hardcode).

It would be better to get the first and last labels from the `Series` like this:

```
first_year = get_first_label(census)
last_year = get_last_label(census)
```

`get_first_label` and `get_last_label` are defined in `modsim.py`; as you might have guessed, they select the first and last labels from `census`. We can use these labels to select the first and last values, then compute `total_growth` and `annual_growth`:

```
total_growth = census[last_year] - census[first_year]
elapsed_time = last_year - first_year
annual_growth = total_growth / elapsed_time
```

The next step is to use this estimate to simulate population growth since 1950.

3.4 Simulation

The result from the simulation is a time series, which is a sequence of times and associated values (see http://modsimpy.com/timeser). In this case, we have a sequence of years and associated population estimates.

To represent a time series, we'll use a `TimeSeries` object:

```
results = TimeSeries()
```

`TimeSeries`, which is defined by `modsim`, is a specialized version of `Series`, which is defined by Pandas.

We can set the first value in the new `TimeSeries` by copying the first value from `census`:

```
results[first_year] = census[first_year]
```

Then we set the rest of the values by simulating annual growth:

```
for t in linrange(first_year, last_year-1):
    results[t+1] = results[t] + annual_growth
```

`linrange` is defined in the `modsim` library. It is similar to `linspace`, but instead of taking parameters `start`, `stop`, and `num`, it takes `start`, `stop`, and `step`.

It returns a NumPy array of values from `start` to `stop`, where `step` is the difference between successive values. The default value of `step` is 1.

In this example, the result from `linrange` is an array of values from `1950` to `2014` (including both).

Each time through the loop, the loop variable `t` gets the next value from the array. Inside the loop, we compute the population for each year by adding the population for the previous year and `annual_growth`. The last time through the loop, the value of `t` is 2014, so the last label in `results` is 2015, which is what we want.

Figure 3.2 shows the result. The model does not fit the data particularly well from 1950 to 1990, but after that, it's pretty good. Nevertheless, there are problems:

- There is no obvious mechanism that could cause population growth to be constant from year to year. Changes in population are determined by the fraction of people who die and the fraction of people who give birth, so they should depend on the current population.
- According to this model, we would expect the population to keep growing at the same rate forever, and that does not seem reasonable.

We'll try out some different models in the next few sections, but first let's clean up the code.

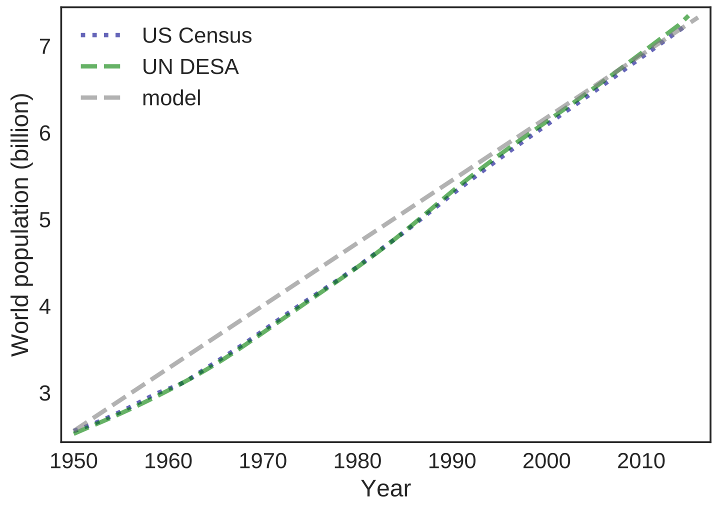


Figure 3.2: Estimates of world population, 1950–2015, and a constant growth model.

3.5 Now with System objects

First, let's put all the information we need to run the model into a `System` object:

```
system = System(t0 = first_year,
                t_end = last_year,
                p0 = census[first_year],
                annual_growth = annual_growth)
```

`t0` and `t_end` are the first and last years; `p0` is the initial population, and `annual_growth` is the estimated annual growth.

Next we'll wrap the code from the previous section in a function:

```
def run_simulation1(system):
    results = TimeSeries()
    results[system.t0] = system.p0

    for t in linrange(system.t0, system.t_end-1):
        results[t+1] = results[t] + system.annual_growth

    system.results = results
```

When `run_simulation1` runs, it creates a new `TimeSeries` that contains the result of the simulation, and stores it as a new system variable, `results`.

To plot the results, we define a new function:

```
def plot_results(system, title):
    newfig()
    plot_estimates(table2)
    plot(system.results, '--', color='gray', label='model')
    decorate(xlabel='Year',
             ylabel='World population (billion)',
             title=title)
```

This function uses `decorate`, which is defined in the `modsim` library. `decorate` takes arguments that specify the title of the figure, labels for the x-axis and y-axis, and limits for the axes.

Finally, we can run it like this.

```
run_simulation1(system)
plot_results(system)
```

The results are the same as Figure 3.2.

3.6 Proportional growth model

The biggest problem with the constant growth model is that it doesn't make any sense. It is hard to imagine how people all over the world could conspire to keep population growth constant from year to year.

On the other hand, if some fraction of the population dies each year, and some fraction gives birth, we can compute the net change in the population like this:

```
def run_simulation2(system):
    results = TimeSeries()
    results[system.t0] = system.p0

    for t in linrange(system.t0, system.t_end-1):
        births = system.birth_rate * results[t]
        deaths = system.death_rate * results[t]
        results[t+1] = results[t] + births - deaths

    system.results = results
```

Now we can choose the values of `birth_rate` and `death_rate` that best fit the data. Without trying too hard, I chose:

```
system.death_rate = 0.01
system.birth_rate = 0.027
```

Then I ran the simulation and and plotted the results:

```
run_simulation2(system)
plot_results(system)
```

Figure 3.3 shows the results. The proportional model fits the data well from 1950 to 1965, but not so well after that. Overall, the **quality of fit** is not as good as the constant growth model, which is surprising, because it seems like the proportional model is more realistic.

There are a few things we could try to improve the model:

- Maybe the birth rate and death rate vary over time.
- Maybe net growth depends on the current population, but the relationship is quadratic, not linear.

We will try out these variations, but first, let's clean up the code one more time.

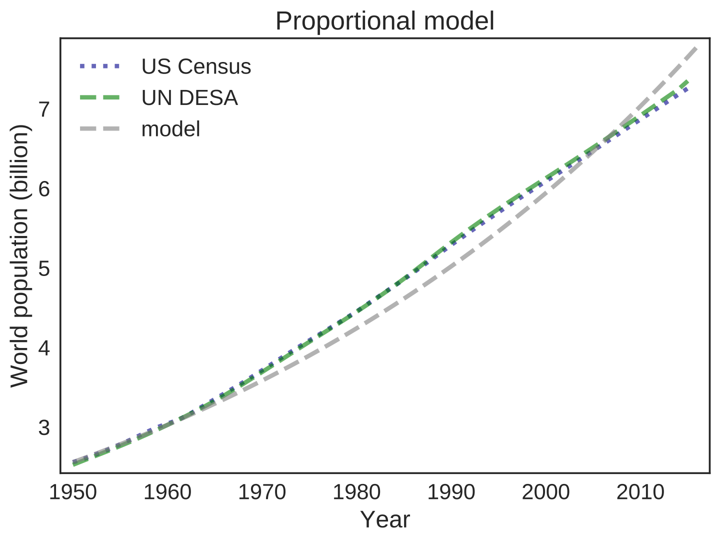


Figure 3.3: Estimates of world population, 1950–2015, and a proportional model.

3.7 Factoring out the update function

`run_simulation1` and `run_simulation2` are nearly identical except for the body of the `for` loop, where we compute the population for the next year.

Rather than repeat identical code, we can separate the things that change from the things that don't. First, we'll pull out the body of the loop and make it a function:

```
def update_func(pop, t, system):
    births = system.birth_rate * pop
    deaths = system.death_rate * pop
    return pop + births - deaths
```

This function takes as arguments the current population, current year, and a `System` object; it returns the computed population for the next year.

Now we can write a function that runs any model:

```
def run_simulation(system, update_func):
    results = TimeSeries()
    results[system.t0] = system.p0
    for t in linrange(system.t0, system.t_end):
        results[t+1] = update_func(results[t], t, system)
    system.results = results
```

This function demonstrates a feature we have not seen before: it takes a function as a parameter! When we call `run_simulation`, the second parameter is a function, like `update_func`, that computes the population for the next year.

Here's how we call it:

```
run_simulation(system, update_func)
```

Passing a function as an argument is the same as passing any other value. The argument, which is `update_func` in this example, gets assigned to the parameter, which is also called `update_func`. Inside `run_simulation`, we can run `update_func` just like any other function.

When you calls `run_simulation`, it calls `update_func` once for each year between `t0` and `t_end`. The result is the same as Figure 3.3.

3.8 Combining birth and death

While we are at it, we can also simplify the code by combining births and deaths to compute the net growth rate. Instead of two parameters, `birth_rate` and `death_rate`, we can write the update function in terms of a single parameter that represents the difference:

```
system.alpha = system.birth_rate - system.death_rate
```

Here's the modified version of `update_func`:

```
def update_func(pop, t, system):
    net_growth = system.alpha  * pop
    return pop + net_growth
```

And here's how we run it:

```
run_simulation(system, update_func)
```

Again, the result is the same as Figure 3.3.

3.9 Quadratic growth

It makes sense that net growth should depend on the current population, but maybe it's not a linear relationship, like this:

```
    net_growth = system.alpha * pop
```

Maybe it's a quadratic relationship, like this:

```
    net_growth = system.alpha * pop + system.beta * pop**2
```

We can test that conjecture with a new update function:

```
def update_func(pop, t, system):
    net_growth = system.alpha * pop + system.beta * pop**2
    return pop + net_growth
```

Now we need two parameters. I chose the following values by trial and error; we will see better ways to do it later.

```
system.alpha = 0.025
system.beta = -0.0018
```

And here's how we run it:

```
run_simulation(system, update_func)
```

Figure 3.4 shows the result. The model fits the data well over the whole range, with just a bit of daylight between them in the 1960s.

Of course, we should expect the quadratic model to fit better than the linear or proportional model because it has two parameters we can choose, where

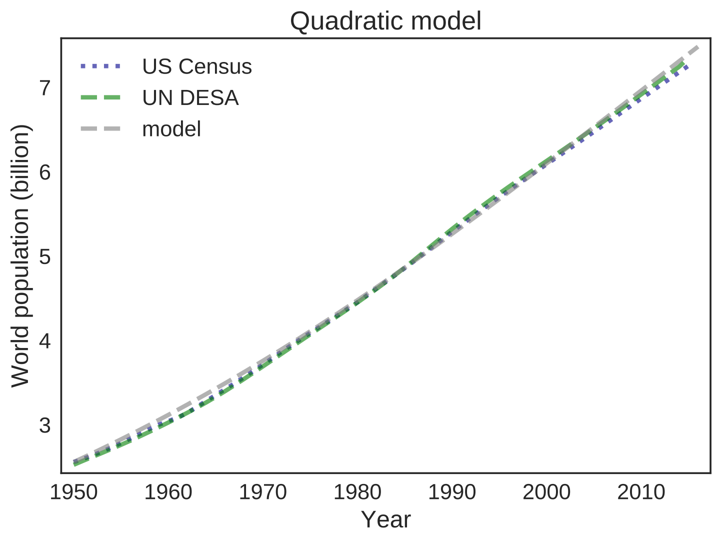


Figure 3.4: Estimates of world population, 1950–2015, and a quadratic model.

the other models have only one. In general, the more parameters you have to play with, the better you should expect the model to fit.

But fitting the data is not the only reason to think the quadratic model might be a good choice. It also makes sense; that is, there is a legitimate reason to expect the relationship between growth and population to have this form.

To understand it, let's look at net growth as a function of population. Here's how we compute it:

```
pop_array = linspace(0.001, 15, 100)
net_growth_array = (system.alpha * pop_array +
                    system.beta * pop_array**2)
```

`pop_array` contains 100 equally spaced values from near 0 to 15. `net_growth_array` contains the corresponding 100 values of net growth. We can plot the results like this:

```
plot(pop_array, net_growth_array, '-')
```

Figure 3.5 shows the result. Note that the x-axis is not time, as in the previous

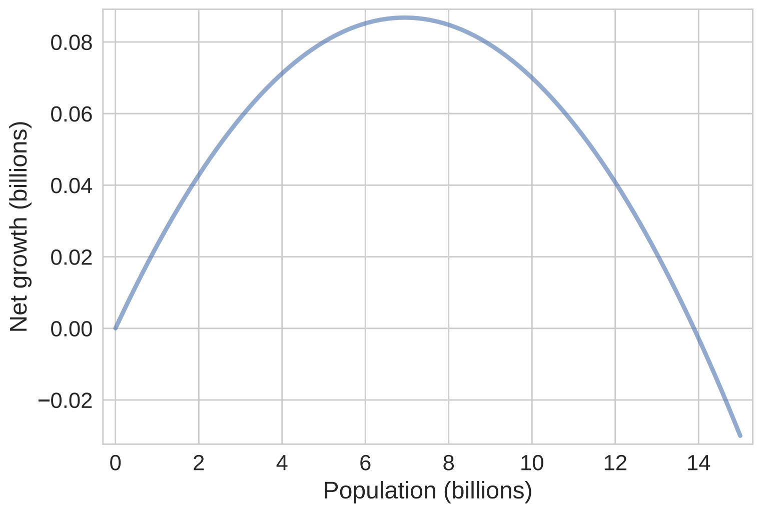


Figure 3.5: Net growth as a function of population.

figures, but population. We can divide this curve into four regimes of behavior:

- When the population is less than 3-4 billion, net growth is proportional to population, as in the proportional model. In this regime, the population grows slowly because the population is small.
- Between 4 billion and 10 billion, the population grows quickly because there are a lot of people, and there are enough resources, like food, water, and space, to sustain high birth rates and low death rates.
- Above 10 billion, population grows more slowly because resource limits start to decrease birth rates, increase death rates, or both.
- Above 14 billion, resources are so limited that the death rate exceeds the birth rate and net growth becomes negative.

Just below 14 billion, there is a point where net growth is 0, which means that the population does not change. At this point, the birth and death rates are equal, so the population is in **equilibrium**.

3.10 Equilibrium

To find this equilibrium point, we can find the roots, or zeros, of this equation:

$$\Delta p = \alpha p + \beta p^2$$

where Δp is net growth, p is current population, and α and β are the parameters of the model. We can rewrite the right hand side like this:

$$\Delta p = p(\alpha + \beta p)$$

which is 0 when $p = 0$ or $p = -\alpha/\beta$. In this example, $\alpha = 0.025$ and $\beta = -0.0018$, so $-\alpha/\beta = 13.9$.

In the context of population modeling, the quadratic model is more conventionally written like this:

$$\Delta p = rp(1 - p/K)$$

This is the same model; it's just a different way to **parameterize** it. Given α and β, we can compute $r = \alpha$ and $K = -\alpha/\beta$.

In this version, it is easier to interpret the parameters: α is the maximum growth rate, observed when p is small, and K is the equilibrium point. K is also called the **carrying capacity**, since it indicates the maximum population the environment can sustain.

In the next chapter we use the models we have developed to generate predictions.

3.11 Disfunctions

When people first learn about functions, there are a few things they often find confusing. In this section I present and explain some common problems with functions.

As an example, suppose you want a function that takes a `System` object, with variables `alpha` and `beta`, as a parameter and computes the carrying capacity, `-alpha/beta`. Here's a good solution:

```
def carrying_capacity(system):
    K = -system.alpha / system.beta
    return K

sys1 = System(alpha=0.025, beta=-0.0018)
pop = carrying_capacity(sys1)
print(pop)
```

Now let's see all the ways that can go wrong.

Disfunction #1: Not using parameters. In the following version, the function doesn't take any parameters; when `system` appears inside the function, it refers to the object we created outside the function.

```
def carrying_capacity():
    K = -system.alpha / system.beta
    return K

system = System(alpha=0.025, beta=-0.0018)
pop = carrying_capacity()
print(pop)
```

This version actually works, but it is not as versatile as it could be. If there are several `System` objects, this function can only work with one of them, and only if it is named `system`.

Disfunction #2: Clobbering the parameters. When people first learn about parameters, they often write functions like this:

```
# WRONG
def carrying_capacity(system):
    system = System(alpha=0.025, beta=-0.0018)
    K = -system.alpha / system.beta
    return K

sys1 = System(alpha=0.03, beta=-0.002)
pop = carrying_capacity(sys1)
print(pop)
```

In this example, we have a System object named sys1 that gets passed as an argument to carrying_capacity. But when the function runs, it ignores the argument and immediately replaces it with a new System object. As a result, this function always returns the same value, no matter what argument is passed.

When you write a function, you generally don't know what the values of the parameters will be. Your job is to write a function that works for any valid values. If you assign your own values to the parameters, you defeat the whole purpose of functions.

Disfunction #3: No return value. Here's a version that computes the value of K but doesn't return it.

```
# WRONG
def carrying_capacity(system):
    K = -system.alpha / system.beta

sys1 = System(alpha=0.025, beta=-0.0018)
pop = carrying_capacity(sys1)
print(pop)
```

A function that doesn't have a return statement always returns a special value called None, so in this example the value of pop is None. If you are debugging a program and find that the value of a variable is None when it shouldn't be, a function without a return statement is a likely cause.

Disfunction #4: Ignoring the return value. Finally, here's a version where the function is correct, but the way it's used is not.

```
# WRONG
def carrying_capacity(system):
    K = -system.alpha / system.beta
    return K

sys1 = System(alpha=0.025, beta=-0.0018)
carrying_capacity(sys1)
print(K)
```

In this example, `carrying_capacity` runs and returns `K`, but the return value is dropped.

When you call a function that returns a value, you should do something with the result. Often you assign it to a variable, as in the previous examples, but you can also use it as part of an expression. For example, you could eliminate the temporary variable `pop` like this:

```
print(carrying_capacity(sys1))
```

Or if you had more than one system, you could compute the total carrying capacity like this:

```
total = carrying_capacity(sys1) + carrying_capacity(sys2)
```

In the notebook for this chapter, you can try out each of these examples and see what happens.

Chapter 4

Prediction

In the previous chapter we developed a quadratic model of world population growth from 1950 to 2015. It is a simple model, but it fits the data well and the mechanisms it's based on are plausible.

In this chapter we'll use the quadratic model to generate projections of future growth, and compare our results to projections from actual demographers. Also, we'll represent the models from the previous chapters as differential equations and solve them analytically.

You can view the code for this chapter at http://modsimpy.com/chap04. For instructions on downloading and running the code, see Section 0.4.

4.1 Generating projections

We'll start with the quadratic model from Section 3.9, which is based on this update function:

```
def update_func(pop, t, system):
    net_growth = system.alpha * pop + system.beta * pop**2
    return pop + net_growth
```

As we saw in the previous chapter, we can get the start date, end date, and initial population from `census`, which is a series that contains world population estimates generated by the U.S. Census:

```
tfirst_year = get_first_label(census)
last_year = get_last_label(census)
```

Now we can create a `System` object:

```
system = System(t0 = first_year,
                t_end = last_year,
                p0 = census[first_year],
                alpha=0.025,
                beta=-0.0018)
```

And run the model:

```
run_simulation(system, update_func)
```

We have already seen the results in Figure 3.4. Now, to generate a projection, the only thing we have to change is `t_end`:

```
system.t_end = 2250
run_simulation(system, update_func)
```

Figure 4.1 shows the result, with a projection until 2250. According to this model, population growth will continue almost linearly for the next 50–100 years, then slow over the following 100 years, approaching 13.9 billion by 2250.

I am using the word “projection” deliberately, rather than “prediction”, with the following distinction: “prediction” implies something like “this is what we should reasonably expect to happen, at least approximately”; “projection” implies something like “if this model is actually a good description of what is happening in this system, and if nothing in the future causes the parameters of the model to change, this is what would happen.”

Using “projection” leaves open the possibility that there are important things in the real world that are not captured in the model. It also suggests that, even if the model is good, the parameters we estimate based on the past might be different in the future.

The quadratic model we’ve been working with is based on the assumption that population growth is limited by the availability of resources; in that scenario,

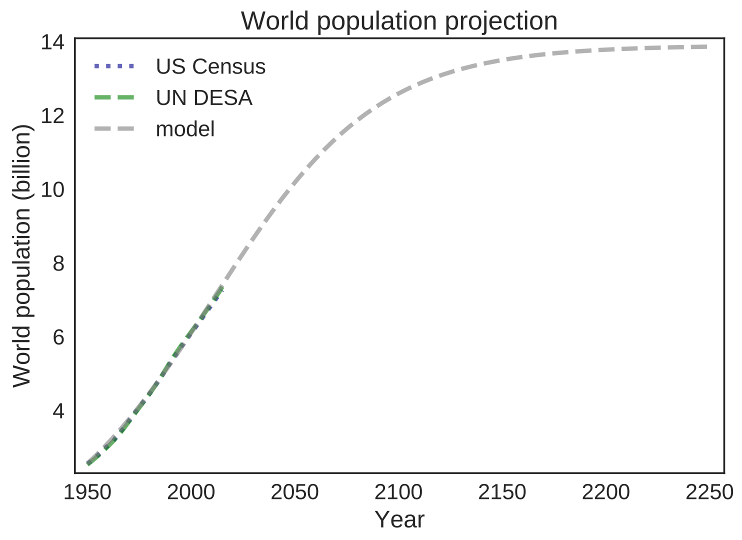


Figure 4.1: Quadratic model of world population growth, with projection from 2016 to 2250.

as the population approaches carrying capacity, birth rates fall and death rates rise because resources become scarce.

If that assumption is valid, we might be able to use actual population growth to estimate carrying capacity, especially if we observe the transition into the regime where the growth rate starts to fall.

But in the case of world population growth, those conditions don't apply. Over the last 50 years, the net growth rate has leveled off, but not yet started to fall, so we don't have enough data to make a credible estimate of carrying capacity. And resource limitations are probably *not* the primary reason growth has slowed. As evidence, consider:

- First, the death rate is not increasing; rather, it has declined from 1.9% in 1950 to 0.8% now (see `http://modsimpy.com/mortality`). So the decrease in net growth is due entirely to declining birth rates.
- Second, the relationship between resources and birth rate is the opposite of what the model assumes; as nations develop and people become more wealthy, birth rates tend to fall.

We should not take too seriously the idea that this model can estimate carrying capacity. But the predictions of a model can be credible even if the assumptions of the model are not strictly true. For example, population growth might behave *as if* it is resource limited, even if the actual mechanism is something else.

In fact, demographers who study population growth often use models similar to ours. In the next section, we'll compare our projections to theirs.

4.2 Comparing projections

Table 3 from `http://modsimpy.com/worldpop` contains projections from the U.S. Census and the United Nations DESA:

```
table3 = tables[3]
```

For some years, one agency or the other has not published a projection, so some elements of `table3` contain the special value `NaN`, which stands for "not a number". `NaN` is often used to indicate missing data.

Pandas provides functions that deal with missing data, including `dropna`, which removes any elements in a series that contain `NaN`. Using `dropna`, we can plot the projections like this:

```
def plot_projections(table):
    census = table.census / 1e9
    un = table.un / 1e9

    plot(census.dropna(), ':',
         color='darkblue', label='US Census')
    plot(un.dropna(), '--',
         color='green', label='UN DESA')
```

We can run our model over the same interval:

```
system.t_end = 2100
run_simulation(system, update_func2)
```

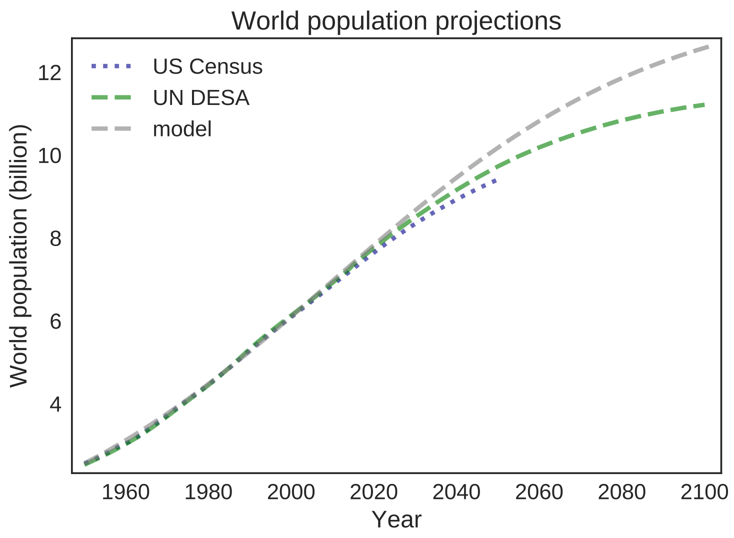


Figure 4.2: Projections of world population generated by the U.S. Census Bureau, the United Nations, and our quadratic model.

And compare our projections to theirs. Figure 4.2 shows the results. Real demographers expect world population to grow more slowly than our model projects, probably because their models are broken down by region and country, where conditions are different, and they take into account expected economic development.

Nevertheless, their projections are qualitatively similar to ours, and theirs differ from each other almost as much as they differ from ours. So the results from this model, simple as it is, are not entirely crazy.

4.3 Recurrence relations

The population models in the previous chapter and this one are simple enough that we didn't really need to run simulations. We could have solved them mathematically. For example, we wrote the constant growth model like this:

```
model[t+1] = model[t] + annual_growth
```

In mathematical notation, we would write the same model like this:

$$x_{n+1} = x_n + c$$

where x_n is the population during year n, x_0 is a given initial population, and c is constant annual growth. This way of representing the model is a **recurrence relation**; see http://modsimpy.com/recur.

Often it is possible to solve a recurrence relation by writing an equation that computes x_n, for a given value of n, directly; that is, without computing the intervening values from x_1 through x_{n-1}.

In the case of constant growth we can see that $x_1 = x_0 + c$, and $x_2 = x_1 + c$. Combining these, we get $x_2 = x_0 + 2c$, then $x_3 = x_0 + 3c$, and it is not hard to conclude that in general

$$x_n = x_0 + nc$$

So if we want to know x_{100} and we don't care about the other values, we can compute it with one multiplication and one addition.

We can also write the proportional model as a recurrence relation:

$$x_{n+1} = x_n + \alpha x_n$$

Or more conventionally as:

$$x_{n+1} = x_n(1 + \alpha)$$

Now we can see that $x_1 = x_0(1 + \alpha)$, and $x_2 = x_0(1 + \alpha)^2$, and in general

$$x_n = x_0(1 + \alpha)^n$$

This result is a **geometric progression**; see http://modsimpy.com/geom. When α is positive, the factor $1 + \alpha$ is greater than 1, so the elements of the sequence grow without bound.

Finally, we can write the quadratic model like this:

$$x_{n+1} = x_n + \alpha x_n + \beta x_n^2$$

or with the more conventional parameterization like this:

$$x_{n+1} = x_n + r x_n (1 - x_n / K)$$

There is no analytic solution to this equation, but we can approximate it with a differential equation and solve that, which is what we'll do in the next section.

4.4 Differential equations

Starting again with the constant growth model

$$x_{n+1} = x_n + c$$

If we define Δx to be the change in x from one time step to the next, we can write:

$$\Delta x = x_{n+1} - x_n = c$$

If we define Δt to be the time step, which is one year in the example, we can write the rate of change per unit of time like this:

$$\frac{\Delta x}{\Delta t} = c$$

This model is **discrete**, which means it is only defined at integer values of n and not in between. But in reality, people are born and die all the time, not once a year, so a **continuous** model might be more realistic.

We can make this model continuous by writing the rate of change in the form of a derivative:

$$\frac{dx}{dt} = c$$

This way of representing the model is a **differential equation**; see `http://modsimpy.com/diffeq`.

We can solve this differential equation if we multiply both sides by dt:

$$dx = c dt$$

And then integrate both sides:

$$x(t) = ct + x_0$$

Similarly, we can write the proportional growth model like this:

$$\frac{\Delta x}{\Delta t} = \alpha x$$

And as a differential equation like this:

$$\frac{dx}{dt} = \alpha x$$

If we multiply both sides by dt and divide by x, we get

$$\frac{1}{x}\, dx = \alpha\ dt$$

Now we integrate both sides, yielding:

$$\ln x = \alpha t + K$$

where ln is the natural logarithm and K is the constant of integration. Exponentiating both sides[1], we have

$$\exp(\log(x)) = x = \exp(\alpha t + K)$$

which we can rewrite

$$x = \exp(\alpha t) \exp(K)$$

Since K is an arbitrary constant, $\exp(K)$ is also an arbitrary constant, so we can write

$$x = C \exp(\alpha t)$$

where $C = \exp(K)$. There are many solutions to this differential equation, with different values of C. The particular solution we want is the one that has the value x_0 when $t = 0$. Well, when $t = 0$, $x(t) = C$, so $C = x_0$ and the solution we want is

$$x(t) = x_0 \exp(\alpha t)$$

If you would like to see this derivation done more carefully, you might like this video: `http://modsimpy.com/khan1`.

[1]The exponential function can be written $\exp(x)$ or e^x. In this book I use the first form because it resembles the Python code.

4.5 Analysis and simulation

Once you have designed a model, there are generally two ways to proceed: simulation and analysis. Simulation often comes in the form of a computer program that models changes in a system over time, like births and deaths, or bikes moving from place to place. Analysis often comes in the form of algebra; that is, symbolic manipulation using mathematical notation.

Analysis and simulation have different capabilities and limitations. Simulation is generally more versatile; it is easy to add and remove parts of a program and test many versions of a model, as we have done in the previous examples.

But there are several things we can do with analysis that are harder or impossible with simulations:

- With analysis we can sometimes compute, exactly and efficiently, a value that we could only approximate, less efficiently, with simulation. For example, in Figure 3.5, we can see that net growth goes to zero near 14 billion, and we could estimate carrying capacity using a numerical search algorithm (more about that later). But with the analysis in Section 3.9, we get the general result that $K = -\alpha/\beta$.
- Analysis often provides "computational shortcuts", that is, the ability to jump forward in time to compute the state of a system many time steps in the future without computing the intervening states.
- We can use analysis to state and prove generalizations about models; for example, we might prove that certain results will always or never occur. With simulations, we can show examples and sometimes find counterexamples, but it is hard to write proofs.
- Analysis can provide insight into models and the systems they describe; for example, sometimes we can identify regimes of qualitatively different behavior and key parameters that control those behaviors.

When people see what analysis can do, they sometimes get drunk with power, and imagine that it gives them a special ability to see past the veil of the material world and discern the laws of mathematics that govern the universe. When they analyze a model of a physical system, they talk about "the math behind it" as if our world is the mere shadow of a world of ideal mathematical entities[2].

This is, of course, nonsense. Mathematical notation is a language designed by humans for a purpose, specifically to facilitate symbolic manipulations like algebra. Similarly, programming languages are designed for a purpose, specifically to represent computational ideas and run programs.

Each of these languages is good for the purposes it was designed for and less good for other purposes. But they are often complementary, and one of the goals of this book is to show how they can be used together.

4.6 Analysis with WolframAlpha

Until recently, most analysis was done by rubbing graphite on wood pulp[3], a process that is laborious and error-prone. A useful alternative is symbolic computation. If you have used services like WolframAlpha, you have used symbolic computation.

For example, if you go to https://www.wolframalpha.com/ and type

```
df(t) / dt = alpha f(t)
```

WolframAlpha infers that `f(t)` is a function of `t` and `alpha` is a parameter; it classifies the query as a "first-order linear ordinary differential equation", and reports the general solution:

$$f(t) = c_1 \exp(\alpha t)$$

If you add a second equation to specify the initial condition:

```
df(t) / dt = alpha f(t),  f(0) = p0
```

WolframAlpha reports the particular solution:

[2] I am not making this up; see http://modsimpy.com/plato.

[3] Or "rubbing the white rock on the black rock", a line I got from Woodie Flowers, who got it from Stephen Jacobsen.

$$f(t) = p_0 \exp(\alpha t)$$

WolframAlpha is based on Mathematica, a powerful programming language designed specifically for symbolic computation.

4.7 Analysis with SymPy

Python has a library called SymPy that provides symbolic computation tools similar to Mathematica. They are not as easy to use as WolframAlpha, but they have some other advantages.

Before we can use SymPy, we have to import it:

```
from sympy import *
```

SymPy defines many functions, and some of them conflict with functions defined in `modsim` and the other libraries we're using, I suggest that you do symbolic computation with SymPy in a separate notebook.

The code for this section and the next is in this notebook: http://modsimpy.com/sympy04.

SymPy defines a `Symbol` object that represents symbolic variable names, functions, and other mathematical entities. object

SymPy provides a function called `symbols` that takes a string and returns a `Symbol` object. So if we run this assignment:

```
t = symbols('t')
```

Python understands that `t` is a symbol, not a numerical value. If we now run

```
expr = t + 1
```

Python doesn't try to perform numerical addition; rather, it creates a new `Symbol` that represents the sum of `t` and `1`. We can evaluate the sum using `subs`, which substitutes a value for a symbol. This example substitutes 2 for `t`:

```
expr.subs(t, 2)
```

The result is 3. Functions in SymPy are represented by a special kind of `Symbol`:

```
f = Function('f')
```

Now if we write `f(t)`, we get an object that represents the evaluation of a function, f, at a value, t. But again SymPy doesn't actually try to evaluate it.

4.8 Differential equations in SymPy

SymPy provides a function, `diff`, that can differentiate a function. We can apply it to `f(t)` like this:

```
dfdt = diff(f(t), t)
```

The result is a `Symbol` that represents the derivative of `f` with respect to `t`. But again, SymPy doesn't try to compute the derivative yet.

To represent a differential equation, we use `Eq`:

```
alpha = symbols('alpha')
eq1 = Eq(dfdt, alpha*f(t))
```

The result is an object that represents an equation, which is displayed like this:

$$\frac{d}{dt} f(t) = \alpha f(t)$$

Now we can use `dsolve` to solve this differential equation:

```
solution_eq = dsolve(eq1)
```

The result is the equation

$$f(t) = C_1 \exp(\alpha t)$$

This is the **general solution**, which still contains an unspecified constant, C_1. To get the **particular solution** where $f(0) = p_0$, we substitute `p0` for `C1`. First, we have to create two more symbols:

```
C1, p0 = symbols('C1 p0')
```

Now we can perform the substitution:

```
particular = solution_eq.subs(C1, p0)
```

The result is

$$f(t) = p_0 \exp(\alpha t)$$

This function is called the **exponential growth curve**; see http://modsimpy.com/expo.

4.9 Solving the quadratic growth model

In the notebook for this chapter, you will see how to use the same tools to solve the quadratic growth model with parameters r and K. The general solution is

$$f(t) = \frac{K \exp(C_1 K + rt)}{\exp(C_1 K + rt) - 1}$$

To get the particular solution where $f(0) = p_0$, we evaluate the general solution at $t = 0$, which yields:

$$f(0) = \frac{K \exp(C_1 K)}{\exp(C_1 K) - 1}$$

Then we set this expression equal to p_0 and solve for C_1. The result is:

$$C_1 = \frac{1}{K} \log\left(-\frac{p_0}{K - p_0}\right)$$

Finally, we substitute this value of C_1 into the general solution, which yields:

$$f(t) = \frac{K p_0 \exp(rt)}{K + p_0 \exp(rt) - p_0}$$

This function is called the **logistic growth curve**; see http://modsimpy.com/logistic. In the context of growth models, the logistic function is often written, equivalently,

$$f(t) = \frac{K}{1 + A\exp(-rt)}$$

where $A = (K - p_0)/p_0$.

If you would like to see this differential equation solved by hand, you might like this video: http://modsimpy.com/khan2

4.10 Summary

The following tables summarize the results so far:

Growth type	Discrete (difference equation)
Constant	linear: $x_n = p_0 + \alpha n$
Proportional	geometric: $x_n = p_0(1 + \alpha)^n$

	Continuous (differential equation)
Constant	linear: $x(t) = p_0 + \alpha t$
Proportional	exponential: $x(t) = p_0 \exp(\alpha t)$
Quadratic	logistic: $x(t) = K/(1 + A\exp(-rt))$

What I've been calling the constant growth model is more commonly called "linear growth" because the solution is a line. Similarly, what I've called proportional is commonly called "exponential", and what I've called quadratic is commonly called "logistic".

I avoided the more common terms until now because I thought it would be strange to use them before we solved the equations and discovered the functional form of the solutions.

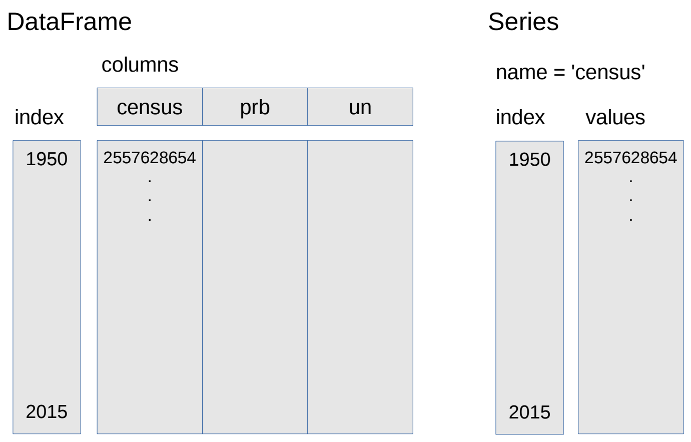


Figure 4.3: The elements that make up a `DataFrame` and a `Series`.

4.11 DataFrames and Series

So far we've been using `DataFrame` and `Series` objects without really understanding how they work. In this section we'll review what we know so far and get into a little more detail.

Each `DataFrame` contains three objects: `index` is a sequence of labels for the rows, `columns` is a sequence of labels for the columns, and `values` is an array that contains the data. Figure 4.3 shows these elements graphically.

A `Series` also contains `index` and `values`; it does not have `columns`, but it does contain `name`, which is a string.

To determine the type of these objects, we can use the Python function `type`:

```
type(table2)
type(table2.index)
type(table2.columns)
type(table2.values)
```

If `table2` is a `DataFrame`, the type of `table2.index` is `Int64Index`, which is a defined by Pandas. The type of `table2.columns` is `Index`. These `Index` objects are similar to `Series` objects.

The type of `table2.values` is `ndarray`, which is the primary array type provided by NumPy; the name indicates that the array can have an arbitrary number of dimensions (N-dimensional).

In a `Series`, the index is an `Index` object and the values are stores in an `ndarray`. Figure 4.3 shows theses elements graphically.

In the `modsim` library, the functions `get_first_label` and `get_last_label` provide a simple way to access the index of a `DataFrame` or `Series`:

```
def get_first_label(series):
    return series.index[0]

def get_last_label(series):
    return series.index[-1]
```

In brackets, the number `0` selects the first label; the number `-1` selects the last label.

Several of the objects defined in `modsim` are modified versions of `Series` objects. A `System` object is a `Series` where the labels are variables names; a `TimeSeries` object is a `Series` where the labels are times.

Defining these objects wasn't necessary; we could do all the same things using `Series` objects. But giving them different names makes the code easier to read and understand, and helps avoid certain kinds of errors (like getting two `Series` objects mixed up).

If you write simulations in Python in the future, you can continue using the objects in `modsim`, if you find them useful, or you can use Pandas objects directly.

4.12 One queue or two?

This section presents an exercise where you can apply what you've learned so far to a question related to **queueing theory** (the study of systems that involve waiting in lines, also known as "queues"). A solution to this exercise is in `queue_soln.ipynb` in the repository for this book.

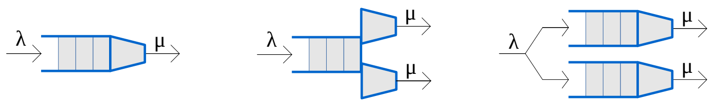


Figure 4.4: One queue, one server (left), one queue, two servers (middle), two queues, two servers (right).

Suppose you are designing the checkout area for a new store. You have enough room for two checkout counters and a waiting area for customers. You can make two lines, one for each counter, or one line that serves both counters.

In theory, you might expect a single line to be better, but it has some practical drawbacks: in order to maintain a single line, you would have to install rope barriers, and customers might be put off by what seems to be a longer line, even if it moves faster.

So you'd like to check whether the single line is really better and by how much. Simulation can help answer this question.

Figure 4.4 shows the three scenarios we'll consider. As we did in the bikeshare model, we'll assume that a customer is equally likely to arrive during any timestep. I'll denote this probability using the Greek letter lambda, λ, or the variable name `lam`. Since it's a new store, we don't know what the value of λ will be, so we'll have to consider a range of possibilities.

Based on data from other stores, you know that it takes 5 minutes for a customer to check out, on average. But checkout times are highly variable: most customers take less than 5 minutes, but some take substantially more. A simple way to model this variability is to assume that when a customer is checking out, they have the same probability of finishing up during each time step. I'll denote this probability using the Greek letter mu, μ, or the variable name `mu`.

If we choose $\mu = 1/5$, the average number of time steps for each checkout will be 5 minutes, which is consistent with the data.

Now we're ready to get started. I'll make some suggestions for how to proceed.

As always, you should practice incremental development: write no more than one or two lines of code a time, and test as you go!

1. Write a function called `make_system` that takes `lam` and `mu` as parameters and returns a `System` object with variables `lam`, `mu`, `x`, and `duration`. `x` is the number if customers in the system, including customers in line and at the checkout counters; `x` should be initialized to `0`. `duration` is the number of time steps to simulate; I set it to 8 hours, in minutes. Test this function by creating a `System` object with `lam=1/8` and `mu=1/5`.

2. Write a function called `run_simulation` that takes a `System` object and simulates the number of time steps specified by `duration`. Start by simulating a single queue with a single checkout counter, which I'll call a "server". During each time step, a customer can finish checking out (but only if there is a customer in the store), and a customer can arrive.

3. In `run_simulation`, add a few lines of code to create a `TimeSeries` and store the number of customers in the store, `x`, at the end of each time step. After the simulation runs, store the `TimeSeries` as a new system variable called `results`. Plot `results` and confirm that the simulation behaves as expected.

4. To compute the average number of customers in the store, L, you can write `system.results.mean()`. You can use the observed value of W to compute the average time customers spend in the store, W, which includes time in queue and time at the counter. L and W are related by Little's Law (see https://en.wikipedia.org/wiki/Little's_law):

$$L = \lambda W$$

Modify `run_simulation` to compute L and W and store them as system variables.

5. Use `linspace` to create an array of values for λ, from about 10% to 90% of μ. Write a function called `sweep_lam` that takes an array of values for λ and a single value for μ. It should call $run_simulation$ once for each value of λ; after each simulation, it should print λ and the resulting value of W. Then modify it to plot the results rather than printing them. Run `sweep_series` with 50 to 100 values of λ to get a sense of how much the results vary from one run to the next. What happens as λ gets close to μ?

6. Next, write a version of `run_simulation` that models the scenario with one queue and two servers. Hint: if there are at least two customers in the store, there are two chances for a customer to finish checking out. Test this version with a wider range of values for λ, maybe going up to 160% of μ.

7. You might want to split `run_simulation` into two parts: and `update_func` that takes a `System` object and simulates one time step, and a general version of `run_simulation` that takes `udpate_func` as a parameter.

8. Write a third version of `run_simulation`, or a third `update_func`, that models the scenario with two queues and two servers. You might have to add system variables, `q1` and `q2`, to keep track of the number of customers in each queue. When a customer arrives, they should join whichever line is shorter.

9. Which system yields shorter wait times, one queue or two? Since the results of a single simulation are so variable, it might not be easy to tell. One option is to run the simulation 50 to 100 times, with a range of values for λ, to model days with different numbers of customers, and compute the average of the daily averages.

Chapter 5

Design

In the previous chapter, we developed a model of world population growth and used it to generate projections for the next 100 years. In this chapter, we develop a model of an epidemic as it spreads in a susceptible population, and use it to evaluate the effectiveness of possible interventions.

My presentation of the SIR model in this chapter, and the analysis in the next chapter, is based on an excellent article by David Smith and Lang Moore[1].

You can view the code for this chapter at `http://modsimpy.com/chap05`. For instructions on downloading and running the code, see Section 0.4.

5.1 The Freshman Plague

Every year at Olin College, about 90 new students come to campus from around the country and the world. Most of them arrive healthy and happy, but usually at least one brings with them some kind of infectious disease. A few weeks later, predictably, some fraction of the incoming class comes down with what we call "The Freshman Plague".

[1]Smith and Moore, "The SIR Model for Spread of Disease," Journal of Online Mathematics and its Applications, December 2001, at `http://modsimpy.com/sir`.

In this chapter we introduce a well-known model of infectious disease, the Kermack-McKendrick model, and use it to explain the progression of the disease over the course of the semester, predict the effect of possible interventions (like immunization) and design the most effective intervention campaign.

So far we have done our own modeling; that is, we've chosen physical systems, identified factors that seem important, and made decisions about how to represent them. In this chapter we start with an existing model and reverse-engineer it. Along the way, we consider the modeling decisions that went into it and identify its capabilities and limitations.

5.2 The SIR model

The Kermack-McKendrick model is a simple version of an **SIR model**, so-named because it considers three categories of people:

- **S**: People who are "susceptible", that is, capable of contracting the disease if they come into contact with someone who is infected.
- **I**: People who are "infectious", that is, capable of passing along the disease if they come into contact with someone susceptible.
- **R**: People who are "recovered".

In the basic version of the model, people who have recovered are considered to be immune to reinfection. That is a reasonable model for some diseases, but not for others, so it should be on the list of assumptions to reconsider later.

Let's think about how the number of people in each category changes over time. Suppose we know that people with the disease are infectious for a period of 4 days, on average. If 100 people are infectious at a particular point in time, and we ignore the particular time each one became infected, we expect about 1 out of 4 to recover on any particular day.

Putting that a different way, if the time between recoveries is 4 days, the recovery rate is about 0.25 recoveries per day, which we'll denote with the Greek letter gamma, γ. If the total number of people in the population is N, and the fraction currently infectious is i, the total number of recoveries we expect per day is $\gamma i N$.

Now let's think about the number of new infections. Suppose we know that each susceptible person comes into contact with 1 person every 3 days, on average, in such a way that they would contract the disease if the other person is infected. We'll denote this contact rate with the Greek letter beta, β.

It's probably not reasonable to assume that we know β ahead of time, but later we'll see how to estimate it based on data from previous outbreaks.

If s is the fraction of the population that's susceptible, sN is the number of susceptible people, βsN is the number of contacts per day, and βsiN is the number of those contacts where the other person is infectious.

In summary:

- The number of recoveries we expect per day is γiN; dividing by N yields the fraction of the population that recovers in a day, which is γi.
- The number of new infections we expect per day is βsiN; dividing by N yields the fraction of the population that gets infected in a day, which is βsi.

This model assumes that the population is closed; that is, no one arrives or departs, so the size of the population, N, is constant.

5.3 The SIR equations

If we treat time as a continuous quantity, we can write differential equations that describe the rates of change for s, i, and r (where r is the fraction of the population that has recovered):

$$\begin{aligned}\frac{ds}{dt} &= -\beta si\\ \frac{di}{dt} &= \beta si - \gamma i\\ \frac{dr}{dt} &= \gamma i\end{aligned}$$

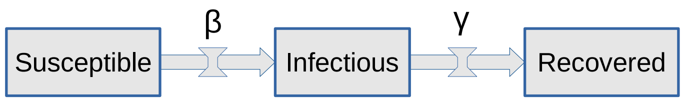


Figure 5.1: Stock and flow diagram for an SIR model.

To avoid cluttering the equations, I leave it implied that s is a function of time, $s(t)$, and likewise for i and r.

SIR models are examples of **compartment models**, so-called because they divide the world into discrete categories, or compartments, and describe transitions from one compartment to another. Compartments are also called **stocks** and transitions between them are called **flows**.

In this example, there are three stocks — susceptible, infectious, and recovered — and two flows — new infections and recoveries. Compartment models are often represented visually using stock-and-flow diagrams (see `http://modsimpy.com/stock`. Figure 5.1 shows the stock and flow diagram for an SIR model.

Stocks are represented by rectangles, flows by arrows. The widget in the middle of the arrows represents a valve that controls the rate of flow; the diagram shows the parameters that control the valves.

5.4 Implementation

For a given physical system, there are many possible models, and for a given model, there are many ways to represent it. For example, we can represent an SIR model as a stock-and-flow diagram, as a set of differential equations, or as a Python program. The process of representing a model in these forms is called **implementation**. In this section, we implement the SIR model in Python.

To get started, I'll represent the initial state of the system using a `State` object, which is defined in the `modsim` library. A `State` object is a collection of **state**

variables; each state variable represents information about the system that changes over time. In this example, the state variables are `S`, `I`, and `R`; they represent the fraction of the population in each compartment.

Creating a `State` object is similar to creating a `System` object. We can initialize the `State` object with the *number* of people in each compartment:

```
init = State(S=89, I=1, R=0)
```

And then convert the numbers to fractions by dividing by the total:

```
init /= sum(init)
```

For now, let's assume we know the time between contacts and time between recoveries:

```
tc = 3              # time between contacts in days
tr = 4              # recovery time in days
```

In that case we can compute the parameters of the model:

```
beta = 1 / tc       # contact rate in per day
gamma = 1 / tr      # recovery rate in per day
```

Now we need a `System` object to store the parameters and initial conditions. The following function takes the system parameters as function parameters and returns a new `System` object:

```
def make_system(beta, gamma):
    init = State(S=89, I=1, R=0)
    init /= sum(init)

    t0 = 0
    t_end = 7 * 14

    return System(init=init, t0=t0, t_end=t_end,
                  beta=beta, gamma=gamma)
```

The default value for `t_end` is 14 weeks, about the length of a semester.

5.5 The update function

At any point in time, the state of the system is represented by a `State` object with three variables, `S`, `I` and `R`. Next we'll define an update function that takes the `State` object as a parameter, along with the `System` object that contains the parameters, and computes the state of the system during the next time step:

```
def update1(state, system):
    s, i, r = state

    infected = system.beta * i * s
    recovered = system.gamma * i

    s -= infected
    i += infected - recovered
    r += recovered

    return State(S=s, I=i, R=r)
```

The first line uses a feature we have not seen before, **multiple assignment**. The value on the right side is a `State` object that contains three values. The left side is a sequence of three variable names. The assignment does just what we want: it assigns the three values from the `State` object to the three variables, in order.

The update function computes `infected` and `recovered` as a fraction of the population, then updates `s`, `i` and `r`. The return value is a `State` that contains the updated values.

When we call `update1` like this:

```
state = update1(init, sir)
```

The result is a `State` object with these values:

	value
S	0.985388
I	0.011865
R	0.002747

5.6 Running the simulation

Now we can simulate the model over a sequence of time steps:

```
def run_simulation(system, update_func):
    state = system.init

    for t in linrange(system.t0, system.t_end-1):
        state = update_func(state, system)

    return state
```

The parameters of `run_simulation` are the `System` object and the update function. The `System` object contains the parameters, initial conditions, and values of `t0` and `t_end`.

The outline of this function should look familiar; it is similar to the function we used for the population model in Section 3.5.

We can call `run_simulation` like this:

```
system = make_system(beta, gamma)
run_simulation(system, update1)
```

The result is the final state of the system:

	value
S	0.520819
I	0.000676
R	0.478505

This result indicates that after 14 weeks (98 days), about 52% of the population is still susceptible, which means they were never infected, less than 1% are actively infected, and 48% have recovered, which means they were infected at some point.

5.7 Collecting the results

The previous version of `run_simulation` only returns the final state, but we might want to see how the state changes over time. We'll consider two ways to do that: first, using three `TimeSeries` objects, then using a new object called a `TimeFrame`.

Here's the first version:

```
def run_simulation(system, update_func):
    S = TimeSeries()
    I = TimeSeries()
    R = TimeSeries()

    state = system.init
    t0 = system.t0
    S[t0], I[t0], R[t0] = state

    for t in linrange(system.t0, system.t_end-1):
        state = update_func(state, system)
        S[t+1], I[t+1], R[t+1] = state

    system.S = S
    system.I = I
    system.R = R
```

First, we create `TimeSeries` objects to store the results. Notice that the variables `S`, `I`, and `R` are `TimeSeries` objects now.

Next we initialize `state`, `t0`, and the first elements of `S`, `I` and `R`.

Inside the loop, we use `update_func` to compute the state of the system at the next time step, then use multiple assignment to unpack the elements of `state`, assigning each to the corresponding `TimeSeries`.

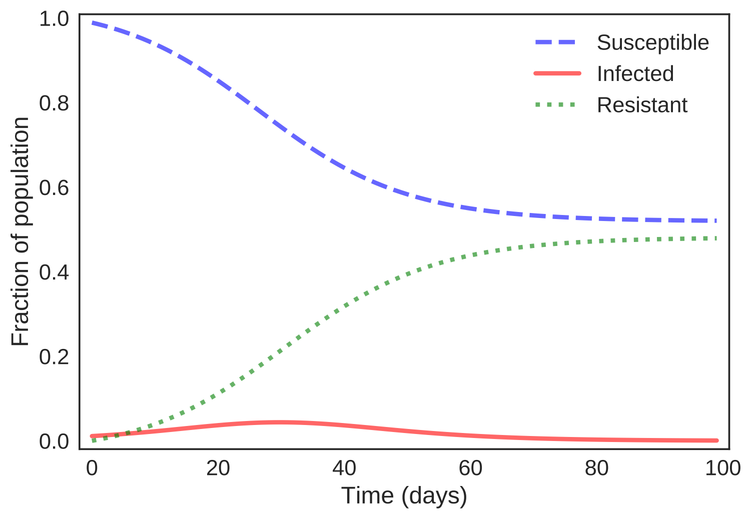


Figure 5.2: Time series for `S`, `I`, and `R` over the course of 98 days.

At the end of the function, we store `S`, `I`, and `R` as system variables.

Now we can run the function like this:

```
system = make_system(beta, gamma)
run_simulation(system, update1)
```

We'll use the following function to plot the results:

```
def plot_results(S, I, R):
    plot(S, '--', color='blue', label='Susceptible')
    plot(I, '-', color='red', label='Infected')
    plot(R, ':', color='green', label='Resistant')
    decorate(xlabel='Time (days)',
             ylabel='Fraction of population')
```

And run it like this:

```
plot_results(system.S, system.I, system.R)
```

Figure 5.2 shows the result. Notice that it takes about three weeks (21 days) for the outbreak to get going, and about six weeks (42 days) before it peaks.

The fraction of the population that's infected is never very high, but it adds up. In total, almost half the population gets sick.

5.8 Now with a TimeFrame

If the number of state variables is small, storing them as separate `TimeSeries` objects might not be so bad. But a better alternative is to use a `TimeFrame`, which is another object are defined in the `modsim` library.

A `TimeFrame` is almost identical to a `DataFrame`, which we used in Section 3.1, with just a few changes I made to adapt it for our purposes. For more details, you can read the `modsim` library source code.

Here's a more concise version of `run_simulation` using a `TimeFrame`:

```
def run_simulation(system, update_func):
    frame = TimeFrame(columns=system.init.index)
    frame.loc[system.t0] = system.init

    for t in linrange(system.t0, system.t_end-1):
        frame.loc[t+1] = update_func(frame.loc[t], system)

    system.results = frame
```

The first line creates an empty `TimeFrame` with one column for each state variable. Then, before the loop starts, we store the initial conditions in the `TimeFrame` at `t0`. Based on the way we've been using `TimeSeries` objects, it is tempting to write:

```
frame[system.t0] = system.init
```

But when you use the bracket operator with a `TimeFrame` or `DataFrame`, it selects a column, not a row. For example, to select a column, we could write:

```
frame['S']
```

To select a row, we have to use `loc`, which stands for "location". `frame.loc[0]` reads a row from a `TimeFrame` and

```
frame.loc[system.t0] = system.init
```

assigns the values from `system.init` to the first row of `df`. Since the value on the right side is a `State`, the assignment matches up the index of the `State` with the columns of the `TimeFrame`; it assigns the `S` value from `system.init` to the `S` column of the `TimeFrame`, and likewise with `I` and `R`.

We can use the same feature to write the loop more concisely, assigning the `State` we get from `update_func` directly to the next row of `df`.

Finally, we store `frame` as a new system variable. We can call this version of `run_simulation` like this:

```
run_simulation(system, update1)
```

And plot the results like this:

```
frame = system.results
plot_results(frame.S, frame.I, frame.R)
```

As with a `DataFrame`, we can use the dot operator to select columns from a `TimeFrame`.

5.9 Metrics

When we plot a time series, we get a view of everything that happened when the model ran, but often we want to boil it down to a few numbers that summarize the outcome. These summary statistics are called **metrics**.

In the SIR model, we might want to know the time until the peak of the outbreak, the number of people who are sick at the peak, the number of students who will still be sick at the end of the semester, or the total number of students who get sick at any point.

As an example, I will focus on the last one — the total number of sick students — and we will consider interventions intended to minimize it.

When a person gets infected, they move from S to I, so we can get the total number of infections by computing the difference in S at the beginning and the end:

```
def calc_total_infected(system):
    frame = system.results
    return frame.S[system.t0] - frame.S[system.t_end]
```

In the notebook that accompanies this chapter, you will have a chance to write functions that compute other metrics. Two functions you might find useful are `max` and `idxmax`.

If you have a `Series` called `S`, you can compute the largest value of the series like this:

```
largest_value = S.max()
```

And the label of the largest value like this:

```
time_of_largest_value = S.idxmax()
```

If the `Series` is a `TimeSeries`, the label you get from `idxmax` is a time or date. You can read more about these functions in the `Series` documentation at http://modsimpy.com/series.

5.10 Immunization

Models like this are useful for testing "what if?" scenarios. As an example, we'll consider the effect of immunization.

Suppose there is a vaccine that causes a patient to become immune to the Freshman Plague without being infected. How might you modify the model to capture this effect?

One option is to treat immunization as a short cut from susceptible to recovered without going through infectious. We can implement this feature like this:

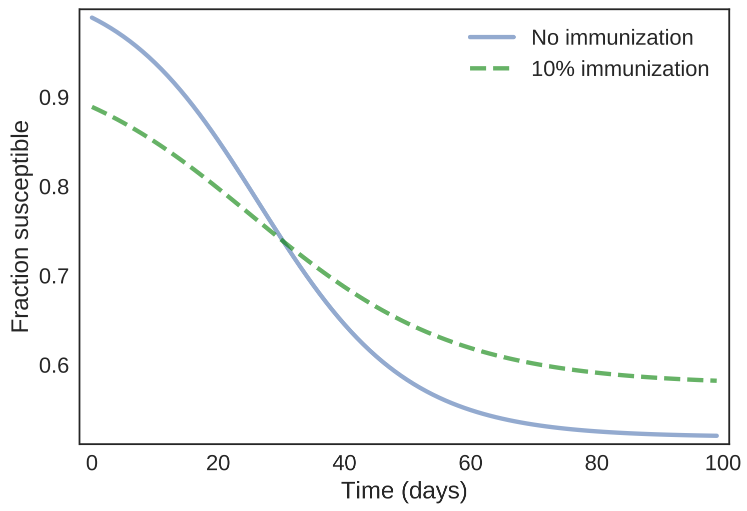


Figure 5.3: Time series for `S`, with and without immunization.

```python
def add_immunization(system, fraction):
    system.init.S -= fraction
    system.init.R += fraction
```

`add_immunization` moves the given fraction of the population from `S` to `R`. If we assume that 10% of students are vaccinated at the beginning of the semester, and the vaccine is 100% effective, we can simulate the effect like this:

```python
system2 = make_system(beta, gamma)
add_immunization(system2, 0.1)
run_simulation(system2, update1)
```

For comparison, we can run the same model without immunization and plot the results. Figure 5.3 shows the results, plotting `S` as a function of time, with and without immunization.

Without immunization, almost 47% of the population gets infected at some point. With 10% immunization, only 31% gets infected. That's pretty good.

So let's see what happens if we administer more vaccines. This following function sweeps a range of immunization rates:

```
def sweep_immunity(immunize_array):
    sweep = SweepSeries()

    for fraction in immunize_array:
        sir = make_system(beta, gamma)
        add_immunization(sir, fraction)
        run_simulation(sir, update1)
        sweep[fraction] = calc_total_infected(sir)

    return sweep
```

The parameter of `sweep_immunity` is an array of immunization rates. The result is a `SweepSeries` object, which is defined in the `modsim` library. `SweepSeries` is similar to `TimeSeries`; the difference is that the index of a `SweepSeries` contains parameter values, not times.

Figure 5.4 shows a plot of the `SweepSeries`. Notice that the x-axis is the immunization rate, not time.

As the immunization rate increases, the number of infections drops steeply. If 40% of the students are immunized, fewer than 4% get sick. That's because immunization has two effects: it protects the people who get immunized, of course, but it also protects the rest of the population.

Reducing the number of "susceptibles" and increasing the number of "resistants" makes it harder for the disease to spread, because some fraction of contacts are wasted on people who cannot be infected. This phenomenon is called **herd immunity**, and it is an important element of public health (see http://modsimpy.com/herd).

The steepness of the curve in Figure 5.4 is a blessing and a curse. It's a blessing because it means we don't have to immunize everyone, and vaccines can protect the "herd" even if they are not 100% effective.

But it's a curse because a small decrease in immunization can cause a big increase in infections. In this example, if we drop from 80% immunization to 60%, that might not be too bad. But if we drop from 40% to 20%, that would trigger a major outbreak, affecting more than 15% of the population. For a serious disease like measles, just to name one, that would be a public health catastrophe.

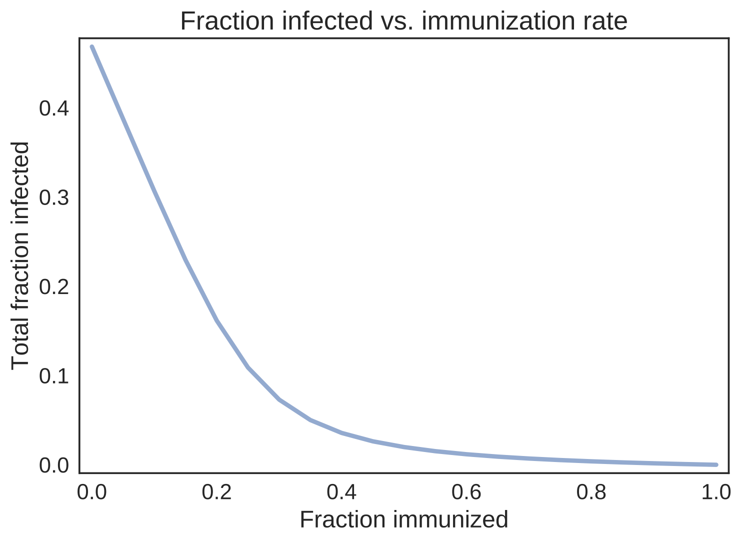


Figure 5.4: Fraction of the population infected as a function of immunization rate.

One use of models like this is to demonstrate phenomena like herd immunity and to predict the effect of interventions like vaccination. Another use is to evaluate alternatives and guide decision making. We'll see an example in the next section.

5.11 Hand washing

Suppose you are the Dean of Student Affairs, and you have a budget of just \$1200 to combat the Freshman Plague. You have two options for spending this money:

1. You can pay for vaccinations, at a rate of \$100 per dose.
2. You can spend money on a campaign to remind students to wash hands frequently.

We have already seen how we can model the effect of vaccination. Now let's think about the hand-washing campaign. We'll have to answer two questions:

1. How should we incorporate the effect of hand washing in the model?
2. How should we quantify the effect of the money we spend on a hand-washing campaign?

For the sake of simplicity, let's assume that we have data from a similar campaign at another school showing that a well-funded campaign can change student behavior enough to reduce the infection rate by 20%.

In terms of the model, hand washing has the effect of reducing `beta`. That's not the only way we could incorporate the effect, but it seems reasonable and it's easy to implement.

Now we have to model the relationship between the money we spend and the effectiveness of the campaign. Again, let's suppose we have data from another school that suggests:

- If we spend $500 on posters, materials, and staff time, we can change student behavior in a way that decreases the effective value of `beta` by 10%.
- If we spend $1000, the total decrease in `beta` is almost 20%.
- Above $1000, additional spending has little additional benefit.

In the notebook for this chapter you will see how I used a logistic curve to fit this data. The result is the following function, which takes spending as a parameter and returns `factor`, which is the factor by which `beta` is reduced:

```python
def compute_factor(spending):
    return logistic(spending, M=500, K=0.2, B=0.01)
```

We use `compute_factor` to write `add_hand_washing`, which takes a `System` object and a budget, and modifies `system.beta` to model the effect of hand washing:

```python
def add_hand_washing(system, spending):
    factor = compute_factor(spending)
    system.beta *= (1 - factor)
```

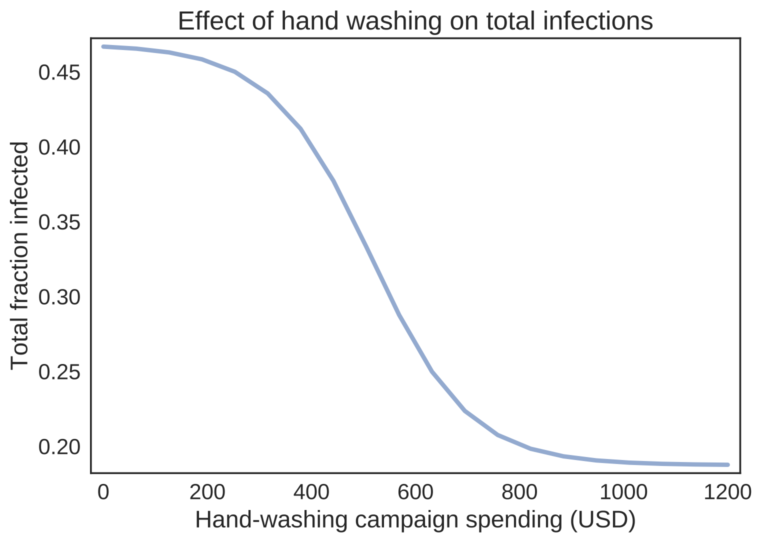


Figure 5.5: Fraction of the population infected as a function of hand-washing campaign spending.

Now we can sweep a range of values for `spending` and use the simulation to compute the effect:

```python
def sweep_hand_washing(spending_array):
    sweep = SweepSeries()

    for spending in spending_array:
        sir = make_system(beta, gamma)
        add_hand_washing(sir, spending)
        run_simulation(sir, update1)
        sweep[spending] = calc_total_infected(sir)

    return sweep
```

Here's how we run it:

```python
spending_array = linspace(0, 1200, 20)
infected_sweep = sweep_hand_washing(spending_array)
```

Figure 5.5 shows the result. Below $200, the campaign has little effect. At $800 it has a substantial effect, reducing total infections from 46% to 20%. Above $800, the additional benefit is small.

5.12 Optimization

Let's put it all together. With a fixed budget of $1200, we have to decide how many doses of vaccine to buy and how much to spend on the hand-washing campaign.

Here are the parameters:

```
num_students = 90
budget = 1200
price_per_dose = 100
max_doses = int(budget / price_per_dose)
```

We'll sweep the range of possible doses:

```
dose_array = linrange(max_doses)
```

And run the simulation for each element of `dose_array`:

```
def sweep_doses(dose_array):
    sweep = SweepSeries()

    for doses in dose_array:
        fraction = doses / num_students
        spending = budget - doses * price_per_dose

        sir = make_system(beta, gamma)
        add_immunization(sir, fraction)
        add_hand_washing(sir, spending)

        run_simulation(sir, update1)
        sweep[doses] = calc_total_infected(sir)

    return sweep
```

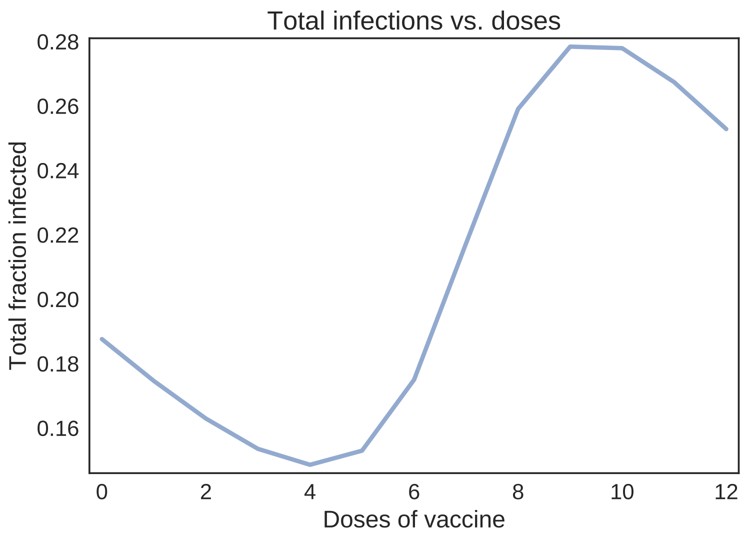


Figure 5.6: Fraction of the population infected as a function of the number of doses.

For each number of doses, we compute the fraction of students we can immunize, `fraction` and the remaining budget we can spend on the campaign, `spending`. Then we run the simulation with those quantities and store the number of infections.

Figure 5.6 shows the result. If we buy no doses of vaccine and spend the entire budget on the campaign, the fraction infected is around 19%. At 4 doses, we have $800 left for the campaign, and this is the optimal point that minimizes the number of students who get sick.

As we increase the number of doses, we have to cut campaign spending, which turns out to make things worse. But interestingly, when we get above 10 doses, the effect of herd immunity starts to kick in, and the number of sick students goes down again.

In the notebook for this chapter, you'll have a chance to run this optimization for a few other scenarios.

5.13 Under the hood

This chapter introduces three new objects, `State`, `TimeFrame`, and `SweepSeries`.

A `State` object is similar to a `System` object. The difference is that the variables in a `State` object change over time; the variables in a `System` object are parameters that usually don't change. At least, they usually don't change during a simulation — they often vary from one simulation to the next.

In previous chapters, we used `System` objects to store both state variables and parameters. Now we are using `State` objects to partition values that play different roles.

A `TimeFrame` is a version of a Pandas `DataFrame`; to be honest, the biggest difference in the name, which is intended as a reminder that the index contains a sequence of times. Usually each row in a `TimeFrame` corresponds to a time step in a simulation, and the columns correspond to the state variables.

Finally, a `SweepSeries` is a version of a Pandas `Series` where

- The index contains a range of values for a system parameter,
- And the values contain metrics that summarize the results of a simulation.

In the next chapter, we'll see a two-dimensional version of a `SweepSeries`, called a `SweepFrame`, where the index contains one parameter, the columns contain a second parameter, and the values contain metrics.

Chapter 6

Analysis

In the previous chapter I presented an SIR model of infectious disease, specifically the Kermack-McKendrick model. We extended the model to include vaccination and the effect of a hand-washing campaign, and used the extended model to allocate a limited budget optimally, that is, to minimize the number of infections.

But we assumed that the parameters of the model, contact rate and recovery rate, were known. In this chapter, we explore the behavior of the model as we vary these parameters, use analysis to understand these relationships better, and propose a method for using data to estimate parameters.

You can view the code for this chapter at `http://modsimpy.com/chap06`. For instructions on downloading and running the code, see Section 0.4.

6.1 Unpack

Before we analyze the SIR model, I want to make a few improvements to the code. In the previous chapter, we used this version of `run_simulation`:

```
def run_simulation(system, update_func):
    frame = DataFrame(columns=system.init.index)
    frame.loc[system.t0] = system.init

    for i in linrange(system.t0, system.t_end):
        frame.loc[i+1] = update_func(frame.loc[i], system)

    system.results = frame
```

Because we read so many variables from `system`, this code is a bit cluttered. We can clean it up using `unpack`, which is defined in the `modsim` library. `unpack` takes a `System` object as a parameter and makes the system variables available without using the dot operator. So we can rewrite `run_simulation` like this:

```
def run_simulation(system, update_func):
    unpack(system)

    frame = TimeFrame(columns=init.index)
    frame.loc[t0] = init

    for i in linrange(t0, t_end):
        frame.loc[i+1] = update_func(frame.loc[i], system)

    system.results = frame
```

The variables you unpack should be treated as read-only. Modifying them is not an error, but it might not have the behavior you expect. In the notebook for this chapter, you can use `unpack` to clean up `update1`.

6.2 Sweeping beta

Recall that β is the contact rate, which captures both the frequency of interaction between people and the fraction of those interactions that result in a new infection. If N is the size of the population and s is the fraction that's susceptible, sN is the number of susceptibles, βsN is the number of contacts per day between susceptibles and other people, and βsiN is the number of those contacts where the other person is infectious.

As β increases, we expect the total number of infections to increase. To quantify that relationship, I'll create a range of values for β:

```
beta_array = linspace(0.1, 0.9, 11)
```

Then run the simulation for each value and print the results.

```
for beta in beta_array:
    sir = make_system(beta, gamma)
    run_simulation(sir, update1)
    print(sir.beta, calc_total_infected(sir))
```

We can wrap that code in a function and store the results in a `SweepSeries` object:

```
def sweep_beta(beta_array, gamma):
    sweep = SweepSeries()
    for beta in beta_array:
        system = make_system(beta, gamma)
        run_simulation(system, update1)
        sweep[system.beta] = calc_total_infected(system)
    return sweep
```

Now we can run `sweep_beta` like this:

```
infected_sweep = sweep_beta(beta_array, gamma)
```

And plot the results:

```
label = 'gamma = ' + str(gamma)
plot(infected_sweep, label=label)
```

The first line uses string operations to assemble a label for the plotted line:

- When the `+` operator is applied to strings, it joins them end-to-end, which is called **concatenation**.

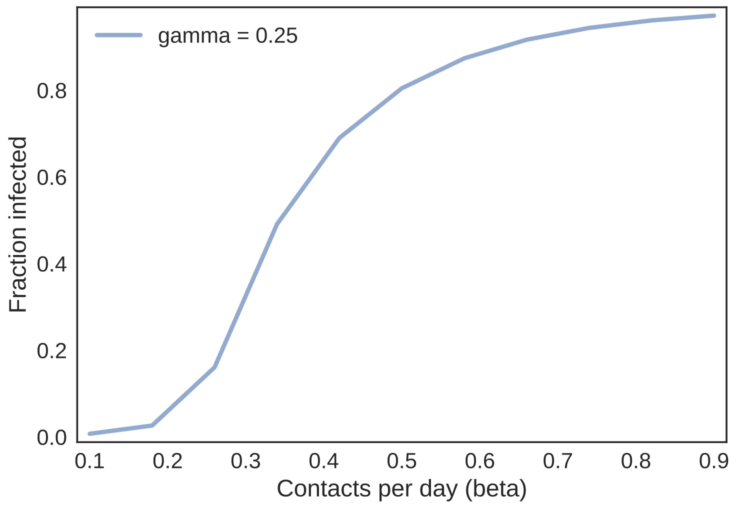


Figure 6.1: Total number of infected students as a function of the parameter `beta`, with `gamma = 0.25`.

- The function `str` converts any type of object to a String representation. In this case, `gamma` is a number, so we have to convert it to a string before trying to concatenate it.

If the value of `gamma` is `0.25`, the value of `label` is the string `'gamma = 0.25'`.

Figure 6.1 shows the results. Remember that this figure is a parameter sweep, not a time series, so the x-axis is the parameter `beta`, not time.

When `beta` is small, the contact rate is low and the outbreak never really takes off; the total number of infected students is near zero. As `beta` increases, it reaches a threshold near 0.3 where the fraction of infected students increases quickly. When `beta` exceeds 0.5, more than 80% of the population gets sick.

6.3 Sweeping gamma

Now let's see what that looks like for a few different values of `gamma`. Again, we'll use `linspace` to make an array of values:

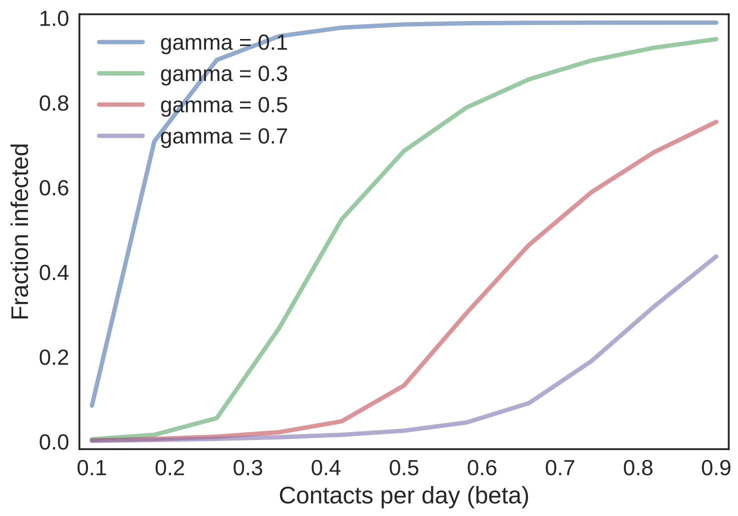


Figure 6.2: Total number of infected students as a function of the parameter `beta`, for several values of `gamma`.

```
gamma_array = linspace(0.1, 0.7, 4)
```

And run `sweep_beta` for each value of `gamma`:

```
for gamma in gamma_array:
    infected_sweep = sweep_beta(beta_array, gamma)
    label = 'gamma = ' + str(gamma)
    plot(infected_sweep, label=label)
```

Figure 6.2 shows the results. When `gamma` is low, the recovery rate is low, which means people are infectious longer. In that case, even low a contact rate (`beta`) results in an epidemic.

When `gamma` is high, `beta` has to be even higher to get things going. That observation suggests that there might be a relationship between `gamma` and `beta` that determines the outcome of the model. In fact, there is. I will demonstrate it first by running simulations, then derive it by analysis.

6.4 Nondimensionalization

Before we go on, let's wrap the code from the previous section in a function:

```
def sweep_parameters(beta_array, gamma_array):
    frame = SweepFrame(columns=gamma_array)
    for gamma in gamma_array:
        frame[gamma] = sweep_beta(beta_array, gamma)
    return frame
```

`sweep_parameters` takes as parameters two arrays: a range of values for `beta` and a range of values for `gamma`.

It creates a `SweepFrame` to store the results, with one column for each value of `gamma` and one row for each value of `beta`. A `SweepFrame` is a kind of `DataFrame`, defined in the `modsim` library. Its purpose is to store results from a two-dimensional parameter sweep.

Each time through the loop, we run `sweep_beta`. The result is a `SweepSeries` object with one element for each value of `gamma`. The assignment

```
frame[gamma] = sweep_beta(beta_array, gamma)
```

stores the values from the `SweepSeries` object as a new column in the `SweepFrame`, corresponding to the current value of `gamma`.

At the end, the `SweepFrame` stores the fraction of students infected for each pair of parameters, `beta` and `gamma`.

We can run `sweep_parameters` like this:

```
frame = sweep_parameters(beta_array, gamma_array)
```

Then we can loop through the results like this:

```
for gamma in frame.columns:
    series = frame[gamma]
    for beta in series.index:
        frac_infected = series[beta]
        print(beta, gamma, frac_infected)
```

This is the first example we've seen with one `for` loop inside another:

- Each time the outer loop runs, it selects a value of `gamma` from the columns of the `DataFrame` and extracts the corresponding column as a `Series`.
- Each time the inner loop runs, it selects a value of `beta` from the `Series` and selects the corresponding element, which is the fraction of student infected.

In this example, `frame` has 4 columns, one for each value of `gamma`, and 11 rows, one for each value of `beta`. So these loops print 44 lines, one for each pair of parameters.

Now let's think about possible relationships between `beta` and `gamma`:

- When `beta` exceeds `gamma`, that means there are more contacts (that is, potential infections) than recoveries. The difference between `beta` and `gamma` might be called the "excess contact rate", in units of contacts per day.
- As an alternative, we might consider the ratio `beta/gamma`, which is the number of contacts per recovery. Because the numerator and denominator are in the same units, this ratio is **dimensionless**, which means it has no units.

Describing physical systems using dimensionless parameters is often a useful move in the modeling and simulation game. It is so useful, in fact, that it has a name: **nondimensionalization** (see `http://modsimpy.com/nondim`).

So we'll try the second option first. In the notebook for this chapter, you can explore the first option as an exercise.

The following function wraps the previous loops and plots the fraction infected as a function of the ratio `beta/gamma`:

```python
def plot_sweep_frame(frame):
    for gamma in frame.columns:
        series = frame[gamma]
        for beta in series.index:
            frac_infected = series[beta]
            plot(beta/gamma, frac_infected, 'ro')
```

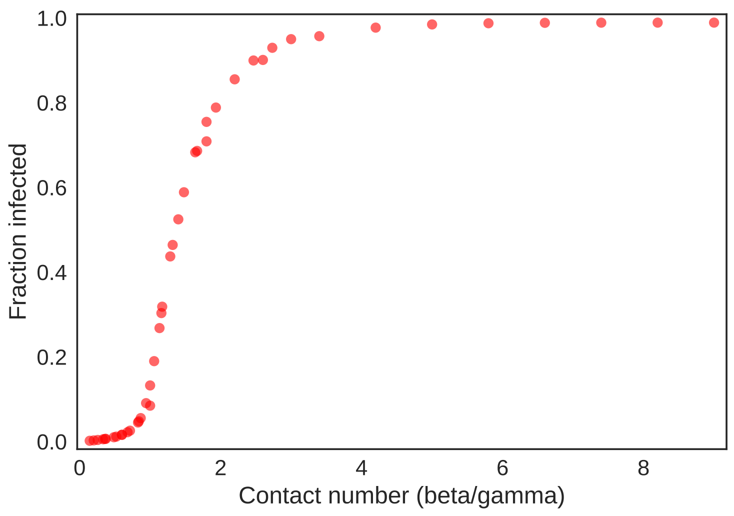


Figure 6.3: Total fraction infected as a function of contact number.

Figure 6.3 shows that the results fall neatly on a single curve, at least approximately. That means that we can predict the fraction of students who will be infected based on a single parameter, the ratio `beta/gamma`. We don't need to know the values of `beta` and `gamma` separately.

6.5 Contact number

Recall that the number of new infections in a given day is βsiN, and the number of recoveries is γiN. If we divide these quantities, the result is $\beta s/\gamma$, which is the number of new infections per recovery (as a fraction of the population).

When a new disease is introduced to a susceptible population, s is approximately 1, so the number of people infected by each sick person is β/γ. This ratio is called the "contact number" or "basic reproduction number" (see `http://modsimpy.com/contact`). By convention it is usually denoted R_0, but in the context of an SIR model, this notation is confusing, so we'll use c instead.

The results in the previous section suggest that there is a relationship between c and the total number of infections. We can derive this relationship by analyzing the differential equations from Section 5.3:

$$\begin{aligned}\frac{ds}{dt} &= -\beta s i \\ \frac{di}{dt} &= \beta s i - \gamma i \\ \frac{dr}{dt} &= \gamma i\end{aligned}$$

In the same way we divided the contact rate by the infection rate to get the dimensionless quantity c, now we'll divide di/dt by ds/dt to get a ratio of rates:

$$\frac{di}{ds} = -1 + \frac{1}{cs}$$

Dividing one differential equation by another is not an obvious move, but in this case it is useful because it gives us a relationship between i, s and c that does not depend on time. We can multiply both sides of the equation by ds:

$$di = \left(-1 + \frac{1}{cs}\right) ds$$

And then integrate both sides:

$$i = -s + \frac{1}{c} \log s + q$$

where q is a constant of integration. Rearranging terms yields:

$$q = i + s - \frac{1}{c} \log s$$

Now let's see if we can figure out what q is. At the beginning of an epidemic, if the fraction infected is small and nearly everyone is susceptible, we can use the approximations $i(0) = 0$ and $s(0) = 1$ to compute q:

$$q = 0 + 1 + \frac{1}{c} \log 1$$

Since $\log 1 = 0$, we get $q = 1$.

Now, at the end of the epidemic, let's assume that $i(\infty) = 0$ and $s(\infty)$ is an unknown quantity s_∞. Now we have:

$$q = 1 = 0 + s_\infty - \frac{1}{c} \log s_\infty$$

Solving for c, we get

$$c = \frac{\log s_\infty}{s_\infty - 1}$$

If we create a range of values for s_∞

```
s_inf_array = linspace(0.0001, 0.9999, 31)
```

we can compute the corresponding values of c:

```
c_array = log(s_inf_array) / (s_inf_array - 1)
```

To get the total infected, we compute the difference between $s(0)$ and $s(\infty)$, then store the results in a `Series`:

```
frac_infected = 1 - s_inf_array
frac_infected_series = Series(frac_infected, index=c_array)
```

Recall from Section **??** that a `Series` object contains an index and a corresponding sequence of values. In this case, the index is `c_array` and the values are from `frac_infected`.

6.6 Analysis and simulation

Now we can plot the results:

```
plot(frac_infected_series)
```

Figure 6.4 compares the analytic results from this section with the simulation results from Section 6.4. Over most of the range they are consistent with each other, with one discrepancy: when the contact number is less than 1, analysis indicates there should be no infections; but in the simulations a small part of the population is affected even when $c < 1$.

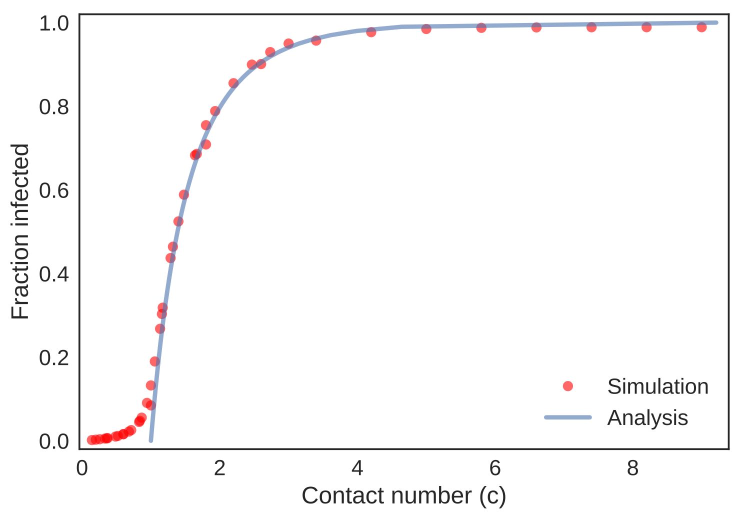


Figure 6.4: Total fraction infected as a function of contact number, showing results from simulation and analysis.

The reason for the discrepancy is that the simulation divides time into a discrete series of days, whereas the analysis treats time as a continuous quantity. In other words, the two methods are actually based on different models. So which model is better?

Probably neither. When the contact number is small, the early progress of the epidemic depends on details of the scenario. If we are lucky, the original infected person, "patient zero", infects no one and there is no epidemic. If we are unlucky, patient zero might have a large number of close friends, or might work in the dining hall (and fail to observe safe food handling procedures).

For contact numbers near or less than 1, we might need a more detailed model. But for higher contact numbers the SIR model might be good enough.

Figure 6.4 shows that if we know the contact number, we can compute the fraction infected. But we can also read the figure the other way; that is, at the end of an epidemic, if we can estimate the fraction of the population that was ever infected, we can use it to estimate the contact number.

Well, at least in theory. In practice, it might not work very well, because of the shape of the curve. When the contact number is near 2, the curve is quite steep, which means that small changes in c yield big changes in the number of infections. If we observe that the total fraction infected is anywhere from 20% to 80%, we would conclude that c is near 2.

On the other hand, for larger contact numbers, nearly the entire population is infected, so the curve is quite flat. In that case we would not be able to estimate c precisely, because any value greater than 3 would yield effectively the same results. Fortunately, this is unlikely to happen in the real world; very few epidemics affect anything like 90% of the population.

In summary, the SIR model has limitations; nevertheless, it provides insight into the behavior of infectious disease, especially the phenomenon of herd resistance. As we saw in the previous chapter, if we know the parameters of the model, we can use it to evaluate possible interventions. And as we saw in this chapter, we might be able to use data from earlier outbreaks to estimate the parameters.

Chapter 7

Thermal systems

So far the systems we have studied have been physical, in the sense that they exist in the world, but they have not been physics, in the sense of what physics classes are usually about. In this chapter, we'll do some physics, starting with **thermal systems**, that is, systems where the temperature of objects changes as heat transfers from one to another.

You can view the code for this chapter at http://modsimpy.com/chap07. For instructions on downloading and running the code, see Section 0.4.

7.1 The coffee cooling problem

The coffee cooling problem was discussed by Jearl Walker in *Scientific American* in 1977[1]; since then it has become a standard example of modeling and simulation.

Here is my version of the problem:

> Suppose I stop on the way to work to pick up a cup of coffee, which I take with milk. Assuming that I want the coffee to be as hot as possible when I arrive at work, should I add the milk at the coffee shop, wait until I get to work, or add the milk at some point in between?

[1]Walker, "The Amateur Scientist", *Scientific American*, Volume 237, Issue 5, November 1977.

To help answer this question, I made a trial run with the milk and coffee in separate containers and took some measurements:

- When served, the temperature of the coffee is 90 °C. The volume is 300 mL.
- The milk is at an initial temperature of 5 °C, and I take about 50 mL.
- The ambient temperature in my car is 22 °C.
- The coffee is served in a well insulated cup. When I arrive at work after 30 minutes, the temperature of the coffee has fallen to 70 °C.
- The milk container is not as well insulated. After 15 minutes, it warms up to 20 °C, nearly the ambient temperature.

To use this data and answer the question, we have to know something about temperature and heat, and we have to make some modeling decisions.

7.2 Temperature and heat

To understand how coffee cools (and milk warms), we need a model of temperature and heat. **Temperature** is a property of an object or a system; in SI units it is measured in degrees Celsius (°C). Temperature quantifies how hot or cold the object is, which is related to the average velocity of the particles that make up the object.

When particles in a hot object contact particles in a cold object, the hot object gets cooler and the cold object gets warmer, as energy is transferred from one to the other. The transferred energy is called **heat**; in SI units it is measured in joules (J).

Heat is related to temperature by the following equation (see http://modsimpy.com/thermass):

$$Q = C \Delta T$$

where Q is the amount of heat transferred to an object, ΔT is resulting change in temperature, and C is the **thermal mass** of the object, which quantifies how much energy it takes to heat or cool it. In SI units, thermal mass is measured in joules per degree Celsius (J/°C).

For objects made primarily from one material, thermal mass can be computed like this:

$$C = mc_p$$

where m is the mass of the object and c_p is the **specific heat capacity** of the material (see http://modsimpy.com/specheat).

We can use these equations to estimate the thermal mass of a cup of coffee. The specific heat capacity of coffee is probably close to that of water, which is 4.2 J/(g °C). Assuming that the density of coffee is close to that of water, which is 1 g/mL, the mass of 300 mL of coffee is 300 g, and the thermal mass is 1260 J/°C.

So when a cup of coffee cools from 90 °C to 70 °C, the change in temperature, ΔT is 20 °C, which means that 25 200 J of heat energy was transferred from the coffee to the surrounding environment (the cup holder and air in my car).

To give you a sense of how much energy that is, if you were able to harness all of that heat to do work (which you cannot[2]), you could use it to lift a cup of coffee from sea level to 8571 m, just shy of the height of Mount Everest, 8848 m.

Assuming that the cup has less mass than the coffee, and is made from a material with lower a specific heat, we can ignore the thermal mass of the cup.

7.3 Heat transfer

In a situation like the coffee cooling problem, there are three ways heat transfers from one object to another (see http://modsimpy.com/transfer):

- Conduction: When objects at different temperatures come into contact, the faster-moving particles of the higher-temperature object transfer kinetic energy to the slower-moving particles of the lower-temperature object.

[2]See http://modsimpy.com/thermo.

- Convection: When particles in a gas or liquid flow from place to place, they carry heat energy with them. Fluid flows can be caused by external action, like stirring, or by internal differences in temperature. For example, you might have heard that hot air rises, which is a form of "natural convection".
- Radiation: As the particles in an object move due to thermal energy, they emit electromagnetic radiation. The energy carried by this radiation depends on the object's temperature and surface properties (see http://modsimpy.com/thermrad).

For objects like coffee in a car, thermal radiation is much smaller than heat transfer due to conduction and convection, so we will ignore it.

Convection can be a complex topic, since it often depends on details of fluid flow in three dimensions. But for this problem we will be able to get away with a simple model called "Newton's law of cooling".

7.4 Newton's law of cooling

Newton's law of cooling asserts that the temperature rate of change for an object is proportional to the difference in temperature between the object and the surrounding environment:

$$\frac{dT}{dt} = -r(T - T_{env})$$

where T, the temperature of the object, is a function of time, t; T_{env} is the temperature of the environment, and r is a constant that characterizes how quickly heats is transferred between the system and the environment.

Newton's so-called "law" is really a model in the sense that it is approximately true in some conditions, only roughly true in others, and not at all true in others.

For example, if the primary mechanism of heat transfer is conduction, Newton's law is "true", which is to say that r is constant over a wide range of temperatures. And sometimes we can estimate r based on the material properties and shape of the object.

When convection contributes a non-negligible fraction of heat transfer, r depends on temperature, but Newton's law is often accurate enough, at least over a narrow range of temperatures. In this case r usually has to be estimated experimentally, since it depends on details of surface shape, air flow, evaporation, etc.

When radiation makes up a substantial part of heat transfer, Newton's law is not a good model at all. This is the case for objects in space or in a vacuum, and for objects at high temperatures (more than a few hundred degrees Celsius, say).

However, for a situation like the coffee cooling problem, we expect Newton's model to be quite good.

7.5 Implementation

To get started, let's forget about the milk temporarily and focus on the coffee. I'll create a `State` object to represent the initial temperature:

```
init = State(temp=90)
```

And a `System` object to contain the parameters of the system:

```
coffee = System(init=init, T_env=22, r=0.01,
                t0=0, t_end=30, dt=1)
```

The values of `T_env`, `t0`, and `t_end` come from the statement of the problem. I chose the value of `r` arbitrarily for now; we will figure out how to estimate it soon.

`dt` is the time step we use to simulate the cooling process. Strictly speaking, Newton's law is a differential equation, but over a short period of time we can approximate it with a difference equation:

$$\Delta T = -r(T - T_{env})\Delta t$$

where Δt is a small time step and ΔT is the change in temperature during that time step.

Note: I use ΔT to denote a change in temperature over time, but in the context of heat transfer, you might also see ΔT used to denote the difference in temperature between an object and its environment, $T - T_{env}$. To minimize confusion, I avoid this second use.

Now we can write an update function:

```
def update(state, system):
    unpack(system)

    T = state.temp
    T += -r * (T - T_env) * dt

    return State(temp=T)
```

Now if we run

```
update(init, coffee)
```

we see that the temperature after one minute is 89.3 °C, so the temperature drops by about 0.7 °C/min, at least for this value of `r`.

Now we can use `run_simulation`, as defined in Section 5.8, to simulate a series of time steps from `t0` to `t_end`:

```
def run_simulation(system, update_func):
    unpack(system)

    frame = TimeFrame(columns=init.index)
    frame.loc[t0] = init
    ts = linrange(t0, t_end-dt, dt)

    for t in ts:
        frame.loc[t+dt] = update_func(frame.loc[t], system)

    system.results = frame
```

and run it like this:

```
run_simulation(coffee, update)
```

The result is a `TimeFrame` object with one row per time step and just one column, `temp`. The temperature after 30 minutes is 72.3 °C, which is a little higher than stated in the problem, 70 °C. We could adjust `r` by hand and find the right value by trial and error, but we can do better, as we'll see in the next section.

First I want to wrap what we have so far in a function:

```
def make_system(T_init=90, r=0.01, volume=300, t_end=30):
    init = State(temp=T_init)

    system = System(init=init,
                    volume=volume,
                    r=r,
                    T_env=22,
                    t0=0,
                    t_end=t_end,
                    dt=1)
    return system
```

`make_system` takes the system parameters and packs them into a `System` object. Now we can simulate the coffee like this:

```
coffee = make_system()
run_simulation(coffee, update)
```

Now let's see a better was to estimate `r`.

7.6 Using fsolve

SciPy provides a method called `fsolve` that finds the roots of non-linear equations. As a simple example, suppose you want to find the roots of the polynomial

$$f(x) = (x-1)(x-2)(x-3)$$

where **root** means a value of x that makes $f(x) = 0$. Because of the way I wrote the polynomial, we can see that if $x = 1$, the first factor is 0; if $x = 2$, the second factor is 0; and if $x = 3$, the third factor is 0, so those are the roots.

But usually it's not that easy. In that case `fsolve` can help. First, we have to write a function that evaluates f:

```
def func(x):
    return (x-1) * (x-2) * (x-3)
```

Now we call `fsolve` like this:

```
fsolve(func, x0=0)
```

The first argument is the function whose roots we want. The second argument, `x0`, is an initial guess about where a root might be. Generally, the closer the initial guess is to an actual root, the faster `fsolve` runs. In this case, with the initial guess `x0=0`, the result is 1.

Often `fsolve` finds the root that's closest to the initial guess. In this example, when `x0=1.9`, `fsolve` returns 2, and when `x0=2.9`, `fsolve` returns 3. But this behavior can be unpredictable; with `x0=1.5`, `fsolve` returns 3.

So how can we use `fsolve` to estimate `r`?

Now, we want to find the value of `r` that yields a final temperature of 70 °C. To work with `fsolve`, we need a function that takes `r` as a parameter and returns the difference between the final temperature and the goal:

```
def error_func1(r):
    system = make_system(r=r)
    run_simulation(system, update)
    return final_temp(system) - 70
```

I call a function like this an "error function" because it returns the difference between what we got and what we wanted, that is, the error. When we find the right value of `r`, this error will be 0.

We can test `error_func1` like this, using our initial guess for `r`:

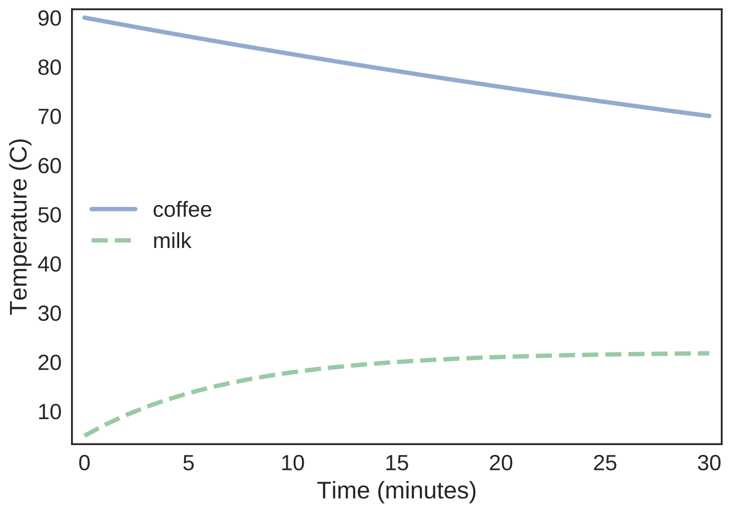


Figure 7.1: Temperature of the coffee and milk over time.

```
error_func1(r=0.01)
```

The result is an error of 2.3 °C, because the final temperature with this value of `r` is too high.

Now we can call `fsolve` like this:

```
solution = fsolve(error_func1, 0.01)
r_coffee = solution[0]
```

The return value from `fsolve` is an array with a single element, which is the root `fsolve` found. In this example, `r_coffee` turns out to be about `0.012`, in units of 1/min.

As one of the exercises for this chapter, you will use the same process to estimate `r_milk`.

With the correct values of `r_coffee` and `r_milk`, the simulation results should look like Figure 7.1, which shows the temperature of the coffee and milk over time.

7.7 Mixing liquids

When we mix two liquids, the temperature of the mixture depends on the temperatures of the ingredients, but it might not be obvious how to compute it.

Assuming there are no chemical reactions between the liquids that either produce or consume heat, the total thermal energy of the system is the same before and after mixing; in other words, thermal energy is **conserved**.

If the temperature of the first liquid is T_1, the temperature of the second liquid is T_2, and the final temperature of the mixture is T, the heat transfer into the first liquid is $C_1(T - T_1)$ and the heat transfer into the second liquid is $C_2(T - T_2)$, where C_1 and C_2 are the thermal masses of the liquids.

In order to conserve energy, these heat transfers must add up to 0:

$$C_1(T - T_1) + C_2(T - T_2) = 0$$

We can solve this equation for T:

$$T = \frac{C_1 T_1 + C_2 T_2}{C_1 + C_2}$$

For the coffee cooling problem, we have the volume of each liquid; if we also know the density, ρ, and the specific heat capacity, c_p, we can compute thermal mass:

$$C = \rho V c_p$$

If we assume that the density and specific heat of the milk and coffee are equal, they drop out of the equation, and we can write:

$$T = \frac{V_1 T_1 + V_2 T_2}{V_1 + V_2}$$

where V_1 and V_2 are the volumes of the liquids. As an exercise, you can look up the density and specific heat of milk to see how good this approximation is.

The following function takes two `System` objects that represent the coffee and milk, and creates a new `System` to represent the mixture:

```python
def mix(s1, s2):
    assert s1.t_end == s2.t_end

    volume = s1.volume + s2.volume

    temp = (s1.volume * final_temp(s1) +
            s2.volume * final_temp(s2)) / volume

    mixture = make_system(T_init=temp,
                          volume=volume,
                          r=s1.r)

    return mixture
```

The first line is an `assert` statement, which is a way of checking for errors. It compares `t_end` for the two systems to confirm that they have been cooling for the same time. If not, `assert` displays an error message and stops the program.

The next two statements compute the total volume of the mixture and its temperature. Fianlly, `mix` makes a new `System` object and returns it.

This function uses the value of `r` from `s1` as the value of `r` for the mixture. If `s1` represents the coffee, and we are adding the milk to the coffee, this is probably a reasonable choice. On the other hand, when we increase the amount of liquid in the coffee cup, that might change `r`. So this is an assumption to we might want to revisit when.

7.8 Mix first or last?

Now we have everything we need to solve the problem. First I'll create objects to represent the coffee and cream, and run for 30 minutes.

```
coffee = make_system(T_init=90, t_end=30,
                     r=r_coffee, volume=300)
run_simulation(coffee, update)

milk = make_system(T_init=5, t_end=30,
                   r=r_milk, volume=50)
run_simulation(milk, update)
```

The final temperatures, before mixing, are 70 °C and 21.7 °C. Then we mix them:

```
mix_last = mix(coffee, milk)
```

After mixing, the temperature is 63.1 °C, which is still warm enough to be enjoyable. Would we do any better if we added the milk first?

To find out, I'll create new objects for the coffee and milk:

```
coffee = run(T_init=90, r=r_coffee, volume=300)
milk = run(T_init=5, r=r_milk, volume=50)
```

Then mix them and simulate 30 minutes:

```
mix_first = mix(coffee, milk)
mix_first.t_end = 30
run_simulation(mix_first, update)
```

The final temperature is only 61.6 °C. So it looks like adding the milk at the end is better, by about 1.5 °C. But is that the best we can do?

7.9 Optimization

Adding the milk after 30 minutes is better than adding immediately, but maybe there's something in between that's even better. To find out, I'll use the following function, which takes `t_add` as a parameter:

```python
def run_and_mix(t_add, t_total=30):
    coffee = make_system(T_init=90, t_end=t_add,
                         r=r_coffee, volume=300)
    run_simulation(coffee, update)

    milk = make_system(T_init=5, t_end=t_add,
                       r=r_milk, volume=50)
    run_simulation(milk, update)

    mixture = mix(coffee, milk)
    mixture.t_end = t_total - t_add
    run_simulation(mixture, update)

    return final_temp(mixture)
```

When `t_add=0`, we add the milk immediately; when `t_add=30`, we add it at the end. Now we can sweep the range of values in between:

```python
sweep = SweepSeries()
for t_add in linrange(0, 30, 2):
    temp = run_and_mix(t_add)
    sweep[t_add] = temp
```

Figure 7.2 shows the result. Again, note that this is a parameter sweep, not a time series. The x-axis is the time when we add the milk, not the index of a `TimeSeries`.

The final temperature is maximized when `t_add=30`, so adding the milk at the end is optimal.

In the notebook for this chapter you will have a chance to explore this solution and try some variations. For example, suppose the coffee shop won't let me take milk in a separate container, but I keep a bottle of milk in the refrigerator at my office. In that case is it better to add the milk at the coffee shop, or wait until I get to the office?

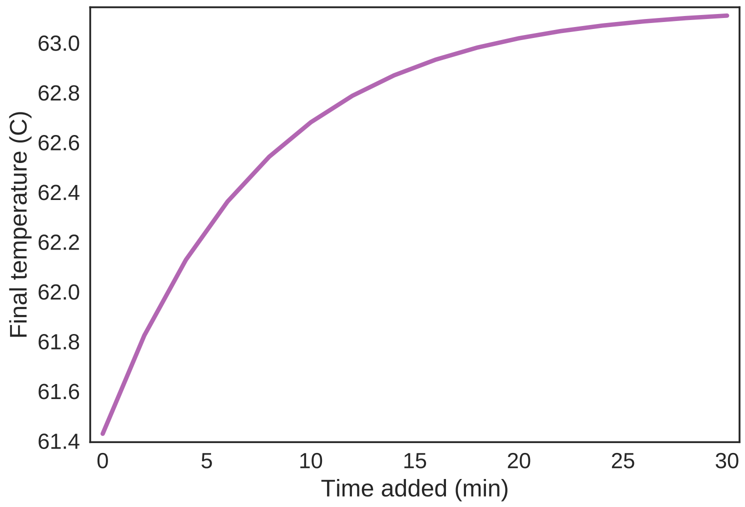


Figure 7.2: Final temperature as a function of the time the milk is added.

7.10 Analysis

Simulating Newton's law of cooling is almost silly, because we can solve the differential equation analytically. If

$$\frac{dT}{dt} = -r(T - T_{env})$$

the general solution is

$$T(t) = C_1 \exp(-rt) + T_{env}$$

and the particular solution where $T(0) = T_init$ is

$$T_{env} + (-T_{env} + T_{init}) \exp(-rt)$$

You can see how I got this solution using SymPy at http://modsimpy.com/sympy07; if you would like to see it done by hand, you can watch this video: http://modsimpy.com/khan3.

Now we can use the observed data to estimate the parameter r. If we observe $T(t_{end}) = T_{end}$, we can plug t_{end} and T_{end} into the particular solution and solve for r. The result is:

$$r = \frac{1}{t_{end}} \log\left(\frac{T_{init} - T_{env}}{T_{end} - T_{env}}\right)$$

Plugging in $t_{end} = 30$ and $T_{end} = 70$ (and again with $T_{init} = 90$ and $T_{env} = 22$), the estimate for r is 0.0116.

We can use the following function to compute the time series:

```
def run_analysis(system):
    unpack(system)

    T_init = init.temp
    ts = linrange(t0, t_end, dt)

    temp_array = T_env + (T_init - T_env) * exp(-r * ts)
    temp_series = TimeSeries(temp_array, index=ts)

    system.results = TimeFrame(temp_series, columns=['temp'])
```

This function is similar to `run_simulation`; it takes a `System` as a parameter, and stores a `TimeFrame` as a result. We can run it like this, with `r_coffee2=0.0116`:

```
init = State(temp=90)
coffee2 = System(init=init, T_env=22, r=r_coffee2,
                 t0=0, t_end=30)
run_analysis(coffee2)
```

The final temperature is 70 °C, as it should be. In fact, the results are identical to what we got by simulation, with very small differences due to round off errors.

Chapter 8

Pharmacokinetics

Pharmacokinetics is the study of how drugs and other substances move around the body, react, and are eliminated. In this chapter, we will implement one of the most widely used pharmacokinetic models: the so-called **minimal model** of glucose and insulin in the blood stream.

We will use this model to fit data collected from a patient, and use the parameters of the fitted model to quantify the patient's ability to produce insulin and process glucose.

My presentation in this chapter follows Bergman (2005) "Minimal Model" (abstract at `http://modsimpy.com/bergman`, PDF at `http://modsimpy.com/minmod`).

You can view the code for this chapter at `http://modsimpy.com/chap08`. For instructions on downloading and running the code, see Section 0.4.

8.1 The glucose-insulin system

Glucose is a form of sugar that circulates in the blood of animals; it is used as fuel for muscles, the brain, and other organs. The concentration of blood sugar is controlled by the hormone system, and especially by **insulin**, which is produced by the pancreas and has the effect of reducing blood sugar.

In people with normal pancreatic function, the hormone system maintains **homeostasis**; that is, it keeps the concentration of blood sugar in a range that is neither too high or too low.

But if the pancreas does not produce enough insulin, or if the cells that should respond to insulin become insensitive, blood sugar can become elevated, a condition called **hyperglycemia**. Long term, severe hyperglycemia is the defining symptom of **diabetes mellitus**, a serious disease that affects almost 10% of the population in the U.S. (see http://modsimpy.com/cdc).

One of the most-used tests for hyperglycemia and diabetes is the frequently sampled intravenous glucose tolerance test (FSIGT), in which glucose is injected into the blood stream of a fasting subject (someone who has not eaten recently), and then blood samples are collected at intervals of 2–10 minutes for 3 hours. The samples are analyzed to measure the concentrations of glucose and insulin.

By analyzing these measurements, we can estimate several parameters of the subject's response; the most important is a parameter denoted S_I, which quantifies the effect of insulin on the rate of reduction in blood sugar.

8.2 The glucose minimal model

The "minimal model" was proposed by Bergman, Ider, Bowden, and Cobelli[1]. It consists of two parts: the glucose model and the insulin model. I will present an implementation of the glucose model; in the notebook for this chapter, you will have the chance to implement the insulin model.

The original model was developed in the 1970s; since then, many variations and extensions have been proposed. Bergman's comments on the development of the model provide insight into their process:

> We applied the principle of Occam's Razor, i.e. by asking what was the simplest model based upon known physiology that could

[1]Bergman RN, Ider YZ, Bowden CR, Cobelli C., "Quantitative estimation of insulin sensitivity", Am J Physiol. 1979 Jun;236(6):E667-77. Abstract at http://modsimpy.com/insulin.

> account for the insulin-glucose relationship revealed in the data. Such a model must be simple enough to account totally for the measured glucose (given the insulin input), yet it must be possible, using mathematical techniques, to estimate all the characteristic parameters of the model from a single data set (thus avoiding unverifiable assumptions).

The most useful models are the ones that achieve this balance: including enough realism to capture the essential features of the system without too much complexity to be practical. In this case the practical limit is the ability to estimate the parameters of the model using data, and to interpret the parameters meaningfully.

Bergman discusses the features he and his colleagues thought were essential:

> (1) Glucose, once elevated by injection, returns to basal level due to two effects: the effect of glucose itself to normalize its own concentration [...] as well as the catalytic effect of insulin to allow glucose to self-normalize (2) Also, we discovered that the effect of insulin on net glucose disappearance must be sluggish — that is, that insulin acts slowly because insulin must first move from plasma to a remote compartment [...] to exert its action on glucose disposal.

To paraphrase the second point, the effect of insulin on glucose disposal, as seen in the data, happens more slowly than we would expect if it depended primarily on the the concentration of insulin in the blood. Bergman's group hypothesized that insulin must move, relatively slowly, from the blood to a "remote compartment" where it has its effect.

At the time, the remote compartment was a modeling abstraction that might, or might not, reflect something physical. Later, according to Bergman, it was "shown to be interstitial fluid", that is, the fluid that surrounds tissue cells. In the history of mathematical modeling, it is common for hypothetical entities, added to models to achieve particular effects, to be found later to correspond to physical entities.

The glucose model consists of two differential equations:

$$\frac{dG}{dt} = -k_1 \left[G(t) - G_b \right] - X(t) G(t)$$

$$\frac{dX}{dt} = k_3 \left[I(t) - I_b\right] - k_2 X(t)$$

where

- G is the concentration of blood glucose as a function of time and dG/dt is its rate of change.
- I is the concentration of insulin in the blood as a function of time, which is taken as an input into the model, based on measurements.
- G_b is the basal concentration of blood glucose and I_b is the basal concentration of blood insulin, that is, the concentrations at equilibrium. Both are constants estimated from measurements at the beginning or end of the test.
- X is the concentration of insulin in the tissue fluid as a function of time, and dX/dt is its rate of change.
- k_1, k_2, and k_3 are positive-valued parameters that control the rates of appearance and disappearance for glucose and insulin.

We can interpret the terms in the equations one by one:

- $-k_1 \left[G(t) - G_b\right]$ is the rate of glucose disappearance due to the effect of glucose itself. When $G(t)$ is above basal level, G_b, this term is negative; when $G(t)$ is below basal level this term is positive. So in the absence of insulin, this term tends to restore blood glucose to basal level.
- $-X(t)G(t)$ models the interaction of glucose and insulin in tissue fluid, so the rate increases as either X or G increases. This term does not require a rate parameter because the units of X are unspecified; we can consider X to be in whatever units would make the parameter of this term 1.
- $k_3 \left[I(t) - I_b\right]$ is the rate at which insulin diffuses between blood and tissue fluid. When $I(t)$ is above basal level, insulin diffuses from the blood into the tissue fluid. When $I(t)$ is below basal level, insulin diffuses from tissue to the blood.
- $-k_2 X(t)$ is the rate of insulin disappearance in tissue fluid as it is consumed or broken down.

The initial state of the model is $X(0) = I_b$ and $G(0) = G_0$, where G_0 is a constant that represents the concentration of blood sugar immediately after the injection. In theory we could estimate G_0 based on measurements, but in practice it takes time for the injected glucose to spread through the blood volume. Since G_0 is not measurable, it is treated as a **free parameter** of the model, which means that we are free to choose it to fit the data.

8.3 Data

To develop and test the model, I'll use data from Pacini and Bergman[2]. The dataset is in a file in the repository for this book, which we can read into a `DataFrame`:

```
data = pd.read_csv('glucose_insulin.csv', index_col='time')
```

`data` has two columns: `glucose` is the concentration of blood glucose in mg/dL; `insulin` is concentration of insulin in the blood in µU/mL (a medical "unit", denoted U, is an amount defined by convention in context). The index is time in min.

Figure 8.1 shows glucose and insulin concentrations over 182 min for a subject with normal insulin production and sensitivity.

8.4 Interpolation

Before we are ready to implement the model, there's one problem we have to solve. In the differential equations, I is a function that can be evaluated at any time, t. But in the `DataFrame`, we only have measurements at discrete times. This is a job for interpolation!

The `modsim` library provides a function named `interpolate`, which is a wrapper for the SciPy function `interp1d`. It takes any kind of `Series` as a parameter, including `TimeSeries` and `SweepSeries`, and returns a function. That's right, I said it returns a *function*.

[2] "MINMOD: A computer program to calculate insulin sensitivity and pancreatic responsivity from the frequently sampled intravenous glucose tolerance test", *Computer Methods and Programs in Biomedicine* 23: 113-122, 1986.

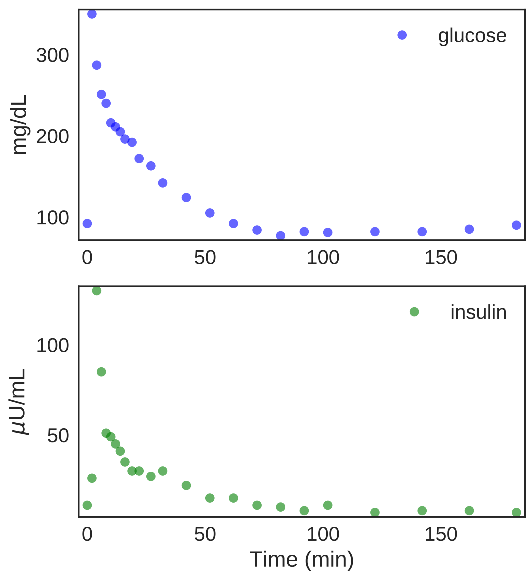


Figure 8.1: Glucose and insulin concentrations measured by FSIGT.

So we can call `interpolate` like this:

```
I = interpolate(data.insulin)
```

Then we can call the new function, `I`, like this:

```
I(18)
```

The result is 31.66, which is a linear interpolation between the actual measurements at `t=16` and `t=19`. We can also pass an array as an argument to `I`:

```
ts = linrange(0, 182, 2)
I(ts)
```

The result is an array of interpolated values for equally-spaced values of `t` between 0 and 182.

`interpolate` can take additional arguments, which it passes along to `interp1d`. You can read about these options at http://modsimpy.com/interp.

8.5 Implementation

To get started, we'll assume that the parameters of the model are known. We'll implement the model and use it to generate time series for `G` and `X`. Then we'll see how to find parameter values that generate series that best fit the data.

Taking advantage of estimates from prior work, I'll start with these values:

```
k1 = 0.03
k2 = 0.02
k3 = 1e-05
G0 = 290
```

And I'll use the measurements at `t=0` as the basal levels:

```
Gb = data.glucose[0]
Ib = data.insulin[0]
```

Now we can create the initial state:

```
init = State(G=G0, X=0)
```

And the `System` object:

```
system = System(init=init,
                k1=k1, k2=k2, k3=k3,
                I=I, Gb=Gb, Ib=Ib,
                t0=0, t_end=182, dt=2)
```

Now here's the update function:

```
def update_func(state, t, system):
    G, X = state
    unpack(system)

    dGdt = -k1 * (G - Gb) - X*G
    dXdt = k3 * (I(t) - Ib) - k2 * X

    G += dGdt * dt
    X += dXdt * dt

    return State(G=G, X=X)
```

As usual, the update function takes a `State` object and a `System` as parameters, but there's one difference from previous examples: this update function also takes `t`. That's because this system of differential equations is **time dependent**; that is, time appears in the right-hand side of at least one equation.

The first line of `update` uses multiple assignment to extract the current values of `G` and `X`. The second line uses `unpack` so we can read the system variables without using the dot operator.

Computing the derivatives `dGdt` and `dXdt` is straightforward; we just have to translate the equations from math notation to Python.

Then, to perform the update, we multiply each derivative by the discrete time step `dt`, which is 2 min in this example. The return value is a `State` object with the new values of `G` and `X`.

Before running the simulation, it is always a good idea to run the update function with the initial conditions:

```
update_func(init, 0, system)
```

If there are no errors, and the results seem reasonable, we are ready to run the simulation. Here's one more version of `run_simulation`. It is almost the same as in Section 7.5, with one change: it passes `t` as an argument to `update_func`.

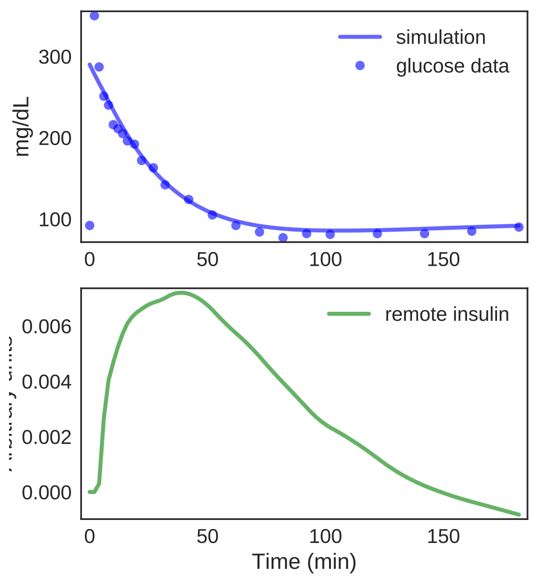


Figure 8.2: Results from simulation of the glucose minimal model.

```python
def run_simulation(system, update_func):
    unpack(system)

    frame = TimeFrame(columns=init.index)
    frame.loc[t0] = init
    ts = linrange(t0, t_end-dt, dt)

    for t in ts:
        frame.loc[t+dt] = update_func(frame.loc[t], t, system)

    system.results = frame
```

And we can run it like this:

```python
run_simulation(system, update_func)
```

The results are shown in Figure 8.2. The top plot shows simulated glucose levels from the model along with the measured data. The bottom plot shows simulated insulin levels in tissue fluid, which is in unspecified units, and not to be confused with measured concentration of insulin in the blood.

With the parameters I chose, the model fits the data reasonably well. We can do better, but first, I want to replace `run_simulation` with a better differential equation solver.

8.6 Numerical solution of differential equations

So far we have been solving differential equations by rewriting them as difference equations. In the current example, the differential equations are:

$$\frac{dG}{dt} = -k_1 \left[G(t) - G_b\right] - X(t)G(t)$$

$$\frac{dX}{dt} = k_3 \left[I(t) - I_b\right] - k_2 X(t)$$

If we multiply both sides by dt, we have:

$$dG = \left[-k_1 \left[G(t) - G_b\right] - X(t)G(t)\right] dt$$

$$dX = \left[k_3 \left[I(t) - I_b\right] - k_2 X(t)\right] dt$$

When dt is very small, or more precisely **infinitesimal**, this equation is exact. But in our simulations, dt is 2 min, which is small but not infinitesimal. In effect, the simulations assume that the derivatives dG/dt and dX/dt are constant during each 2 min time step. That's not exactly true, but it can be a good enough approximation.

This method, evaluating derivatives at discrete time steps and assuming that they are constant in between, is called **Euler's method** (see http://modsimpy.com/euler).

Euler's method is good enough for some simple problems, but there are many better ways to solve differential equations, including an entire family of methods called linear multistep methods (see http://modsimpy.com/lmm).

Rather than implement these methods ourselves, we will use functions from SciPy. The `modsim` library provides a function called `run_odeint`, which is a wrapper for `scipy.integrate.odeint`. The name `odeint` stands for "ordinary differential equation integrator". The equations we are solving are "ordinary" because all the derivatives are with respect to the same variable; in other words, there are no partial derivatives. And the solver is called an integrator because solving differential equations is considered a form of integration.

`scipy.integrate.odeint` is a wrapper for `LSODA`, which is from ODEPACK, a venerable collection of ODE solvers written in Fortran (for some of the history of ODEPACK, see http://modsimpy.com/hindmarsh).

To use `odeint`, we have to provide a "slope function":

```
def slope_func(state, t, system):
    G, X = state
    unpack(system)

    dGdt = -k1 * (G - Gb) - X*G
    dXdt = k3 * (I(t) - Ib) - k2 * X

    return dGdt, dXdt
```

`slope_func` is similar to `update_func`; in fact, it takes the same parameters in the same order. But `slope_func` is simpler, because all we have to do is compute the derivatives, that is, the slopes. We don't have to do the updates; `odeint` does them for us.

Before we call `run_odeint`, we have to create a `System` object:

```
system2 = System(init=init,
                 k1=k1, k2=k2, k3=k3,
                 I=I, Gb=Gb, Ib=Ib,
                 ts=data.index)
```

When we were using `run_simulation`, we created a `System` object with variables `t0`, `t_end`, and `dt`. When we use `run_odeint`, we don't need those variables, but we do have to provide `ts`, which is an array or `Series` that contains the times where we want the solver to evaluate G and X.

Now we can call `run_odeint` like this:

```
run_odeint(system2, slope_func)
```

Like `run_simulation`, `run_odeint` puts the results in a `TimeFrame` and stores it as a system variable named `results`. The columns of `results` match the state variables in `init`, `G` and `X`. The index of `results` matches the values from `ts`; in this example, `ts` contains the timestamps of the measurements.

The results are similar to what we saw in Figure 8.2. The difference is about 1% on average and never more than 2%.

8.7 Least squares

So far we have been taking the parameters as given, but in general we don't have that luxury. Normally we are given the data and we have to search for the parameters that yield a time series that best matches the data.

We will do that now, in two steps:

1. First we'll define an **error function** that takes a set of possible parameters, simulates the system with the given parameters, and computes the errors, that is, the differences between the simulation results and the data.

2. Then we'll use a SciPy function, `leastsq`, to search for the parameters that minimize mean squared error (MSE).

Here's an outline of the functions we'll use:

- The `modsim` library provides `fit_leastsq`, which takes a function called `error_func` as a parameter. It does some error-checking, then calls `scipy.optimize.leastsq`, which does the real work.

- `scipy.optimize.leastsq` uses functions called `lmdif` and `lmdir`, which implement the Levenberg-Marquardt algorithm for non-linear least squares problems (see http://modsimpy.com/levmarq). These functions are provided by another venerable FORTRAN library called MINPACK (see http://modsimpy.com/minpack).

- When `scipy.optimize.leastsq` runs, it calls `error_func` many times, each time with a different set of parameters, until it converges on the set of parameters that minimizes MSE.

Each time the error function runs, it creates a `System` object with the given parameters, so let's wrap that operation in a function:

```
def make_system(G0, k1, k2, k3, data):
    init = State(G=G0, X=0)
    system = System(init=init,
                    k1=k1, k2=k2, k3=k3,
                    Gb=Gb, Ib=Ib,
                    I=interpolate(data.insulin),
                    ts=data.index)
    return system
```

`make_system` takes `G0` and the rate constants as parameters, as well as `data`, which is the `DataFrame` containing the measurements. It creates and returns a `System` object.

Now here's the error function:

```
def error_func(params, data):
    system = make_system(*params, data)
    run_odeint(system, slope_func)
    error = system.results.G - data.glucose
    return error
```

The parameters of `error_func` are

- `params`, which is a sequence of four system parameters, and
- `data`, which is the `DataFrame` containing the measurements.

`error_func` uses `make_system` to create the `System` object. This line demonstrates a feature we have not seen before, the **scatter operator**, `*`. Applied to `params`, the scatter operator unpacks the sequence, so instead of being considered a single value, it is treated as four separate values.

`error_func` calls `run_odeint` using the same slope function we saw in Section 8.6. Then it computes the difference between the simulation results and the data. Since `system.results.G` and `data.glucose` are both `Series` objects, the result of subtraction is also a `Series`.

Now, to do the actual minimization, we run `fit_leastsq`:

```
k1 = 0.03
k2 = 0.02
k3 = 1e-05
G0 = 290
params = G0, k1, k2, k3
best_params = fit_leastsq(error_func, params, data)
```

`error_func` is the function we just defined. `params` is a sequence containing an initial guess for the four system parameters, and `data` is the `DataFrame` containing the measurements.

Actually, the third parameter can be any object we like. `fit_leastsq` and `leastsq` don't do anything with this parameter except to pass it along to `error_func`, so in general it contains whatever information `error_func` needs to do its job.

8.8 Interpreting parameters

The return value from `fit_leastsq` is `best_params`, which we can pass along to `make_system`, again using the scatter operator, and then run the simulation:

```
system = make_system(*best_params, data)
run_odeint(system, slope_func)
```

Figure 8.3 shows the results. The simulation matches the measurements well, except during the first few minutes after the injection. But we don't expect the model to do well in this regime.

The reason is that the model is **non-spatial**; that is, it does not take into account different concentrations in different parts of the body. Instead, it

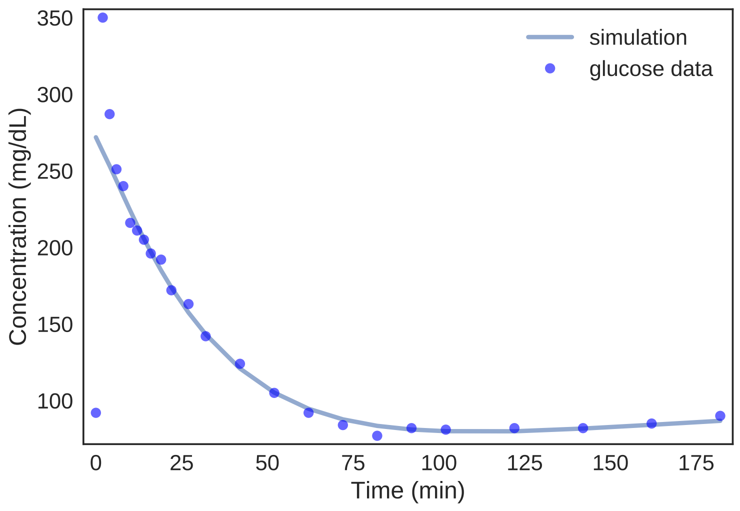


Figure 8.3: Simulation of the glucose minimal model with parameters that minimize MSE.

assumes that the concentrations of glucose and insulin in blood, and insulin in tissue fluid, are the same throughout the body. This way of representing the body is known among experts as the "bag of blood" model.

Immediately after injection, it takes time for the injected glucose to circulate. During that time, we don't expect a non-spatial model to be accurate. For this reason, we should not take the estimated value of `G0` too seriously; it is useful for fitting the model, but not meant to correspond to a physical, measurable quantity.

On the other hand, the other parameters are meaningful; in fact, they are the reason the model is useful. Using the best-fit parameters, we can estimate two quantities of interest:

- "Glucose effectiveness", E, which is the tendency of elevated glucose to cause depletion of glucose.
- "Insulin sensitivity", S, which is the ability of elevated blood insulin to enhance glucose effectiveness.

Glucose effectiveness is defined as the change in dG/dt as we vary G:

$$E \equiv -\frac{\delta \dot{G}}{\delta G}$$

where $\dot{G}$ is shorthand for dG/dt. Taking the derivative of dG/dt with respect to G, we get

$$E = k_1 + X$$

The **glucose effectiveness index**, S_G, is the value of E in when blood insulin is near its basal level, I_b. In that case, X approaches 0 and E approaches k_1. So we can use the best-fit value of k_1 as an estimate of S_G.

Insulin sensitivity is defined as the change in E as we vary I:

$$S \equiv -\frac{\delta E}{\delta I}$$

The **insulin sensitivity index**, S_I, is the value of S when E and I are at steady state:

$$S_I \equiv \frac{\delta E_{SS}}{\delta I_{SS}}$$

E and I are at steady state when dG/dt and dX/dt are 0, but we don't actually have to solve those equations to find S_I. If we set $dX/dt = 0$ and solve for X, we find the relation:

$$X_{SS} = \frac{k_3}{k_2} I_{SS}$$

And since $E = k_1 + X$, we have:

$$S_I = \frac{\delta E_{SS}}{\delta I_{SS}} = \frac{\delta X_{SS}}{\delta I_{SS}}$$

Taking the derivative of X_{SS} with respect to I_{SS}, we have:

$$S_I = k_3/k_2$$

So if we find parameters that make the model fit the data, we can use k_3/k_2 as an estimate of S_I.

For the example data, the estimated values of S_G and S_I are 0.029 and for 8.9×10^{-4}. According to Pacini and Bergman, these values are within the normal range.

8.9 The insulin minimal model

Along with the glucose minimal mode, Berman et al. developed an insulin minimal model, in which the concentration of insulin, I, is governed by this differential equation:

$$\frac{dI}{dt} = -kI(t) + \gamma \left[G(t) - G_T\right] t$$

where

- k is a parameter that controls the rate of insulin disappearance independent of blood glucose.
- $G(t)$ is the measured concentration of blood glucose at time t.
- G_T is the glucose threshold; when blood glucose is above this level, it triggers an increase in blood insulin.
- γ is a parameter that controls the rate of increase (or decrease) in blood insulin when glucose is above (or below) G_T.

The initial condition is $I(0) = I_0$. As in the glucose minimal model, we treat the initial condition as a parameter which we'll choose to fit the data.

The parameters of this model can be used to estimate, ϕ_1 and ϕ_2, which are values that "describe the sensitivity to glucose of the first and second phase pancreatic responsivity". They are related to the parameters as follows:

$$\phi_1 = \frac{I_{max} - I_b}{k(G_0 - G_b)}$$

$$\phi_2 = \gamma \times 10^4$$

where I_{max} is the maximum measured insulin level, and I_b and G_b are the basal levels of insulin and glucose.

In the notebook for this chapter, you will have a chance to implement this model, find the parameters that best fit the data, and estimate these values.

Chapter 9

Projectiles

So far the differential equations we've worked with have been **first order**, which means they involve only first derivatives. In this chapter, we turn our attention to second order ODEs, which can involve both first and second derivatives.

We'll revisit the falling penny example from Chapter 1, and use `odeint` to find the position and velocity of the penny as it falls, with and without air resistance.

You can view the code for this chapter at `http://modsimpy.com/chap09`. For instructions on downloading and running the code, see Section 0.4.

9.1 Newton's second law of motion

First order ODEs can be written

$$\frac{dy}{dx} = G(x, y)$$

where G is some function of x and y (see `http://modsimpy.com/ode`). Second order ODEs can be written

$$\frac{d^2y}{dx^2} = H(x, y, y')$$

where H is another function and y' is shorthand for dy/dx. In particular, we will work with one of the most famous and useful second order ODEs, Newton's second law of motion:

$$F = ma$$

where F is a force or the total of a set of forces, m is the mass of a moving object, and a is its acceleration.

Newton's law might not look like a differential equation, until we realize that acceleration, a, is the second derivative of position, y, with respect to time, t. With the substitution

$$a = \frac{d^2y}{dt^2}$$

Newton's law can be written

$$\frac{d^2y}{dt^2} = F/m$$

And that's definitely a second order ODE. In general, F can be a function of time, position, and velocity.

Of course, this "law" is really a model, in the sense that it is a simplification of the real world. Although it is often approximately true:

- It only applies if m is constant. If mass depends on time, position, or velocity, we have to use a more general form of Newton's law (see http://modsimpy.com/varmass).
- It is not a good model for very small things, which are better described by another model, quantum mechanics.
- And it is not a good model for things moving very fast, which are better described by relativistic mechanics.

But for medium to large things with constant mass, moving at speeds that are medium to slow, Newton's model is phenomenally useful. If we can quantify the forces that act on such an object, we can figure out how it will move.

9.2 Dropping pennies

As a first example, let's get back to the penny falling from the Empire State Building, which we considered in Section 1.1. We will implement two models of this system: first without air resistance, then with.

Given that the Empire State Building is 381 m high, and assuming that the penny is dropped with velocity zero, the initial conditions are:

```
init = State(y=381 * m,
             v=0 * m/s)
```

where `y` is height above the sidewalk and `v` is velocity. The units `m` and `s` are from the `UNITS` object provided by Pint:

```
m = UNITS.meter
s = UNITS.second
kg = UNITS.kilogram
```

The only system parameter is the acceleration of gravity:

```
g = 9.8 * m/s**2
```

In addition, we'll specify the sequence of times where we want to solve the differential equation:

```
duration = 10 * s
dt = 1 * s
ts = linrange(0, duration, dt)
```

`ts` contains equally spaced points between 0 s and 10 s, including both endpoints.

Next we need a `System` object to contain the system parameters:

```
system = System(init=init, g=g, ts=ts)
```

Now we need a slope function, and here's where things get tricky. As we have seen, `odeint` can solve systems of first order ODEs, but Newton's law is a second order ODE. However, if we recognize that

1. Velocity, v, is the derivative of position, dy/dt, and
2. Acceleration, a, is the derivative of velocity, dv/dt,

we can rewrite Newton's law as a system of first order ODEs:

$$\frac{dy}{dt} = v$$

$$\frac{dv}{dt} = a$$

And we can translate those equations into a slope function:

```python
def slope_func(state, t, system):
    y, v = state
    unpack(system)

    dydt = v
    dvdt = -g

    return dydt, dvdt
```

The first parameter, `state`, contains the position and velocity of the penny. The last parameter, `system`, contains the system parameter `g`, which is the magnitude of acceleration due to gravity.

The second parameter, `t`, is time. It is not used in this slope function because none of the factors of the model are time dependent (see Section 8.5). I include it anyway because this function will be called by `odeint`, and `odeint` always provides the same arguments, whether they are needed or not.

The rest of the function is a straightforward translation of the differential equations, with the substitution $a = -g$, which indicates that acceleration is due to gravity, in the direction of decreasing y. `slope_func` returns a sequence containing the two derivatives.

Before calling `run_odeint`, it is always a good idea to test the slope function with the initial conditions:

```python
slope_func(init, 0, system)
```

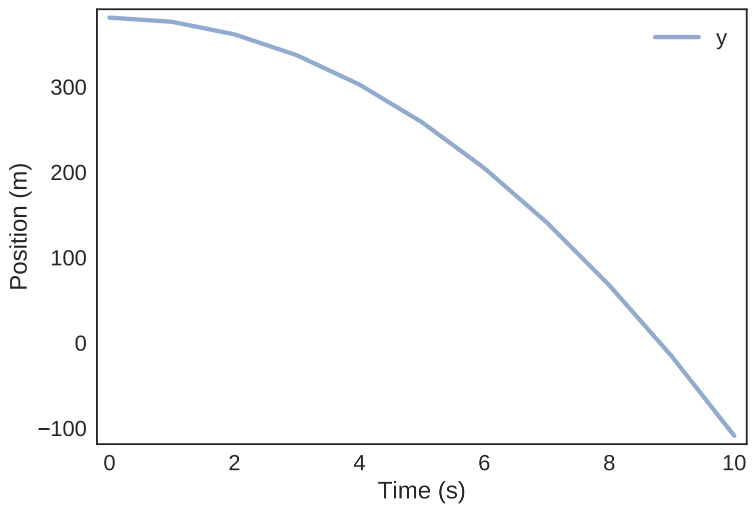


Figure 9.1: Height of the penny versus time, with no air resistance.

The result is a sequence containing 0 m/s for velocity and 9.8 m/s^2 for acceleration. Now we can run `odeint` like this:

```
run_odeint(system, slope_func)
```

`run_odeint` stores the results in a `TimeFrame` with two columns: `y` contains the height of the penny; `v` contains its velocity.

`plot_position`, which is defined in the notebook for this chapter, plots height versus time:

```
plot_position(system.results)
```

Figure 9.1 shows the result. Since acceleration is constant, velocity increases linearly and position decreases quadratically; as a result, the height curve is a parabola.

In this model, height can be negative, because we have not included the effect of the sidewalk!

9.3 Onto the sidewalk

To avoid negative heights, we can use the results from the previous section to estimate when the penny hits the sidewalk, and run the simulation for the estimated time.

From the results, we can extract `y`, which is a `Series` that represents height as a function of time.

```
y = system.results.y
```

To interpolate the values of `y`, we could use `interpolate`, which we saw in Section 8.4.

```
Y = interpolate(y)
```

If we do that, we get a function that computes height as a function of time, but that's not what we want. Rather, we want the inverse function, time as a function of height. The `modsim` library provides a function that computes it:

```
T = interp_inverse(y, kind='cubic')
```

The second parameter, `kind`, indicates what kind of interpolation we want: `cubic` means we want a cubic spline (see http://modsimpy.com/spline).

The result is a function that maps from height to time. Now we can evaluate the interpolating function at `y=0`

```
T_sidewalk = T(0)
```

The result is 8.8179 m, which agrees with the exact answer to 4 decimal places.

One caution about `interpolate` and `interp_inverse`: the function you provide has to be single valued (see http://modsimpy.com/singval).

In this example, height decreases monotonically, so for every height there is only one corresponding time. But if we threw the penny upward and then it fell down, the penny would pass through some heights more than once. In that case the inverse function represented by `T` would not be single valued, and the interpolation function would behave unpredictably.

9.4 With air resistance

As an object moves through a fluid, like air, the object applies force to the air and, in accordance with Newton's third law of motion, the air applies an equal and opposite force to the object (see http://modsimpy.com/newton).

The direction of this **drag force** is opposite the direction of travel, and its magnitude is given by the drag equation (see http://modsimpy.com/drageq):

$$F_d = \frac{1}{2}\, \rho\, v^2\, C_d\, A$$

where

- F_d is force due to drag, in newtons (N).
- ρ is the density of the fluid in kg/m^3.
- v is velocity in m/s.
- A is the **reference area** of the object, in m^2. In this context, the reference area is the projected frontal area, that is, the visible area of the object as seen from a point on its line of travel (and far away).
- C_d is the **drag coefficient**, a dimensionless quantity that depends on the shape of the object (including length but not frontal area), its surface properties, and how it interacts with the fluid.

For objects moving at moderate speeds through air, typical drag coefficients are between 0.1 and 1.0, with blunt objects at the high end of the range and streamlined objects at the low end (see http://modsimpy.com/dragco).

For simple geometric objects we can sometimes guess the drag coefficient with reasonable accuracy; for more complex objects we usually have to take measurements and estimate C_d from the data.

Of course, the drag equation is itself a model, based on the assumption that C_d does not depend on the other terms in the equation: density, velocity, and area. For objects moving in air at moderate speeds (below 45 mph or 20 m/s), this model might be good enough, but we should remember to revisit this assumption.

For the falling penny, we can use measurements to estimate C_d. In particular, we can measure **terminal velocity**, v_{term}, which is the speed where drag force equals force due to gravity:

$$\frac{1}{2}\ \rho\ v_{term}^2\ C_d\ A = mg$$

where m is the mass of the object and g is acceleration due to gravity. Solving this equation for C_d yields:

$$C_d = \frac{2\ mg}{\rho\ v_{term}^2\ A}$$

According to *Mythbusters*, the terminal velocity of a penny is between 35 and 65 mph (see `http://modsimpy.com/mythbust`). Using the low end of their range, 40 mph or about 18 m/s, the estimated value of C_d is 0.44, which is close to the drag coefficient of a smooth sphere.

Now we are ready to add air resistance to the model.

9.5 Implementation

As the number of system parameters increases, and as we need to do more work to compute them, we will find it useful to define a `Condition` object to contain the quantities we need to make a `System` object. `Condition` objects are similar to `System` and `State` objects; in fact, all three have the same capabilities. I have given them different names to document the different roles they play.

Here's the `Condition` object for the falling penny:

```
condition = Condition(height = 381 * m,
                      v_init = 0 * m / s,
                      g = 9.8 * m/s**2,
                      mass = 2.5e-3 * kg,
                      diameter = 19e-3 * m,
                      rho = 1.2 * kg/m**3,
                      v_term = 18 * m / s,
                      duration = 30 * s)
```

The mass and diameter are from http://modsimpy.com/penny. The density of air depends on temperature, barometric pressure (which depends on altitude), humidity, and composition (http://modsimpy.com/density). I chose a value that might be typical in New York City at 20 °C.

Here's a version of `make_system` that takes a `Condition` object and returns a `System`:

```
def make_system(condition):
    unpack(condition)

    init = State(y=height, v=v_init)
    area = np.pi * (diameter/2)**2
    C_d = 2 * mass * g / (rho * area * v_term**2)
    ts = linspace(0, duration, 101)

    return System(init=init, g=g, mass=mass, rho=rho,
                  C_d=C_d, area=area, ts=ts)
```

It might not be obvious why we need `Condition` objects. One reason is to minimize the number of variables in the `System` object. In this example, we use `diameter` to compute `area` and `v_term` to compute `C_d`, but then we don't need `diameter` and `v_term` in the `System` object.

Using a `Condition` object is also useful because we can modify it iteratively and create a sequence of `System` objects, each with a different set of conditions.

But for now, you might have to take my word that this is a good idea (see http://modsimpy.com/zen).

We can make a `System` like this:

```
system = make_system(condition)
```

And write a version of the slope function that includes drag:

```
def slope_func(state, t, system):
    y, v = state
    unpack(system)

    f_drag = rho * v**2 * C_d * area / 2
    a_drag = f_drag / mass

    dydt = v
    dvdt = -g + a_drag

    return dydt, dvdt
```

`f_drag` is force due to drag, based on the drag equation. `a_drag` is acceleration due to drag, based on Newton's second law.

To compute total acceleration, we add accelerations due to gravity and drag, where `g` is negated because it is in the direction of decreasing `y`, and `a_drag` is positive because it is in the direction of increasing `y`. In the next chapter we will use `Vector` objects to keep track of the direction of forces and add them up in a less error-prone way.

After we test the slope function, we can run the simulation like this:

```
run_odeint(system, slope_func)
```

Figure 9.2 shows the result. It only takes a few seconds for the penny to accelerate up to terminal velocity; after that, velocity is constant, so height as a function of time is a straight line.

9.6 Dropping quarters

In the previous sections, we were given an estimate of terminal velocity, based on measurements, and we used it to estimate the drag coefficient, C_d. Now

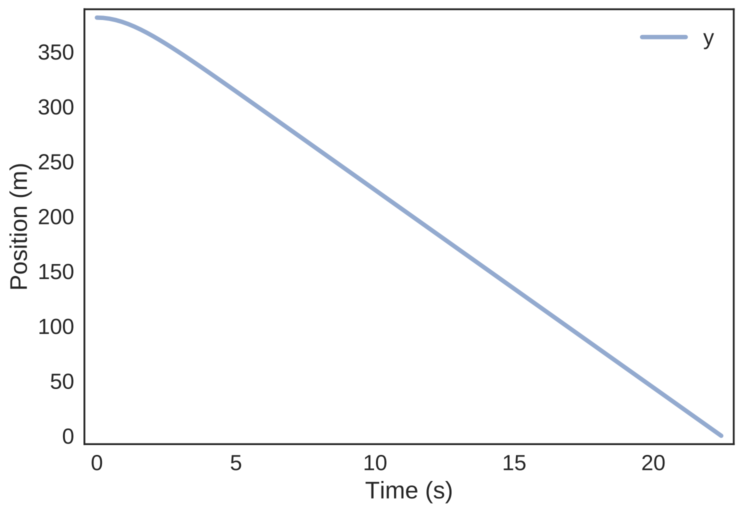


Figure 9.2: Height of the penny versus time, with air resistance.

suppose that we are given flight time, instead. Can we use that to estimate C_d and terminal velocity?

Suppose I drop a quarter off the Empire State Building and find that it takes 19.1 s to reach the sidewalk. Here's a `Condition` object with the parameters of a quarter (from http://modsimpy.com/quarter) and the measured duration:

```
condition = Condition(height = 381 * m,
                      v_init = 0 * m / s,
                      g = 9.8 * m/s**2,
                      mass = 5.67e-3 * kg,
                      diameter = 24.26e-3 * m,
                      rho = 1.2 * kg/m**3,
                      duration = 19.1 * s)
```

And here's a revised version of `make_system`:

```
def make_system(condition):
    unpack(condition)

    init = State(y=height, v=v_init)
    area = np.pi * (diameter/2)**2
    ts = linspace(0, duration, 101)

    return System(init=init, g=g, mass=mass, rho=rho,
                  C_d=C_d, area=area, ts=ts)
```

This version does not expect the `Condition` object to contain `v_term`, but it does expect `C_d`. We don't know what `C_d` is, so we'll start with an initial guess and go from there:

```
condition.set(C_d=0.4)
system = make_system(condition)
run_odeint(system, slope_func)
```

`Condition` objects provide a function called `set` that we can use to modify the condition variables. With `C_d=0.4`, the height of the quarter after 19.1 s is −11 m. That means the quarter is moving a bit too fast, which means our estimate for the drag coefficient is too low. We could improve the estimate by trial and error, or we could get `fsolve` to do it for us.

To use `fsolve`, we need an error function, which we can define by encapsulating the previous lines of code:

```
def height_func(C_d, condition):
    condition.set(C_d=C_d)
    system = make_system(condition)
    run_odeint(system, slope_func)
    y, v = final_state(system.results)
    return y
```

`height_func` takes a hypothetical value of `C_d` as a parameter. It runs the simulation with the given value of `C_d` and returns the final height after 19.1 s.

When we get the value of `C_d` right, the result should be 0, so we can use `fsolve` to find it:

```
fsolve(height_func, 0.4, condition)
```

As we saw in Section 7.6, `fsolve` takes the error function and the initial guess as parameters. Any additional parameters we give to `fsolve` are passed along to `height_func`. In this case, we provide `condition` as an argument to `fsolve` so we can use it inside `height_func`.

The result from `fsolve` is 0.43, which is very close to the drag coefficient we computed for the penny, 0.44. Although it is plausible that different coins would have similar drag coefficients, we should not take this result too seriously. Remember that I chose the terminal velocity of the penny arbitrarily from the estimated range. And I completely fabricated the flight time for the quarter.

Nevertheless, the methods we developed for estimating `C_d`, based on terminal velocity or flight time, are valid, subject to the precision of the measurements.

These methods demonstrate two ways to use models to solve problems, sometimes called **forward** and **inverse** problems. In a forward problem, you are given the parameters of the system and asked to predict how it will behave. In an inverse problem, you are given the behavior of the system and asked to infer the parameters. See http://modsimpy.com/inverse.

Chapter 10

Two dimensions

In the previous chapter we modeled objects moving in one dimension, with and without drag. Now let's move on to two dimensions, and baseball!

You can view the code for this chapter at http://modsimpy.com/chap10. For instructions on downloading and running the code, see Section 0.4.

10.1 The Manny Ramirez problem

Manny Ramirez is a former member of the Boston Red Sox (an American baseball team) who was notorious for a relaxed attitude and a taste for practical jokes that his managers did not always appreciate. Our objective in this chapter is to solve the following Manny-inspired problem:

What is the minimum effort required to hit a home run in Fenway Park?

Fenway Park is a baseball stadium in Boston, Massachusetts. One of its most famous features is the "Green Monster", which is a wall in left field that is unusually close to home plate, only 310 feet. To compensate for the short distance, the wall is unusually high, at 37 feet (see http://modsimpy.com/wally).

We want to find the minimum velocity at which a ball can leave home plate and still go over the Green Monster. We'll proceed in the following steps:

1. We'll model the flight of a baseball through air.
2. For a given velocity, we'll find the optimal **launch angle**, that is, the angle the ball should leave home plate to maximize its height when it reaches the wall.
3. Then we'll find the minimal velocity that clears the wall, given that it has the optimal launch angle.

As usual, we'll have to make some modeling decisions. To get started, we'll ignore any spin that might be on the ball, and the resulting Magnus force (see http://modsimpy.com/magnus).

As a result, we'll assume that the ball travels in the plane above the left field line, so we'll run simulations in two dimensions, rather than three.

But we will take into account air resistance. Based on what we learned about falling coins, it seems likely that air resistance has a substantial effect on the flight of a baseball.

To model air resistance, we'll need the mass, frontal area, and drag coefficient of a baseball. Mass and diameter are easy to find (see http://modsimpy.com/baseball). Drag coefficient is only a little harder; according to a one-pager from NASA[1], the drag coefficient of a baseball is approximately 0.3.

However, this value *does* depend on velocity[2]. At low velocities it might be as high as 0.5, and at high velocities as low as 0.29. Furthermore, the transition between these regimes typically happens exactly in the range of velocities we are interested in, around 40 m/s.

To get started, I'll assume that the drag coefficient does not depend on velocity, but this is an issue we might want to revisit.

10.2 Vectors

Now that we are working in two dimensions, we will find it useful to work with **vector quantities**, that is, quantities that represent both a magnitude and a

[1] "Drag on a Baseball", available from http://modsimpy.com/nasa
[2] Adair, *The Physics of Baseball*, Third Edition, Perennial, 2002

direction. We will use vectors to represent positions, velocities, accelerations, and forces in two and three dimensions.

The `modsim` library provides a `Vector` object that represents a vector quantity. A `Vector` object is a like a NumPy array; it contains elements that represent the **components** of the vector. For example, in a `Vector` that represents a position in space, the components are the x and y coordinates (and a z coordinate in 3-D). A `Vector` object also has units, like the quantities we've seen in previous chapters.

You can create a `Vector` by specifying its components. The following `Vector` represents a point 3 m to the right (or east) and 4 m up (or north) from an implicit origin:

```
A = Vector(3, 4) * m
```

You can access the components of a `Vector` by name, using the dot operator; for example, `A.x` or `A.y`. You can also access them by index, using brackets, like `A[0]` or `A[1]`.

Similarly, you can get the magnitude and angle using the dot operator, `A.mag` and `A.angle`. **Magnitude** is the length of the vector: if the `Vector` represents position, magnitude is the distance from the origin; if it represents velocity, magnitude is speed, that is, how fast the object is moving, regardless of direction.

The **angle** of a `Vector` is its direction, expressed as the angle in radians from the positive x-axis. In the Cartesian plane, the angle 0 rad is due east, and the angle π rad is due west.

`Vector` objects support most mathematical operations, including addition and subtraction:

```
B = Vector(1, 2) * m
A + B
A - B
```

For the definition and graphical interpretation of these operations, see http://modsimpy.com/vecops.

When you add and subtract `Vector` objects, the `modsim` library uses NumPy and Pint to check that the operands have the same number of dimensions and units. The notebook for this chapter shows examples for working with `Vector` objects.

One note on working with angles: in mathematics, we almost always represent angle in radians, and most Python functions expect angles in radians. But people often think more naturally in degrees. It can be awkward, and error-prone, to use both units in the same program. Fortunately, Pint makes it possible to represent angles using quantities with units.

As an example, I'll get the `degree` unit from `UNITS`, and create a quantity that represents 45 degrees:

```
degree = UNITS.degree
angle = 45 * degree
```

Then if we need to convert to radians we can use the `to` function

```
radian = UNITS.radian
rads = angle.to(radian)
```

Alternatively, if we know that a quantity is represented in degrees, we can use `np.deg2rad` to convert to radians. However, unlike the `to` function, `np.deg2rad` does no error checking!

If you are given an angle and velocity, you can make a `Vector` by converting to Cartesian coordinates using `pol2cart`. To demonstrate, I'll extract the angle and magnitude of `A`:

```
mag = A.mag
angle = A.angle
```

And then make a new `Vector` with the same components:

```
x, y = pol2cart(angle, mag)
Vector(x, y)
```

10.3 Modeling baseball flight

Now we're ready to simulate the flight of the baseball. As in Section 9.5, I'll create a `Condition` object that contains the parameters of the system:

```
condition = Condition(x = 0 * m,
                      y = 1 * m,
                      g = 9.8 * m/s**2,
                      mass = 145e-3 * kg,
                      diameter = 73e-3 * m,
                      rho = 1.2 * kg/m**3,
                      C_d = 0.3,
                      angle = 45 * degree,
                      velocity = 40 * m / s,
                      duration = 5.1 * s)
```

Using the center of home plate as the origin, the initial height is about 1 m. The initial velocity is 40 m/s at a launch angle of 45°. The mass, diameter, and drag coefficient of the baseball are from the sources in Section 10.1. The acceleration of gravity, `g`, is a well-known quantity, and the density of air, `rho`, is based on a temperature of 20 °C at sea level (see http://modsimpy.com/tempress). I chose the value of `duration` to run the simulation long enough for the ball to land on the ground.

The following function uses the `Condition` object to make a `System` object. Again, this two-step process reduces the number of variables in the `System` object, and makes it easier to work with functions like `fsolve`.

```
def make_system(condition):
    unpack(condition)

    theta = np.deg2rad(angle)
    vx, vy = pol2cart(theta, velocity)
    init = State(x=x, y=y, vx=vx, vy=vy)
    area = np.pi * (diameter/2)**2
    ts = linspace(0, duration, 101)

    return System(init=init, g=g, mass=mass,
                  area=area, rho=rho, C_d=C_d, ts=ts)
```

After unpacking `Condition`, we can access the variables it contains without using the dot operator.

`make_system` uses `np.deg2rad` to convert `angle` to radians and `pol2cart` to compute the x and y components of the initial velocity. Then it makes the initial `State` object, computes `area` and `ts`, and creates the `System` object.

Now we're ready for a slope function:

```
def slope_func(state, t, system):
    x, y, vx, vy = state
    unpack(system)

    a_grav = Vector(0, -g)

    v = Vector(vx, vy)
    f_drag = -rho * v.mag * v * C_d * area / 2
    a_drag = f_drag / mass

    a = a_grav + a_drag

    return v.x, v.y, a.x, a.y
```

As usual, the parameters of the slope function are a `State` object, time, and a `System` object. In this example, we don't use `t`, but we can't leave it out because when `odeint` calls the slope function, it always provides the same arguments, whether they are needed or not.

The `State` object has four variables: `x` and `y` are the components of position; `vx` and `vy` are the components of velocity.

The return values from the slope function are the derivatives of these components. The derivative of position is velocity, so the first two return values are just `vx` and `vy`, the values we extracted from the `State` object. The derivative of velocity is acceleration, and that's what we have to compute.

The total acceleration of the baseball is the sum of accelerations due to gravity and drag. These quantities have both magnitude and direction, so we'll use `Vector` objects to represent them. Here's how it works:

- `a_grav` is the `Vector` representation of acceleration due to gravity, with magnitude `g` and direction along the negative y-axis.
- `v` is the `Vector` representation of velocity, which we create using the components `vx` and `vy`. This representation makes it easier to compute the drag force, which I explain in more detail below.
- `f_drag` is drag force, which is also a `Vector` quantity, with units of $\mathrm{kg\,m/s^2}$, also known as newtons (N).
- `a_drag` is acceleration due to drag, which we get by dividing `f_drag` by mass. The result is in units of acceleration, $\mathrm{m/s^2}$.
- `a` is total acceleration due to all forces, from which we can extract the components `a.x` and `a.y`.

The last thing I have to explain is the vector form of the drag equation. In Section 9.4 we saw the scalar form (a **scalar** is a single value, as contrasted with a vector, which contains components):

$$F_d = \frac{1}{2}\ \rho\ v^2\ C_d\ A$$

This form was sufficient when `v` represented the magnitude of velocity and all we wanted was the magnitude of drag force. But now `v` is a `Vector` and we want both the magnitude and angle of drag.

We can do that by replacing v^2, in the equation, with a vector that has the opposite direction as `v` and magnitude `v.mag**2`. In math notation, we can write

$$\vec{F}_d = -\frac{1}{2}\ \rho\ |v|\ \vec{v}\ C_d\ A$$

Where $|v|$ indicates the magnitude of v and the arrows on $\vec{F}_d$ and $\vec{v}$ indicate that they are vectors. Negation reverses the direction of a vector, so $\vec{F}_d$ is in the opposite direction of $\vec{v}$.

Translating to Python we have:

```
f_drag = -rho * v.mag * v * C_d * area / 2
```

Using vectors to represent forces and accelerations makes the code concise, readable, and less error-prone. In particular, when we add `a_grav` and `a_drag`, the directions are likely to be correct, because they are encoded in the `Vector` objects. And the units are certain to be correct, because otherwise Pint would report an error.

As always, we can test the slope function by running it with the initial conditions:

```
slope_func(system.init, 0, system)
```

10.4 Trajectories

Now we're ready to run the simulation:

```
run_odeint(system, slope_func)
```

The result is a `TimeFrame` object with one column for each of the state variables, `x`, `y`, `vx`, and `vy`. We can extract the x and y components like this:

```
xs = system.results.x
ys = system.results.y
```

And plot them like this:

```
plot(xs, label='x')
plot(ys, label='y')
```

Figure 10.1 shows the result. As expected, the x component increases monotonically, with decreasing velocity. And the y position climbs initially and then descends, falling slightly below 0 m after 5.1 s.

Another way to view the same data is to plot the x component on the x-axis and the y component on the y-axis, so the plotted line follows the trajectory of the ball through the plane:

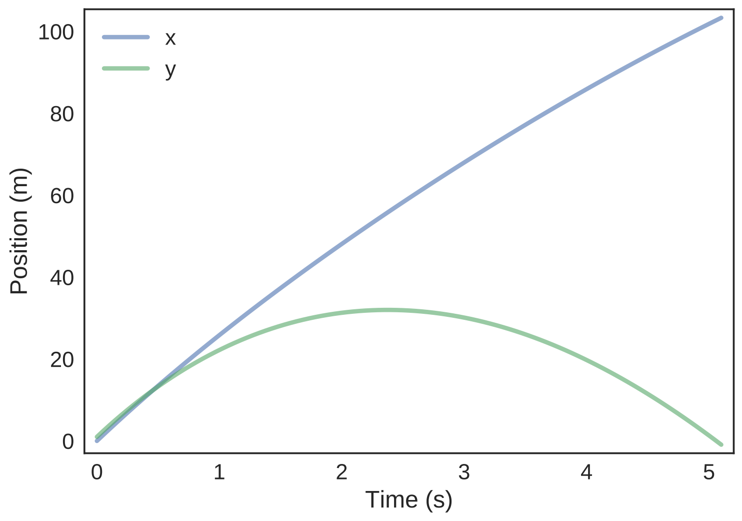


Figure 10.1: Simulated baseball flight, x and y components of position as a function of time.

```
plot(xs, ys, label='trajectory')
```

Figure 10.2 shows this way of visualizing the results, which is called a **trajectory plot** (see `http://modsimpy.com/trajec`).

A trajectory plot can be easier to interpret than a time series plot, because it shows what the motion of the projectile would look like (at least from one point of view). Both plots can be useful, but don't get them mixed up! If you are looking at a time series plot and interpreting it as a trajectory, you will be very confused.

Another useful way to visualize the results is animation. You can create animations using the `plot` function from the `modsim` library, with the `update` argument, which tells `plot` that the coordinates you provide should update the old coordinates. Here's an example:

```
for x, y in zip(xs, ys):
    plot(x, y, 'bo', update=True)
    sleep(0.01)
```

This example uses two features we have not seen before:

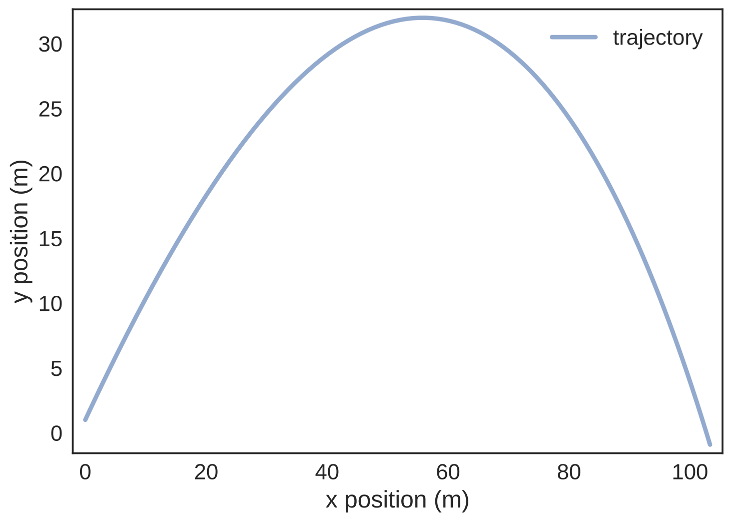


Figure 10.2: Simulated baseball flight, trajectory plot.

- `zip` takes two sequences (in this case they are `Series` objects) and "zips" them together; that is, it loops through both of them at the same time, selecting corresponding elements from each. So each time through the loop, `x` and `y` get the next elements from `xs` and `ys`.
- `sleep` causes the program to pause for a given duration, in seconds.

You can see what the results look like in the notebook for this chapter.

10.5 Finding the range

Suppose we want to find the launch angle that maximizes **range**, that is, the distance the ball travels in the air before landing. Assuming that the simulation runs long enough for the ball to land, we can compute the range like this:

1. Find the time when the height of the ball is maximized and select the part of the trajectory where the ball is falling. We have to do this in order to avoid problems with interpolation (see Section 9.3).

2. Then we use `interpolate` to find the time when the ball hits the ground, `t_land`.

3. Finally, we compute the x component at `t_land`.

Here's the function that does all that:

```
def interpolate_range(results):
    xs = results.x
    ys = results.y

    t_peak = ys.idxmax()

    descent = ys.loc[t_peak:]
    T = interp_inverse(descent)
    t_land = T(0)

    X = interpolate(xs, kind='cubic')
    return X(t_land)
```

`interpolate_range` uses `idxmax` to find the time when the ball hits its peak (see Section 5.9).

Then it uses `ys.loc` to extract only the points from `t_peak` to the end. The index in brackets includes a colon (`:`), which indicates that it is a **slice index**. In general, a slice selects a range of elements from a `Series`, specifying the start and end indices. For example, the following slice selects elements from `t_peak` to `t_land`, including both:

```
ys.loc[t_peak:t_land]
```

If we omit the first index, like this:

```
ys.loc[:t_land]
```

we get everything from the beginning to `t_land`. If we omit the second index, as in `interpolate_range`, we get everything from `t_peak` to the end of the `Series`. For more about indexing with `loc`, see `http://modsimpy.com/loc`.

Next it uses `interp_inverse`, which we saw in Section 9.3, to make `T`, which is an interpolation function that maps from height to time. So `t_land` is the time when height is 0.

Finally, it uses `interpolate` to make `X`, which is an interpolation function that maps from time to x component. So `X(t_land)` is the distance from home plate when the ball lands.

We can call `interpolate_range` like this:

```
interpolate_range(system.results)
```

The result is 103 m, which is about 337 feet.

10.6 Optimization

To find the angle that optimizes range, we need a function that takes launch angle as a parameter and returns range:

```
def range_func(angle, condition):
    condition.set(angle=angle)
    system = make_system(condition)
    run_odeint(system, slope_func)
    x_range = interpolate_range(system.results)
    return x_range
```

We can call `range_func` directly like this:

```
range_func(45, condition)
```

And we can sweep a sequence of angles like this:

```
angles = linspace(30, 60, 11)
sweep = SweepSeries()

for angle in angles:
    x_range = range_func(angle, condition)
    print(angle, x_range)
    sweep[angle] = x_range
```

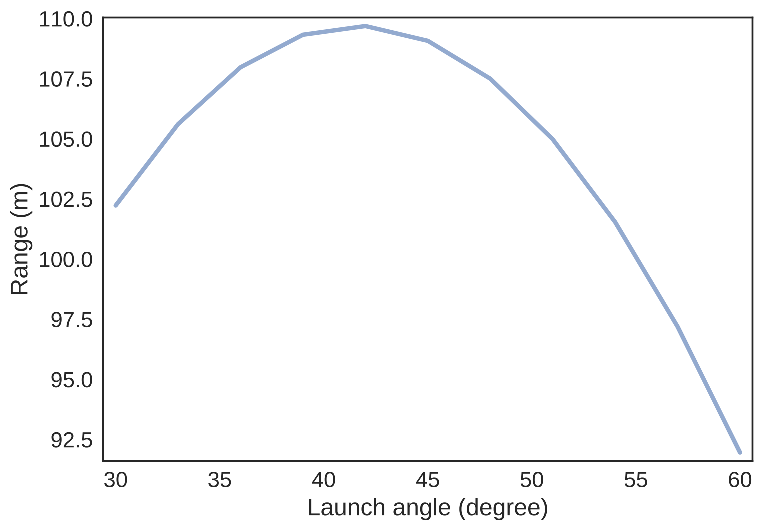


Figure 10.3: Distance from home plate as a function of launch angle, with fixed velocity.

Figure 10.3 shows the results. It looks like the optimal angle is between 40° and 45° (at least for this definition of "optimal").

We can find the optimal angle more precisely and more efficiently using `max_bounded`, which is a function in the `modsim` library that uses `scipy.opimize.minimize_scalar` (see `http://modsimpy.com/minimize`).

Here's how we run it:

```
res = max_bounded(range_func, [0, 90], condition)
```

The first parameter is the function we want to maximize. The second is the range of values we want to search; in this case it's the range of angles from 0° to 90°. The third argument is the `Condition` object, which gets passed along as an argument when `max_bounded` calls `range_func`.

The result from `max_bounded` is an `OptimizeResult` object, which contains several variables. The ones we want are `x`, which is the angle that yielded the highest range, and `fun`, which is the value of `range_func` when it's evaluated at `x`, that is, range when the baseball is launched at the optimal angle.

10.7 Finishing off the problem

In the notebook for this chapter, you'll have to chance to finish off the Manny Ramirez problem. There are a few things you'll have to do:

- In the previous section the "optimal" launch angle is the one that maximizes range, but that's not what we want. Rather, we want the angle that maximizes the height of the ball when it gets to the wall (310 feet from home plate). So you'll have to write a height function to compute it, and then use `max_bounded` to find the revised optimum.
- Once you can find the optimal angle for any velocity, you have to find the minimum velocity that gets the ball over the wall. You'll write a function that takes a velocity as a parameter, computes the optimal angle for that velocity, and returns the height of the ball, at the wall, using the optimal angle.
- Finally, you'll use `fsolve` to find the velocity that makes the height, at the wall, just barely 37 feet.

The notebook provides some additional hints, but at this point you should have everything you need. Good luck!

If you enjoy this exercise, you might be interested in this paper: "How to hit home runs: Optimum baseball bat swing parameters for maximum range trajectories", by Sawicki, Hubbard, and Stronge, at `http://aapt.scitation.org/doi/abs/10.1119/1.1604384`.

Chapter 11

Rotation

In this chapter we model systems that involve rotating objects. In general, rotation is complicated: in three dimensions, objects can rotate around three axes; objects are often easier to spin around some axes than others; and they may be stable when spinning around some axes but not others.

If the configuration of an object changes over time, it might become easier or harder to spin, which explains the surprising dynamics of gymnasts, divers, ice skaters, etc.

And when you apply a twisting force to a rotating object, the effect is often contrary to intuition. For an example, see this video on gyroscopic precession `http://modsimpy.com/precess`.

In this chapter, we will not take on the physics of rotation in all its glory. Rather, we will focus on simple scenarios where all rotation and all twisting forces are around a single axis. In that case, we can treat some vector quantities as if they were scalars (in the same way that we sometimes treat velocity as a scalar with an implicit direction).

This approach makes it possible to simulate and analyze many interesting systems, but you will also encounter systems that would be better approached with the more general toolkit.

The fundamental ideas in this chapter are **angular velocity**, **angular acceleration**, **torque**, and **moment of inertia**. If you are not already familiar

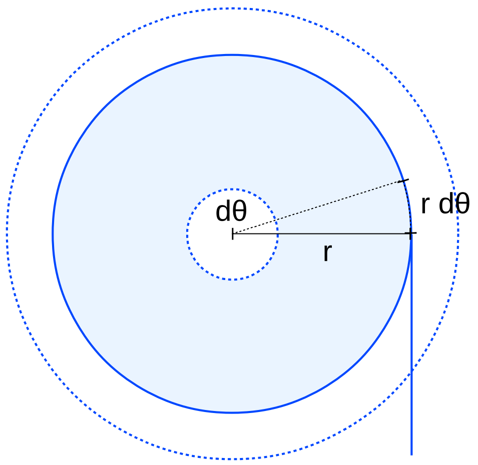


Figure 11.1: Diagram of a roll of toilet paper, showing change in paper length as a result of a small rotation, $d\theta$.

with these concepts, I will define them as we go along, and I will point to additional reading.

As an exercise at the end of the chapter, you will use these tools to simulate the behavior of a yo-yo (see `http://modsimpy.com/yoyo`). But we'll work our way up to it gradually, starting with toilet paper.

You can view the code for this chapter at `http://modsimpy.com/chap11`. For instructions on downloading and running the code, see Section 0.4.

11.1 The physics of toilet paper

As a simple example of a system with rotation, we'll simulate the manufacture of a roll of toilet paper. Starting with a cardboard tube at the center, we will roll up 47 m of paper, the typical length of a roll of toilet paper in the U.S. (see `http://modsimpy.com/paper`).

Figure 11.1 shows a diagram of the system: r represents the radius of the roll at a point in time. Initially, r is the radius of the cardboard core, R_{min}. When the roll is complete, r is R_{max}.

I'll use θ to represent the total rotation of the roll in radians. In the diagram, $d\theta$ represents a small increase in θ, which corresponds to a distance along the circumference of the roll of $r\ d\theta$.

Finally, I'll use y to represent the total length of paper that's been rolled. Initially, $\theta = 0$ and $y = 0$. For each small increase in θ, there is a corresponding increase in y:

$$dy = r\ d\theta$$

If we divide both sides by a small increase in time, dt, we get a differential equation for y as a function of time.

$$\frac{dy}{dt} = r\frac{d\theta}{dt}$$

As we roll up the paper, r increases, too. Assuming that r increases by a fixed amount per revolution, we can write

$$dr = k\ d\theta$$

Where k is an unknown constant we'll have to figure out. Again, we can divide both sides by dt to get a differential equation in time:

$$\frac{dr}{dt} = k\frac{d\theta}{dt}$$

Finally, let's assume that θ increases at a constant rate of 10 rad/s (about 95 revolutions per minute):

$$\frac{d\theta}{dt} = 10$$

This rate of change is called an **angular velocity**. Now we have a system of three differential equations we can use to simulate the system.

11.2 Implementation

At this point we have a pretty standard process for writing simulations like this. First, we'll get the units we need from Pint:

```
radian = UNITS.radian
m = UNITS.meter
s = UNITS.second
```

And create a `Condition` object with the parameters of the system:

```
condition = Condition(Rmin = 0.02 * m,
                      Rmax = 0.055 * m,
                      L = 47 * m,
                      duration = 130 * s)
```

`Rmin` and `Rmax` are the initial and final values for the radius, `r`. `L` is the total length of the paper, and `duration` is the length of the simulation in time.

Then we use the `Condition` object to make a `System` object:

```
def make_system(condition):
    unpack(condition)

    init = State(theta = 0 * radian,
                 y = 0 * m,
                 r = Rmin)

    k = estimate_k(condition)
    ts = linspace(0, duration, 101)

    return System(init=init, k=k, ts=ts)
```

The initial state contains three variables, `theta`, `y`, and `r`.

To get started, we'll estimate a reasonable value for `k`; then in Section 11.3 we'll figure it out exactly. Here's how we compute the estimate:

```
def estimate_k(condition):
    unpack(condition)

    Ravg = (Rmax + Rmin) / 2
    Cavg = 2 * pi * Ravg
    revs = L / Cavg
    rads = 2 * pi * revs
    k = (Rmax - Rmin) / rads
    return k
```

`Ravg` is the average radius, half way between `Rmin` and `Rmax`, so `Cavg` is the circumference of the roll when `r` is `Ravg`.

`revs` is the total number of revolutions it would take to roll up length `L` if `r` were constant at `Ravg`. And `rads` is just `revs` converted to radians.

Finally, `k` is the change in `r` for each radian of revolution. For these parameters, `k` is about `2.8e-5` m/rad.

Now we can use the differential equations from Section 11.1 to write a slope function:

```
def slope_func(state, t, system):
    theta, y, r = state
    unpack(system)

    omega = 10 * radian / s
    dydt = r * omega
    drdt = k * omega

    return omega, dydt, drdt
```

As usual, the slope function takes a `State` object, a time, and a `System` object. The `State` object contains the hypothetical values of `theta`, `y`, and `r` at time `t`. The job of the slope function is to compute the time derivatives of these values. The time derivative of `theta` is angular velocity, which is often denoted `omega`.

Now we can run the simulation like this:

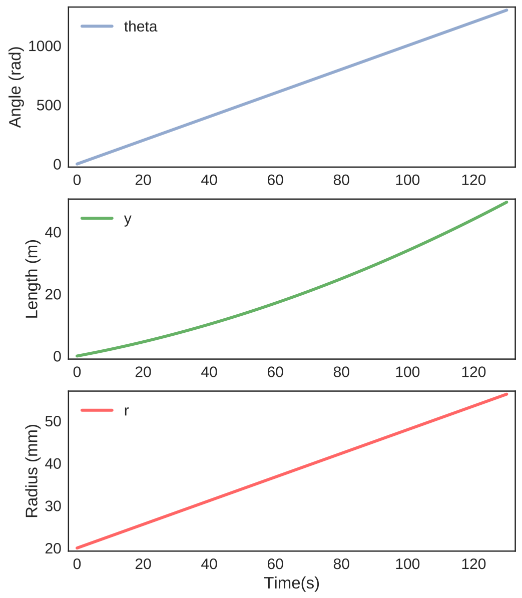


Figure 11.2: Results from paper rolling simulation, showing rotation, length, and radius over time.

```
run_odeint(system, slope_func)
```

Figure 11.2 shows the results. `theta` grows linearly over time, as we should expect. As a result, `r` also grows linearly. But since the derivative of `y` depends on `r`, and `r` is increasing, `y` grows with increasing slope.

Because this system is so simple, it is almost silly to simulate it. As we'll see in the next section, it is easy enough to solve the differential equations analytically. But it is often useful to start with a simple simulation as a way of exploring and checking assumptions.

In order to get the simulation working, we have to get the units right, which can help catch conceptual errors early. And by plugging in realistic parameters, we can detect errors that cause unrealistic results. For example, in this system we can check:

- The total time for the simulation is about 2 minutes, which seems plausible for the time it would take to roll 47 m of paper.

- The final value of `theta` is about 1250 rad, which corresponds to about 200 revolutions, which also seems plausible.
- The initial and final values for `r` are consistent with `Rmin` and `Rmax`, as we intended when we chose `k`.

But now that we have a working simulation, it is also useful to do some analysis.

11.3 Analysis

The differential equations in Section 11.1 are simple enough that we can just solve them. Since angular velocity is constant:

$$\frac{d\theta}{dt} = \omega$$

We can find θ as a function of time by integrating both sides:

$$\theta(t) = \omega t + C_1$$

With the initial condition $\theta(0) = 0$, we find $C_1 = 0$. Similarly,

$$\frac{dr}{dt} = k\omega \tag{11.1}$$

So

$$r(t) = k\omega t + C_2$$

With the initial condition $r(0) = R_{min}$, we find $C_2 = R_{min}$. Then we can plug the solution for r into the equation for y:

$$\begin{aligned} \frac{dy}{dt} &= r\omega \\ &= [k\omega t + R_{min}]\,\omega \end{aligned} \tag{11.2}$$

Integrating both sides yields:

$$y(t) = \left[k\omega t^2/2 + R_{min}t\right]\omega + C_3$$

So y is a parabola, as you might have guessed. With initial condition $y(0) = 0$, we find $C_3 = 0$.

We can also use these equations to find the relationship between y and r, independent of time, which we can use to compute k. Using a move we saw in Section 6.5, I'll divide Equations 11.1 and 11.2, yielding

$$\frac{dr}{dy} = \frac{k}{r}$$

Separating variables yields

$$r\ dr = k\ dy$$

Integrating both sides yields

$$r^2/2 = ky + C$$

When $y = 0$, $r = R_{min}$, so

$$C = \frac{1}{2} R_{min}^2$$

Solving for y, we have

$$y = \frac{1}{2k}(r^2 - R_{min}^2) \tag{11.3}$$

When $y = L$, $r = R_{max}$; substituting in those values yields

$$L = \frac{1}{2k}(R_{max}^2 - R_{min}^2)$$

Solving for k yields

$$k = \frac{1}{2L}(R_{max}^2 - R_{min}^2) \tag{11.4}$$

Plugging in the values of the parameters yields `2.8e-5` m/rad, the same as the "estimate" we computed in Section 11.2. In this case the estimate turns out to be exact.

11.4 Torque

Now that we've rolled up the paper, let's unroll it. Specifically, let's simulate a kitten unrolling toilet paper. As reference material, see this video: `http://modsimpy.com/kitten`.

The interactions of the kitten and the paper roll are complex. To keep things simple, let's assume that the kitten pulls down on the free end of the roll with constant force. Also, we will neglect the friction between the roll and the axle. This will not be a particularly realistic model, but it will allow us to explore two new concepts, angular acceleration and torque.

Just as linear acceleration is the derivative of velocity, **angular acceleration** is the derivative of angular velocity. And just as linear acceleration is caused by force, angular acceleration is caused by the rotational version of force, **torque**. If you are not familiar with torque, you can read about it at http://modsimpy.com/torque.

In general, torque is a vector quantity, defined as the **cross product** of $\vec{r}$ and $\vec{F}$, where $\vec{r}$ is the **lever arm**, a vector from the point of rotation to the point where the force is applied, and $\vec{F}$ is the vector that represents the magnitude and direction of the force.

However, for the problems in this chapter, we only need the *magnitude* of torque; we don't care about the direction. In that case, we can compute

$$\tau = rF \sin\theta$$

where τ is torque, r is the length of the lever arm, F is the magnitude of force, and θ is the angle between $\vec{r}$ and $\vec{F}$. In the toilet paper scenario, if the kitten pulls on the loose end of the paper, the force on the roll is always perpendicular to the lever arm, so $\sin\theta = 1$.

Since torque is the product of a length and a force, it is expressed in newton meters (N m).

Figure 11.3 shows the paper roll with r, F, and τ. As a vector quantity, the direction of τ is into the page, but we only care about its magnitude for now.

11.5 Moment of inertia

In the same way that linear acceleration is related to force by Newton's second law of motion, $F = ma$, angular acceleration is related to torque by another form of Newton's law:

$$\tau = I\alpha$$

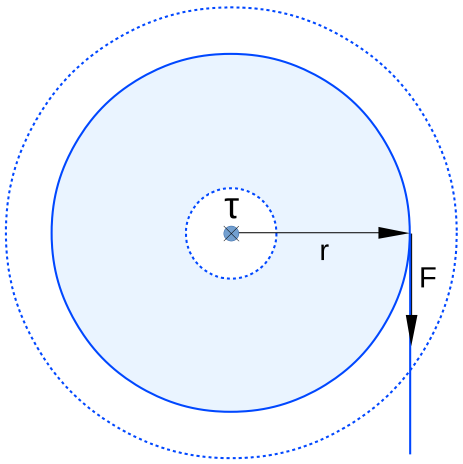


Figure 11.3: Diagram of a roll of toilet paper, showing a force, lever arm, and the resulting torque.

Where α is angular acceleration and I is **moment of inertia**. Just as mass is what makes it harder to accelerate an object[1], moment of inertia is what makes it harder to spin an object.

In the most general case, a 3-D object rotating around an arbitrary axis, moment of inertia is a tensor, which is a function that takes a vector as a parameter and returns a vector as a result.

Fortunately, in a system where all rotation and torque happens around a single axis, we don't have to deal with the most general case. We can treat moment of inertia as a scalar quantity.

For a small point with mass m, rotating around a point at distance r, the moment of inertia is $I = mr^2$, in SI units $\mathrm{kg\,m^2}$. For more complex objects, we can compute I by dividing the object into small masses, computing moments of inertia for each mass, and adding them up.

However, for most simple shapes, people have already done the calculations; you can just look up the answers.

[1] That might sound like a dumb way to describe mass, but its actually one of the fundamental definitions.

11.6 Unrolling

Let's work on simulating the kitten unrolling the toilet paper. Here's the `Condition` object with the parameters we'll need:

```
condition = Condition(Rmin = 0.02 * m,
                      Rmax = 0.055 * m,
                      L = 47 * m,
                      Mcore = 15e-3 * kg,
                      Mroll = 215e-3 * kg,
                      tension = 2e-4 * N,
                      duration = 180 * s)
```

As before, `Rmin` is the minimum radius and `Rmax` is the maximum. `L` is the length of the paper. `Mcore` is the mass of the cardboard tube at the center of the roll; `Mroll` is the mass of the paper. `tension` is the force applied by the kitten, in N. I chose a value that yields plausible results.

At http://modsimpy.com/moment you can find moments of inertia for simple geometric shapes. I'll model the cardboard tube at the center of the roll as a "thin cylindrical shell", and the paper roll as a "thick-walled cylindrical tube with open ends".

The moment of inertia for a thin shell is just mr^2, where m is the mass and r is the radius of the shell.

For a thick-walled tube the moment of inertia is

$$I = \frac{\pi \rho h}{2}(r_2^4 - r_1^4)$$

where ρ is the density of the material, h is the height of the tube, r_2 is the outer diameter, and r_1 is the inner diameter.

Since the outer diameter changes as the kitten unrolls the paper, we have to compute the moment of inertia, at each point in time, as a function of the current radius, `r`. Here's the function that does it:

```
def moment_of_inertia(r, system):
    unpack(system)
    Icore = Mcore / 2 * Rmin**2
    Iroll = pi * rho_h / 2 * (r**4 - Rmin**4)
    return Icore + Iroll
```

`rho_h` is the product of density and height, ρh, which is the mass per area. `rho_h` is computed in `make_system`:

```
def make_system(condition):
    unpack(condition)

    init = State(theta = 0 * radian,
                 omega = 0 * radian/s,
                 y = L)

    area = pi * (Rmax**2 - Rmin**2)
    rho_h = Mroll / area
    k = (Rmax**2 - Rmin**2) / 2 / L / radian
    ts = linspace(0, duration, 101)

    return System(init=init, k=k, rho_h=rho_h,
                  Rmin=Rmin, Rmax=Rmax,
                  Mcore=Mcore, Mroll=Mroll,
                  ts=ts)
```

`make_system` also computes `k`, using Equation 11.4. Now we can write the slope function:

```
def slope_func(state, t, system):
    theta, omega, y = state
    unpack(system)

    r = sqrt(2*k*y + Rmin**2)
    I = moment_of_inertia(r, system)
    tau = r * tension
    alpha = tau / I
    dydt = -r * omega

    return omega, alpha, dydt
```

This slope function is similar to the previous one (Section 11.2), with a few changes:

- `r` is no longer part of the `State` object. Instead, we compute `r` at each time step, based on the current value of `y`, by Equation 11.3.
- Because `r` changes over time, we have to compute moment of inertia, `I`, at each time step[2].
- Angular velocity, `omega`, is no longer constant. Instead, we compute torque, `tau`, and angular acceleration, `alpha`, at each time step.
- I quietly changed the definition of `theta` so positive values of `theta` correspond to clockwise rotation, so `dydt = -r * omega`; that is, positive values of `omega` yield decreasing values of `y`, the amount of paper still on the roll.

`slope_func` returns `omega`, `alpha`, and `dydt`, which are the derivatives of `theta`, `omega`, and `y`, respectively.

Now we're ready to run the simulation. Figure 11.4 shows the results. Again, we can check the results to see if they seem plausible:

[2]Actually, this is more of a problem than I have made it seem. In the same way that $F = ma$ only applies when m is constant, $\tau = I\alpha$ only applies when I is constant. When I varies, we usually have to use a more general version of Newton's law. However, in this example, mass and moment of inertia vary together in a way that makes the simple approach work out.

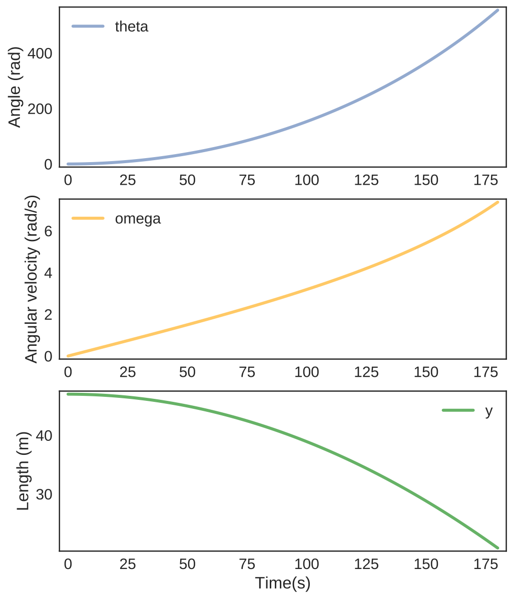


Figure 11.4: Simulation results showing rotation, angular velocity, and length over time.

- Angular velocity, `omega`, increases almost linearly at first, as constant force yields almost constant torque. Then, as the radius decreases, the lever arm decreases, yielding lower torque, but moment of inertia decreases even more, yielding higher angular acceleration.

- The final value of `omega` is 7.4 rad/s, which is close to one revolution per second, so that seems plausible.

- The final value of `theta` is 555 rad, which is about 88 revolutions.

- The final value of `y` is 21 m of paper left on the roll, which means the kitten pulled off 26 m in two minutes. That doesn't seem impossible, although it is based on a level of consistency and focus that is unlikely in a kitten.

This model yields results that seem reasonable, but remember that I chose the force applied by the kitten arbitrarily, and the model ignores friction between

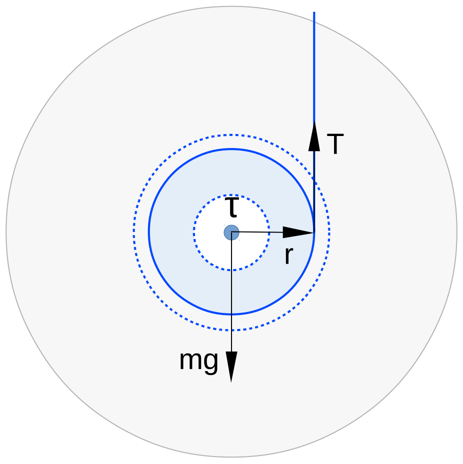


Figure 11.5: Diagram of a yo-yo showing forces due to gravity and tension in the string, the lever arm of tension, and the resulting torque.

the paper roll and the axle. This example is not meant to be particularly serious, but it is good preparation for the next problem, which is a little more interesting.

11.7 Simulating a yo-yo

Suppose you are holding a yo-yo with a length of string wound around its axle, and you drop it while holding the end of the string stationary. As gravity accelerates the yo-yo downward, tension in the string exerts a force upward. Since this force acts on a point offset from the center of mass, it exerts a torque that causes the yo-yo to spin.

Figure 11.5 is a diagram of the forces on the yo-yo and the resulting torque. The outer shaded area shows the body of the yo-yo. The inner shaded area shows the rolled up string, the radius of which changes as the yo-yo unrolls.

In this model, we can't figure out the linear and angular acceleration independently; we have to solve a system of equations:

$$\sum F = ma$$
$$\sum \tau = I\alpha$$

where the summations indicate that we are adding up forces and torques.

As in the previous examples, linear and angular velocity are related because of the way the string unrolls:

$$\frac{dy}{dt} = -r\frac{d\theta}{dt}$$

In this example, the linear and angular accelerations have opposite sign. As the yo-yo rotates counter-clockwise, θ increases and y, which is the length of the rolled part of the string, decreases.

Taking the derivative of both sides yields a similar relationship between linear and angular acceleration:

$$\frac{d^2y}{dt^2} = -r\frac{d^2\theta}{dt^2}$$

Which we can write more concisely:

$$a = -r\alpha$$

This relationship is not a general law of nature; it is specific to scenarios like this where there is rolling without stretching or slipping.

Because of the way we've set up the problem, y actually has two meanings: it represents the length of the rolled string and the height of the yo-yo, which decreases as the yo-yo falls. Similarly, a represents acceleration in the length of the rolled string and the height of the yo-yo.

We can compute the acceleration of the yo-yo by adding up the linear forces:

$$\sum F = T - mg = ma$$

Where T is positive because the tension force points up, and mg is negative because gravity points down.

Because gravity acts on the center of mass, it creates no torque, so the only torque is due to tension:

$$\sum \tau = Tr = I\alpha$$

Positive (upward) tension yields positive (counter-clockwise) angular acceleration.

Now we have three equations in three unknowns, T, a, and α, with I, m, g, and r as known quantities. It is simple enough to solve these equations by hand, but we can also get SymPy to do it for us:

```
T, a, alpha, I, m, g, r = symbols('T a alpha I m g r')
eq1 = Eq(a, -r * alpha)
eq2 = Eq(T - m*g, m * a)
eq3 = Eq(T * r, I * alpha)
soln = solve([eq1, eq2, eq3], [T, a, alpha])
```

The results are

$$\begin{aligned} T &= mgI/I^* \\ a &= -mgr^2/I^* \\ \alpha &= mgr/I^* \end{aligned}$$

where I^* is the augmented moment of inertia, $I + mr^2$.

To simulate the system, we don't really need T; we can plug a and α directly into the slope function.

At this point you have everything you need to simulate the descent of a yo-yo. In the notebook for this chapter you will have a chance to finish off the exercise.

Chapter 12

Second order systems

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