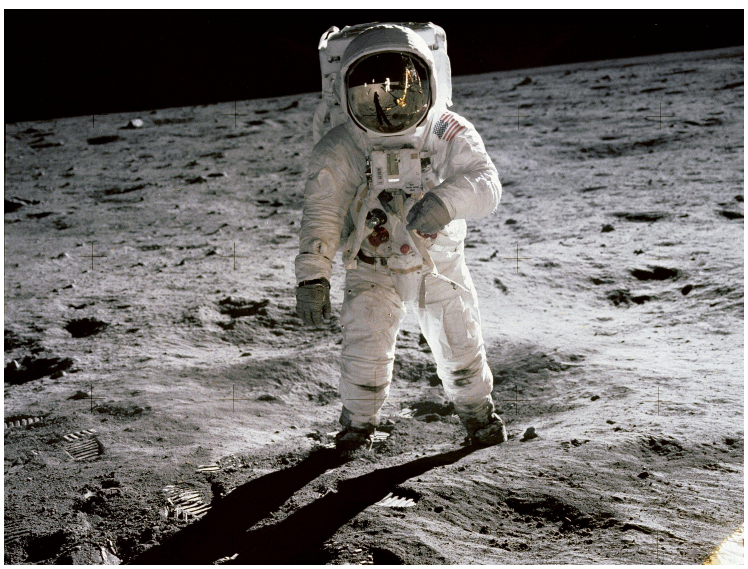
Labs for Foundations of Applied Mathematics

Volume 4
Modeling with Dynamics and Control

Jeffrey Humpherys & Tyler J. Jarvis, managing editors



List of Contributors

B. Barker
Brigham Young University

E. Evans
Brigham Young University

R. Evans
Brigham Young University

J. Grout
Drake University

J. Humpherys
Brigham Young University

T. Jarvis
Brigham Young University

J. Whitehead
Brigham Young University

J. Adams
Brigham Young University

J. Bejarano
Brigham Young University

Z. Boyd
Brigham Young University

M. Brown
Brigham Young University

A. Carr
Brigham Young University

C. Carter
Brigham Young University

T. Christensen
Brigham Young University

M. Cook
Brigham Young University

R. Dorff
Brigham Young University

B. Ehlert
Brigham Young University

M. Fabiano
Brigham Young University

K. Finlinson
Brigham Young University

J. Fisher
Brigham Young University

R. Flores
Brigham Young University

R. Fowers
Brigham Young University

A. Frandsen
Brigham Young University

R. Fuhriman
Brigham Young University

T. Gledhill
Brigham Young University

S. Giddens
Brigham Young University

C. Gigena
Brigham Young University

M. Graham
Brigham Young University

F. Glines
Brigham Young University

C. Glover
Brigham Young University

M. Goodwin
Brigham Young University

R. Grout
Brigham Young University

D. Grundvig
Brigham Young University

E. Hannesson
Brigham Young University

K. Harmer
Brigham Young University

J. Hendricks
Brigham Young University

A. Henriksen
Brigham Young University

I. Henriksen
Brigham Young University

C. Hettinger
Brigham Young University

S. Horst
Brigham Young University

K. Jacobson
Brigham Young University

R. Jenkins
Brigham Young University

J. Leete
Brigham Young University

J. Lytle
Brigham Young University

E. Manner
Brigham Young University

R. McMurray
Brigham Young University

S. McQuarrie
Brigham Young University

D. Miller
Brigham Young University

J. Morrise
Brigham Young University

M. Morrise
Brigham Young University

A. Morrow
Brigham Young University

R. Murray
Brigham Young University

J. Nelson
Brigham Young University

E. Parkinson
Brigham Young University

M. Probst
Brigham Young University

M. Proudfoot
Brigham Young University

D. Reber
Brigham Young University

H. Ringer
Brigham Young University

C. Robertson
Brigham Young University

M. Russell
Brigham Young University

R. Sandberg
Brigham Young University

C. Sawyer
Brigham Young University

M. Stauffer
Brigham Young University

E. Steadman
Brigham Young University

J. Stewart
Brigham Young University

S. Suggs
Brigham Young University

A. Tate
Brigham Young University

T. Thompson
Brigham Young University

M. Victors
Brigham Young University

E. Walker
Brigham Young University

J. Webb
Brigham Young University

R. Webb
Brigham Young University

J. West
Brigham Young University

A. Zaitzeff
Brigham Young University

This project is funded in part by the National Science Foundation, grant no. TUES Phase II DUE-1323785.

Preface

This lab manual is designed to accompany the textbook *Foundations of Applied Mathematics Volume 4: Modeling with Dynamics and Control* by Humpherys, Jarvis and Whitehead. The labs focus on numerical methods for solving ordinary and partial differential equations, including applications to optimal control problems. The reader should be familiar with Python [VD10] and its NumPy [Oli06, ADH$^+$01, Oli07] and Matplotlib [Hun07] packages before attempting these labs. See the Python Essentials manual for introductions to these topics.

Contents

Part I

Labs

1 Introduction to Matplotlib: 3D Plotting and Animations

Lab Objective: *3D plots and animations are useful in visualizing solutions to ODEs and PDEs found in many dynamics and control problems. In this lab we explore the functionality contained in the 3D plotting and animation libraries in Matplotlib.*

Introduction

Matplotlib is a Python library that contains tools for creating plots in multiple dimensions. The library contains important classes that are needed to create plots. The most important objects to understand in this lab are figure objects, axes objects, and line objects. These three objects are created using the following code.

```
>>> import matplotlib.pyplot as plt
>>> fig = plt.figure()              # Create figure object.
>>> ax = fig.add_subplot(111)       # Create axes object.
>>> line2d, = plt.plot([],[])       # Create empty 2D Line object
>>> line3d, = plt.plot([],[],[])    # Create empty 3D line object
```

Recall that `plt.figure()` creates a `matplotlib.figure.Figure` object, which is the window that is displayed when `plt.show()` is called. 3D plotting and animation both require explicitly defining the `Figure` object, as shown above. This allows for the object to be updated and modified, as will be explained later in the lab.

`Figure` objects contain `matplotlib.axes._subplots.AxesSubplot` objects, called *axes*. Axes are spaces to plot on, and are created by the `add_subplot()` method of a `Figure` object. Figures can have multiple axes.

Calling `plt.plot()` returns a list of line objects. For example, supposing `x1`, `y1`, `x2`, and `y2` are arrays containing data for two separate curves, then calling `plt.plot(x1, y1, x2, y2)` will return a list with two elements. Each element of the list is a `matplotlib.lines.Line2D` object. If the axes is three-dimensional, then the returned list will contain `matplotlib.lines.Line3D` objects. Because this function call returns a list, if only one line is plotted, adding a trailing comma to the variable name will assign the name to the first element of the returned list. You can alternatively reference the zero index of the returned list, but using a trailing comma is standard.

Animation Background

The animation library in Matplotlib contains a class called `FuncAnimation`. We will use this class throughout this lab. `FuncAnimation` requires a user-defined *update* function that controls the plot for each frame of the animation. This grants the user wide flexibility and control of the resulting animation. The following steps describe the process of creating a simple animated plot using the `FuncAnimation` class.

1. Compute all data to be plotted.
2. Explicitly define figure object.
3. Define line objects to be altered dynamically.
4. Create function to update line objects.
5. Create `FuncAnimation` object.
6. Display using `plt.show()`.

These steps will be explained by way of an example. The arrays `x` and `y` contain data giving the location of a particle moving in the plane. To visualize this motion, one could animate the particle as well as display the trajectory that the particle has traveled. For this animation, two separate `Line2D` objects must be created on an axes object. The first, `particle` will be for the position of the particle itself, and the second, `traj` will be for the trajectory that the particle has traveled. Note that these objects are created with empty lists of data. The update function will be used to dynamically set the data to be plotted in these line objects.

```
>>> import matplotlib.animation as animation
>>> import numpy as np
>>> t = np.linspace(0,2*np.pi,100)
>>> x = np.sin(t)
>>> y = t**2
>>> fig = plt.figure()
>>> ax = fig.add_subplot(111)
>>> ax.set_xlim((-1.1,1.1))
>>> ax.set_ylim((0,40))
>>> particle, = plt.plot([],[], marker='o', color='r')
>>> traj, = plt.plot([],[], color='r', alpha=0.5)
```

The update function must be defined a specific way in order to interact properly with the `matplotlib.animation.FuncAnimation` object. The update function must accept the current frame index as its first input parameter and it must return a list or tuple of line objects. The current frame index is used to access the data to be plotted in the current frame. Both 2D and 3D line objects have the built-in method `.set_data()`. This function takes in two one-dimensional arrays representing x and y values to plot. This allows a single line object to display different data for each frame. Inside the update function, `.set_data()` is called on the line objects with the relevant data as inputs.

```
>>> def update(i):
>>>     particle.set_data(x[i],y[i])
>>>     traj.set_data(x[:i+1],y[:i+1])
>>>     return particle,traj
```

Next, the `FuncAnimation` object is created. The argument `frames` specifies the iterable representing the frame indices. If `frames` is an integer, it is treated as the iterable `range(frames)`. After the `FuncAnimation` object is created, `plt.show()` displays the animation.

```
>>> ani = FuncAnimation(fig, update, frames=range(100), interval=25)
>>> plt.show()
```

The following table shows more parameters that can be passed into FuncAnimation.

Parameter	Description
`fargs` (tuple)	Additional arguements to pass update function
`interval` (float)	Delay between frames in milliseconds
`repeat` (bool)	Determines whether animation repeats (Default True)
`blit` (bool)	Determines whether blitting is used (Default False)

Note

When using FuncAnimation, it is essential that a reference is kept to the instance of the class. The animation is advanced by a timer and if a reference is not held for the object, `Python` will automatically garbage collect and the animation will stop.

Problem 1. Use the FuncAnimation class to animate the function $y = \sin(x + 0.1t)$ where $x \in [0, 2\pi]$, and t ranges from 0 to 100 seconds.

3D Plotting Introduction

3D plotting is very similar to 2D plotting. The main difference is that a set of 3D axes must be created within the figure object. A 3D axes object is created using the additional keyword argument `projection='3d'`, as shown below. Note that the Axes3D submodule must first be imported in order to create the 3D axis.

```
>>> from mpl_toolkits.mplot3d import Axes3D
>>>
>>> # Create figure object.
>>> fig = plt.figure()
>>>
>>> # Create 3D axis object using add_subplot().
>>> ax = fig.add_subplot(111, projection='3d')
```

3D Static Plotting

When the axes object is explicitly defined, plots are generated by calling the chosen plot function (such as `ax.plot()` on the axes object. Additional information on the use of axes objects can be found here: https://matplotlib.org/api/axes_api.html.

Problem 2. The orbits for Mercury, Venus, Earth, and Mars are stored in the file `orbits.npz`. The file contains four NumPy arrays: `mercury`, `venus`, `earth`, and `mars`. The first column of each array contains the x-coordinates, the second column contains the y-coordinates, and the third column contians the z-coordinates of each planet, all relative to the Sun, and expressed in AU (astronomical units, the average distance between Earth and the Sun, approximately 150 million kilometers).

Use `np.load('orbits.npz')` to load the data for the four planets' orbits. Create a 3D plot of the orbits, and compare your results with Figure 1.1.

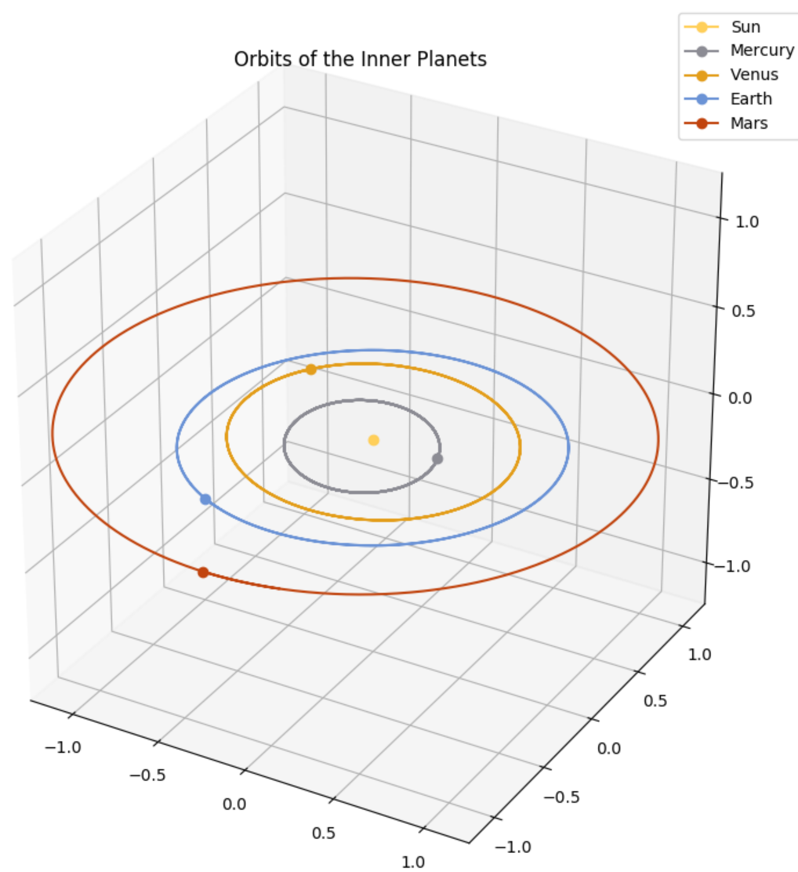


Figure 1.1: The solution to Problem 2.

3D Animations

The key difference between 2D and 3D animations is that the `.set_data()` method does not support setting the `z` values. Instead, set the `x` and `y` values with `.set_data()` as before, and then set the `z` values with `.set_3d_properties()`. The `.set_3d_properties()` function call is also made inside the update function.

Saving Animations

Animation in 3D requires more careful consideration than in the 2D case. When `matplotlib` displays a 3D plot, it does so in an interactive figure that allows the user to change the camera angle and position. Since 3D rendering is more computationally expensive than 2D rendering, interactive views of 3D animations often have poor framerates and choppy rendering. The solution is to use the `matplotlib.animation` module's `FuncAnimation.save()` method. With an installed video encoder, this allows Matplotlib to render a video file of the animation, which can then be displayed inline inside a Jupyter Notebook, or viewed using any video player supporting the chosen filetype.

Unfortunately, Matplotlib does not come with a built-in video encoder. The `matplotlib.animation` module supports several third-party encoders. FFmpeg is a lightweight solution which can be obtained from: https://www.ffmpeg.org/download.html.

To prevent the animation from displaying while it is being rendered as video, use `plt.ioff()`. This turns off matplotlib's interactive mode until `plt.ion()` is called. After creating the animation object, use its `.save()` method with the desired filename to render and save the video. The following code is given for reference:

```
>>> animation.writer = animation.writers['ffmpeg']
>>> plt.ioff()    # Turn off interactive mode to hide rendering animations
>>>
>>> # Code to create figure, axes, update function
>>>
>>> ani = animation.FuncAnimation(fig,update,frames)
>>> ani.save('my_animation.mp4')
```

Problem 3. Each row of the arrays in `orbits.npz` gives the position of the planets at evenly spaced time points. The arrays correspond to 1400 points in time over a 700 day period (beginning on 2018-5-30). Create a 3D animation of the planet orbits. Display lines for the trajectories of the orbits and points for the current positions of the planets at each point in time. Your `update()` function will need to return a list of Line3D objects, one for each orbit trajectory and one for each planet position marker. Using `animation.save()`, save your animated plot as "planet_ani.mp4".

To display the mp4 video in a Jupyter Notebook, run the following code in a markdown cell:

```
<video src="planet_ani.mp4" controls>
```

Surface Plotting

3D surface plotting is very similar to regular 3D plotting discussed earlier. The difference with surface plots is that they require first creating a *meshgrid* for X and Y. Meshgrids are created using the NumPy command `np.meshgrid(x, y)` where `x` and `y` are 1D arrays representing the x and y coordinates of the grid. This function creates 2D arrays `X` and `Y` that combined give cartesian cordinates for every point made from the `x` and `y` arrays.

Once a meshgrid is defined, a surface plot is generated by calling `ax.plot_surface(X, Y, Z)`, where `Z` is a 2D array of height values that is the same shape as `X` and `Y`.

Problem 4. Make a surface plot of the bivariate normal density function given by:

$$f(\mathbf{x}) = \frac{1}{\sqrt{det(2\pi\Sigma)}} \exp\left[-\frac{1}{2}(\mathbf{x}-\mu)^T\Sigma^{-1}(\mathbf{x}-\mu)\right]$$

where $\mathbf{x} = [x, y]^T$, $\mu = [0, 0]^T$ is the mean vector, and

$$\Sigma = \begin{bmatrix} 1 & 3/5 \\ 3/5 & 2 \end{bmatrix}$$

is the covariance matrix. Compare your results with Figure 1.2.

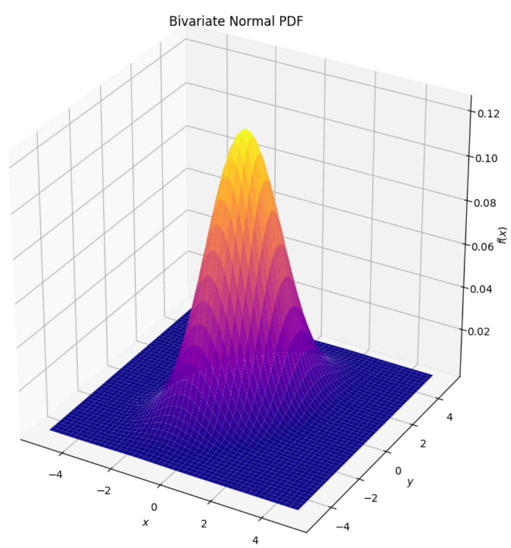


Figure 1.2: The solution to Problem 4.

Surface Animations

Animating a 3D surface is slightly different from animating a parametric curve in 3D. The object created by `.plot_surface()` does not have a `.set_data()` method. Instead, use `ax.clear()` to empty the axes at each frame, followed by a new call to `ax.plot_surface()`. Note that the axes limits must be reset after `ax.clear()` is called.

Problem 5. Use the data in `vibration.npz` to produce a surface animation of the solution to the wave equation for an elastic rectangular membrane. The file contains three NumPy arrays: `X`, `Y`, `Z`. `X` and `Y` are meshgrids of shape `(300,200)` corresponding to 300 points in the y-direction and 200 points in the x-direction, giving a 2x3 rectangle with one corner at the origin. `Z` is of shape `(150,300,200)`, giving the height of the vibrating membrane at each (x,y) point for 150 values of time. In the language of partial differential equations, this is the solution to the following initial/boundary value problem:

$$u_{tt} = 6^2(u_{xx} + u_{yy})$$

$$(x, y) \in [0, 2] \times [0, 3], t \in [0, 5]$$

$$u(t, 0, y) = u(t, 2, y) = u(t, x, 0) = u(t, x, 3) = 0$$

$$u(0, x, y) = xy(2 - x)(3 - y)$$

2 Modelling the spread of an epidemic: SIR models

Numerical Solvers

we often rely on numerical solvers to numerically integrate ODEs, Because of the complexity of many ODE systems. These numerical solvers allow us to solve complex ODE systems that may not be solvable symbolically, or are high dimensional. In this lab we will be using `solve_ivp`, which is a part of `scipy.integrate`, to solve ODE systems related to epidemic models. You can read the documentation for `solve_ivp` here.

`solve_ivp` takes the ODE as a function, a tuple containing the start and end time, and an array with the initial conditions as arguments, and returns a bunch object containing the solution and other information. If were were trying to solve the following ODE system

$$\begin{aligned} \begin{bmatrix} y_1(t) \\ y_2(t) \end{bmatrix}' &= \begin{bmatrix} y_2(t) \\ \sin(t) - 5y_2(t) - y_1(t) \end{bmatrix} \\ y_1(0) &= 0, \quad y_2(0) = 1, \quad t \in [0, 3\pi] \end{aligned} \tag{2.1}$$

we would write the following code.

```
import numpy as np
from scipy.integrate import solve_ivp

# define the ode system as given in the problem
def ode(t,y):
    return np.array([y[1], np.sin(t) - 5*y[1] - y[0]])

# define the t0 and tf parameters
t0 = 0
tf = 3*np.pi

# define the initial conditions
y0 = np.array([0,1])

# solve the system
sol = solve_ivp(ode, (t0,tf), y0)
```

And to plot the solution we would write this code

```
import matplotlib.pyplot as plt

# plot y_1 against y_2
plt.plot(sol.y[0],sol.y[1])
plt.xlabel('$y_1$')
plt.ylabel('$y_2$')
plt.show()
```

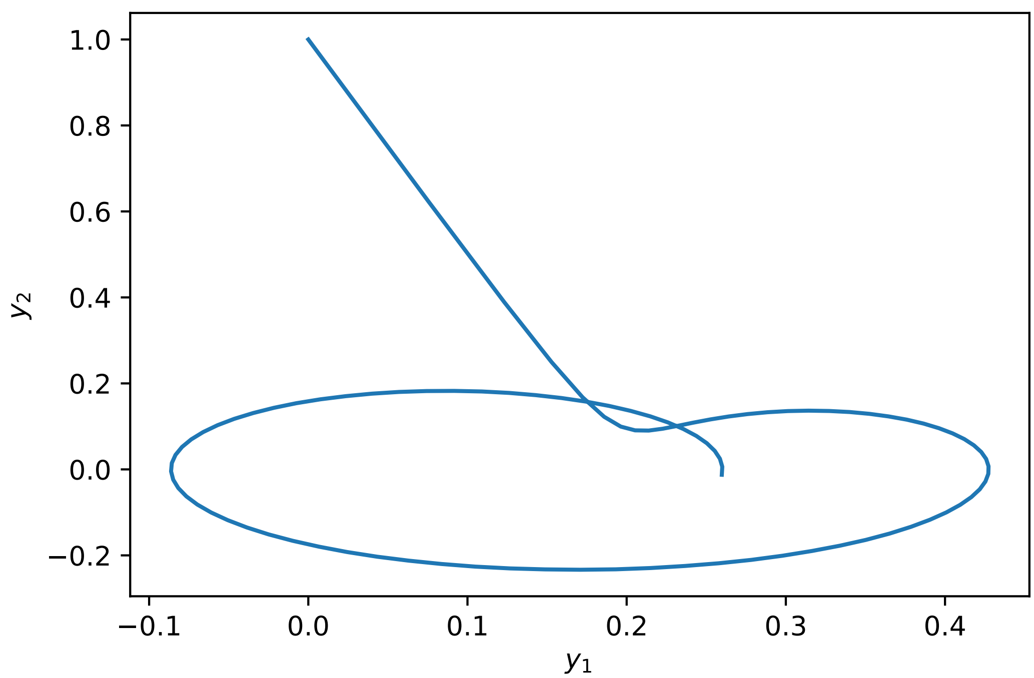


Figure 2.1: Solution to (2.1)

The SIR Model

The SIR model describes the spread of an epidemic through a large population. It does this by describing the movement of the population through three phases of the disease: those individuals who are *susceptible*, those who are *infectious*, and those who have been *removed* from the disease. Those individuals in the removed class have either died, or have recovered from the disease and are now immune to it. If the outbreak occurs over a short period of time, we may reasonably assume that the total population is fixed, so that $S'(t) + I'(t) + R'(t) = 0$. We may also assume that $S(t) + I(t) + R(t) = 1$, so that $S(t)$ represents the *fraction* of the population that is susceptible, etc.

Individuals may move from one class to another as described by the flow

$$S \to I \to R.$$

Let us consider the transition rate between S and I. Let β represent the average number of contacts made per unit time period (one day perhaps) that could spread the disease. The proportion of these contacts that are with a susceptible individual is $S(t)$. Thus, one infectious individual will on average infect $\beta S(t)$ others per day. Let N represent the total population size. Then we obtain the differential equation

$$\frac{d}{dt}(S(t)N) = -\beta S(t)(I(t)N)$$

Now consider the transition rate between I and R. We assume that there is a fixed proportion γ of the infectious group who will recover on a given day, so that

$$\frac{d}{dt}R(t) = \gamma I(t).$$

Note that γ is the reciprocal of the average length of time spent in the infectious phase.

Since the derivatives sum to 0, we have $I'(t) = -S'(t) - R'(t)$, so the differential equations are given by

$$\frac{dS}{dt} = -\beta IS, \tag{2.2}$$

$$\frac{dI}{dt} = \beta IS - \gamma I, \tag{2.3}$$

$$\frac{dR}{dt} = \gamma I. \tag{2.4}$$

Problem 1. Suppose that, in a city of approximately three million, five have recently entered the city carrying a certain disease. (Suppose they have just entered the infectious state.)

Each of those individuals has one contact each day that could spread the disease, and an average of three days is spent in the infectious state. Find the solution of the corresponding SIR equations for the next fifty days and plot your results.

At the peak of the infection, how many in the city will still be able to work (assume for simplicity that those who are in the infectious state either cannot go to work or are unproductive, etc.)?

SIR is an effective model for epidemic spread under certain assumptions. For example, we assume that the network is what's called "fully mixed". This implies that no group of members of a network are more likely to encounter each other than any other group. Because of this assumption, we should not use SIR to model networks we know to be poorly mixed. In fact, we should be clear in stating that almost no network is truly fully mixed; however this model is still effective for networks that are reasonably well mixed. In the next problem we will be using SIR to model data from the recent Covid-19 outbreak. To adhere to the "reasonably well mixed" criteria, we will be using only data from one county at a time.

Problem 2. On March 11, 2020, New York City had 52 confirmed cases of Covid-19. On that day New York started its lock-down measures. Using the following information, model what the spread of the virus could have been if New York did not implement any measures to curb the spread of the virus over the next 150 days: there are approximately 8.399 million people in New York city, the average case of Covid-19 lasts for 10 days, and each infected person can spread the virus to 2-3 people.

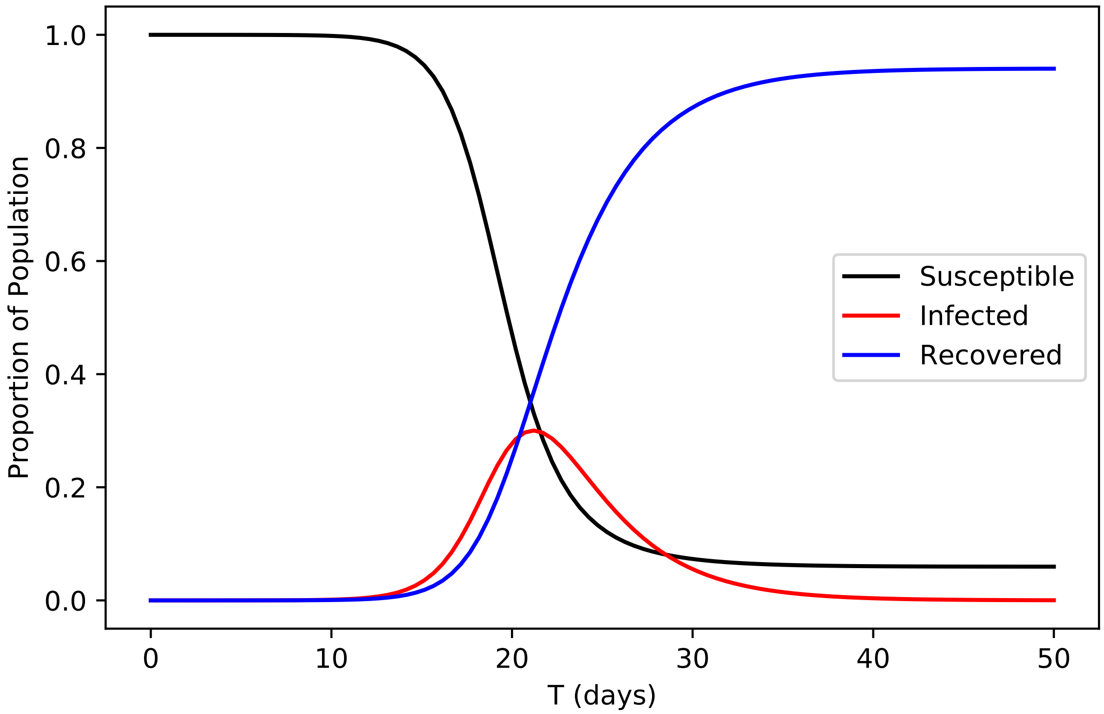


Figure 2.2: Solution to Problem (1)

Plot your results.

At the projected peak, how many concurrent active cases are there?

Assuming that about 5% of Covid-19 cases require hospitalization, and using the fact that there are about 58,000 hospital beds in NYC, how much over capacity will the hospitals in NYC be at the projected peak?

Variations on the SIR Model

The SIS model is a common variation of the SIR model. SIS Models describe diseases where individuals who have recovered from the disease do not gain any lasting immunity. There are only two compartments in this model: those who are *susceptible*, and those who are *infectious*.

The basic equations are given by

$$\frac{dS}{dt} = -\beta IS + fI,$$
$$\frac{dI}{dt} = \beta IS - fI$$

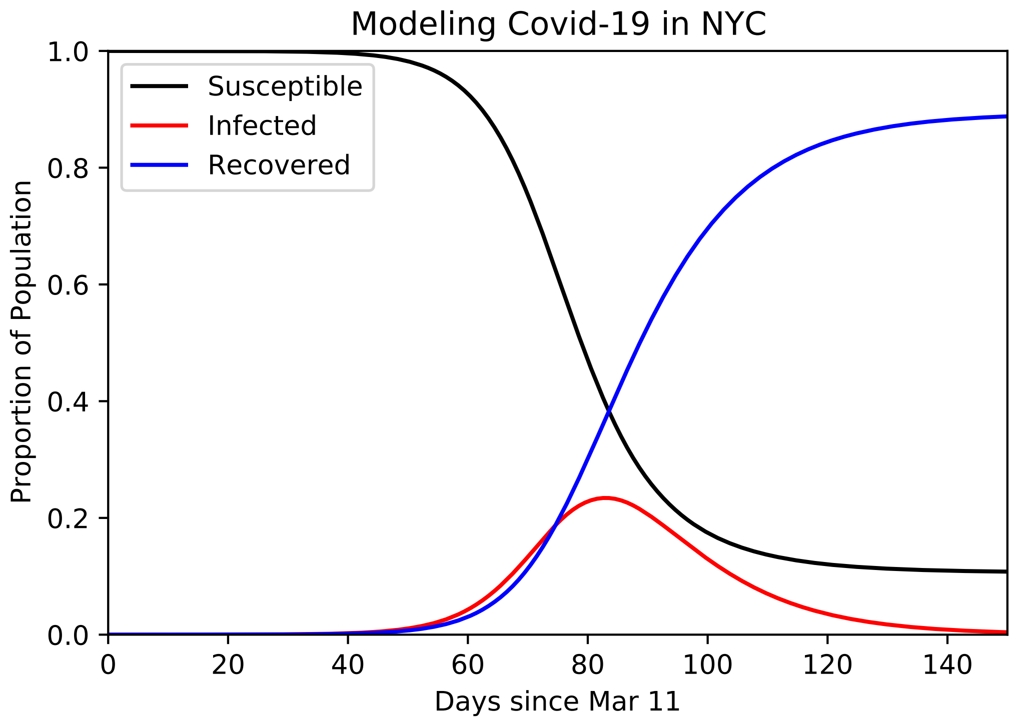


Figure 2.3: Solution to Problem (2).

Another alteration we can make to the SIR model is to add a birth and death rate. In the equations below we are assuming that the natural death rate together with the death rate caused by the disease is equal to the birth rate. This model is given by

$$\frac{dS}{dt} = \mu(1-S) - \beta IS,$$
$$\frac{dI}{dt} = \beta IS - (\gamma+\mu)I,$$
$$\frac{dR}{dt} = \gamma I - \mu R$$

where μ represents the death rate and equal birth rate, noting that any new person born is born into the susceptible population.

If we combine the last two variations we made on the SIR model we come to this formulation, which is an SIRS model. This SIRS model allows the transfer of individuals from the recovered/removed class to the susceptible class and includes modeling of the birth and death rates.

$$\frac{dS}{dt} = fR + \mu(1-S) - \beta IS, \tag{2.5}$$
$$\frac{dI}{dt} = \beta IS - (\gamma+\mu)I, \tag{2.6}$$
$$\frac{dR}{dt} = -fR + \gamma I - \mu R. \tag{2.7}$$

Problem 3. In the world there are 7 billion people. Influenza, or the flu, is one of those viruses that everyone can be susceptible to, even after recovering from their last sickness. The flu virus is able to change in order to evade our immune system and we become susceptible once more (although technically it is now a different strain). Suppose the virus originates with 1000 people in Texas after Hurricane Harvey flooded Houston and stagnant water allowed the virus to proliferate. According to WebMD (trustworthy source, right?), once you get the virus you are contagious up to a week, and kids up to 2 weeks. For this lab, suppose you are contagious for 10 days before recovering. Also suppose that on average someone makes one contact every two days that could spread the flu. Since we can catch a new strain of the flu, suppose that a recovered individual becomes susceptible again with probability $f = 1/50$. The flu is also known to be deadly, killing hundreds of thousands every year on top of the normal death rate. To assure a steady population, let the birth rate balance out the death rate, and in particular let $\mu = .0001$.

Using the SIRS model above, plot the proportion of population that is Susceptible, Infected, and Recovered over a year span (365 days).

Modeling Covid-19 with Social Distancing

Social distancing upsets the main assumption that is made when trying to model epidemic spread using SIR models. During the periods of lockdown instituted by governments, the interaction networks between people in a city or county were disrupted to the point that standard SIR models were no longer effective at modeling the spread of Covid-19. A paper released in May of 2020 presented some alternative models for Covid-19 that have some success in modeling its spread during periods of social distancing.

This model claims that the growth of $I(t)$ is polynomial with exponential decay (PGED). So we get the following form

$$I(t) \approx Bt^{\alpha}e^{-t/T_G},$$

which results in the following SIR type model

$$\frac{dS}{dt} = -\frac{\alpha}{t}I, \tag{2.8}$$

$$\frac{dI}{dt} = \left(\frac{\alpha}{t} - \frac{1}{T_G}\right)I, \tag{2.9}$$

$$\frac{dR}{dt} = \frac{1}{T_G}I, \tag{2.10}$$

where α and T_G are simply model parameters. In this model αT_G can be interpreted as the time of epidemic peak.

Fitting Models

Model fitting can be a frustrating task if we only use our intuition and guess and check. Thankfully, SciPy's `optimize` library has tools we can use to make these problems a lot easier. Many of the functions in this library are designed to take an arbitrary function and find whatever input makes the output close to zero. Our job is to create a function that outputs zero at the right values.

Suppose we have some data that we believe to follow a cubic trend with the following model

$$\alpha x^3 + \beta(x^2 + 2x) + \delta.$$

In order to fit the data to this model we can use `scipy.optimize.minimize` and create a function that will output zero when the correct parameters are input. `scipy.optimize.minimize` will then return an `OptimizeResult` object, which contains the optimal paramters.

```
# import the minimizer function
from scipy.optimize import minimize

# load the data and get the x and y values
data = np.load('to_fit.npy')
xs = data[:,0]
ys = data[:,1]

# define the function we want to minimize
def fun(params):
    # unpack the parameters
    a,b,d = params

    # get the model output based on the parameters
    out = a*xs**3 + b*(xs**2 + 2*xs) + d

    # find the difference between out and the data
    diff = out - ys

    # must return a float
    return np.linalg.norm(diff)

# make a guess for the parameters
p0 = (1,1,1)

# find the best parameters for this model
minimize(fun,p0)
```

Problem 4. Fit the PGED model to the Covid-19 data provided in `new_york_cases.csv`. Print the optimal values of α and T_G, and plot your results.

Notice that the data provided are the cumulative cases in NYC, which should be equal to $1 - S(t)$.

Hint: Set $t_0 = 1$ as the PEGD model requires to divide by t, so we must have $t \neq 0$.

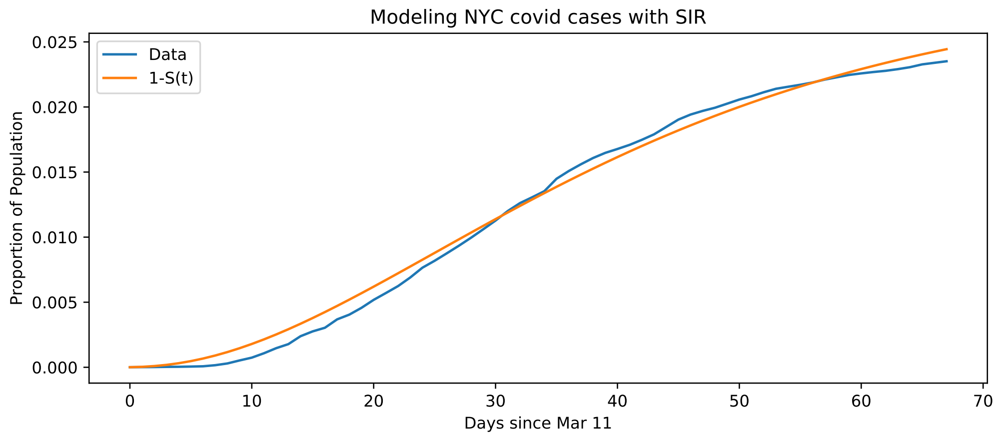


Figure 2.4: Solution to (4)

Boundary Value Problems

The next exercise uses a variation of the SIR model called an SEIR model to describe the spread of measles (see [1]). This new model adds another compartment, called the *exposed* or *latency* phase. It assumes that the rate at which measles is contracted depends on the season, i.e. the rate is periodic. That allows us to formulate the yearly occurrence rate for measles as a boundary value problem. The boundary value problem looks like

$$\begin{bmatrix} S \\ E \\ I \end{bmatrix}' = \begin{bmatrix} \mu - \beta(t)SI \\ \beta(t)SI - E/\lambda \\ E/\lambda - I/\eta \end{bmatrix}, \tag{2.11}$$

$$\begin{aligned} S(0) &= S(1), \\ E(0) &= E(1), \\ I(0) &= I(1) \end{aligned} \tag{2.12}$$

Parameters μ and λ represent the birth rate of the population and the latency period of measles, respectively. η represents the infectious period before an individual moves from the infectious class to the recovered class. After recovery an individual remains immune, which is why $R(t)$ is not included in the system. The set up of this problem is not normal since we are excluding $R(t)$, but it results in a nice graph.

To solve this problem we will use a full-featured BVP solver that is available in `SciPy`. The code below demonstrates how to use `solve_bvp` to solve the BVP

$$\varepsilon y'' + yy' - y = 0, \quad y(-1) = 1, \quad y(1) = -1/3, \quad \varepsilon = .1 \tag{2.13}$$

Look at figure 2.5 for the solution.

[1] Numerical Solution of Boundary Value Problems for Ordinary Differential Equations, by Aescher, Mattheij, and Russell

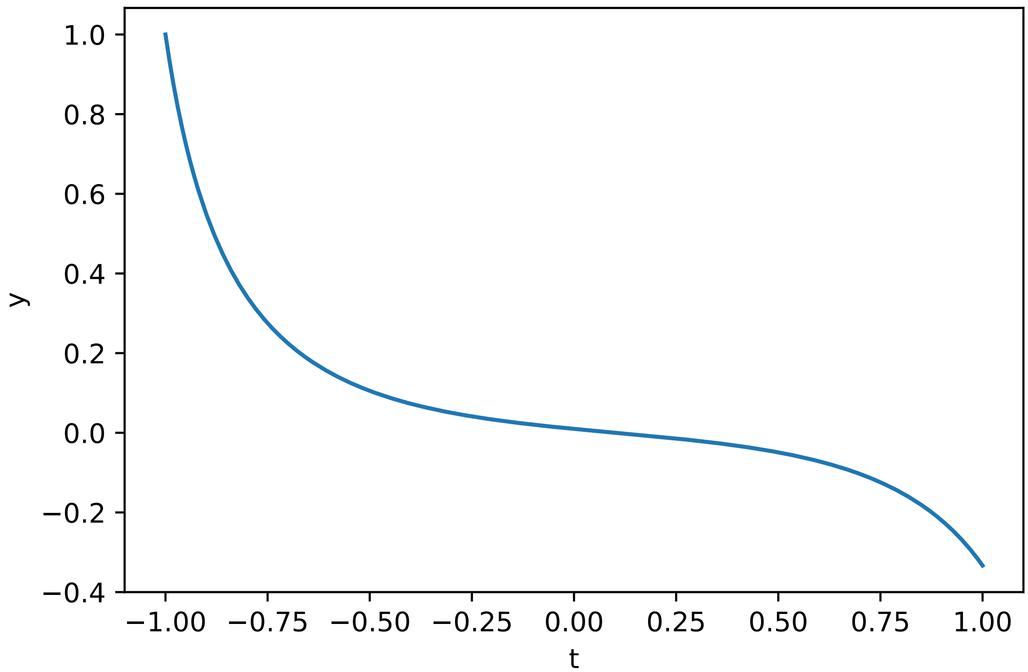


Figure 2.5: Solution to (2.13)

The BVP solver expects you to pass it the boundary conditions as a callable function that computes the difference between a guess at the boundary conditions and the desired boundary conditions. When we use the BVP solver, we will tell it how many constraints there should be on each side of the domain so it knows how many entries to expect. In this case, we have one boundary condition on either side. These constraints are expected to evaluate to 0 when the boundary condition is satisfied.

```
import numpy as np
from scipy.integrate import solve_bvp
import matplotlib.pyplot as plt

epsilon, lbc, rbc = .1, 1, - 1/3

# The ode function takes the independent variable first
# It has return shape (n,)
def ode(x , y):
    return np.array([y[1] , (1/epsilon) * (y[0] - y[0] * y[1])])

# The return shape of bcs() is (n,)
def bcs(ya, yb):
    BCa = np.array([ya[0] - lbc])   # 1 Boundary condition on the left
    BCb = np.array([yb[0] - rbc])   # 1 Boundary condition on the right
    # The return values will be 0s when the boundary conditions are met exactly
    return np.hstack([BCa, BCb])
```

```python
# The independent variable has size (m,) and goes from a to b with some step ←
    size
X = np.linspace(-1, 1, 200)
# The y input must have shape (n,m) and includes our initial guess for the ←
    boundaries
y = np.array([-1/3, -4/3]).reshape((-1,1))*np.ones((2, len(X)))

# There are multiple returns from solve_bvp(). We are interested in the y ←
    values which can be found in the sol field.
solution = solve_bvp(ode, bcs, X, y)
# We are interested in only y, not y', which is found in the first row of sol.
y_plot = solution.sol(X)[0]

plt.plot(X, y_plot)
plt.xlabel('t')
plt.ylabel('y')
plt.show()
```

Problem 5. Consider equations (2.11) and (2.12). Let the periodic function for our measles case be $\beta(t) = \beta_0(1 + \beta_1 \cos 2\pi t)$. Use parameters $\beta_1 = 1$, $\beta_0 = 1575$, $\eta = 0.01$, $\lambda = .0279$, and $\mu = .02$. Note: in this case, time is measured in years, so run the solution over the interval $[0, 1]$ to show a one-year cycle. The boundary conditions in (2.12) are just saying that the year will begin and end in the same state.

One issue that we encounter with this problem is that we have 6 boundary conditions but we only have 3 free variables. The 6 boundary counditions are the initial and final conditions of S, E, and I. `solve_bvp` only allows as many boundary conditions as there are free variables, so what we can do is include "dummy" variables in the ODE. This allows more boundary conditions in the BVP solver, while not changing the ODE system that we are solving. To deal with this, let $C(t) = [C_1(t), C_2(t), C_3(t)]$, and add the equation

$$C'(t) = 0$$

to the system of ODEs given above (for a total of 6 equations) resulting in this final 6 variable system

$$\begin{bmatrix} S(t) \\ E(t) \\ I(t) \\ C_1 \\ C_2 \\ C_3 \end{bmatrix}' = \begin{bmatrix} \mu - \beta(t)SI \\ \beta(t)SI - E/\lambda \\ E/\lambda - I/\eta \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

We can then apply all 6 of the boundary conditions that we need. The boundary conditions can be separated using the following trick:

$$\begin{pmatrix} C_1(0) \\ C_2(0) \\ C_3(0) \end{pmatrix} = \begin{pmatrix} S(0) \\ E(0) \\ I(0) \end{pmatrix}, \quad \begin{pmatrix} C_1(1) \\ C_2(1) \\ C_3(1) \end{pmatrix} = \begin{pmatrix} S(1) \\ E(1) \\ I(1) \end{pmatrix}.$$

Now C_1, C_2, C_3 become the 4th, 5th, and 6th rows of your solution matrix, so the 3 boundary conditions for the left are obtained by subtracting the last three entries of $y(0)$ from the first three entries, giving you $ya[0:3] - ya[3:]$. Similarly, your right boundary conditions will look like $yb[0:3] - yb[3:]$.

When you code your boundary conditions, note that `solve_bvp` changes the initial conditions to force all the entries in the return of `bcs()` to be zero. You can use the initial conditions from Fig. 2.6 as your initial guess (which will be an array of 6 elements). Remember that the initial infected proportion is small, not 0.

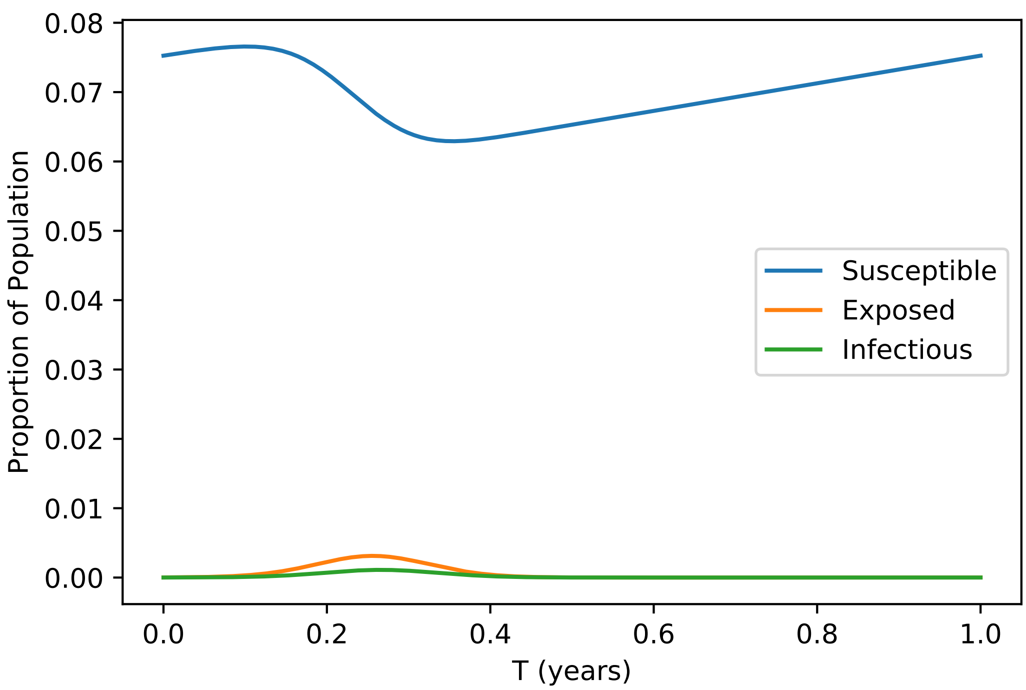


Figure 2.6: Solution to Problem (5)

3 Numerical Methods for Initial Value Problems; Harmonic Oscillators

Lab Objective: *Implement several basic numerical methods for initial value problems (IVPs) and use them to study harmonic oscillators.*

Methods for Initial Value Problems

Consider the *initial value problem* (IVP)

$$\begin{aligned} \mathbf{x}'(t) &= f(\mathbf{x}(t), t), \quad t_0 \leq t \leq t_f \\ \mathbf{x}(t_0) &= \mathbf{x}_0, \end{aligned} \tag{3.1}$$

where f is a suitably continuous function. A solution of (3.1) is a continuously differentiable, and possibly vector-valued, function $\mathbf{x}(t) = [x_1(t), \ldots, x_m(t)]^\mathsf{T}$, whose derivative $\mathbf{x}'(t)$ equals $f(\mathbf{x}(t), t)$ for all $t \in [t_0, t_f]$, and for which the *initial value* $\mathbf{x}(t_0)$ equals $\mathbf{x}_0$.

Under the right conditions, namely that f is uniformly Lipschitz continuous in $\mathbf{x}(t)$ near $\mathbf{x}_0$ and continuous in t near t_0, (3.1) is well-known to have a unique solution. However, for many IVPs, it is difficult, if not impossible, to find a closed-form, analytic expression for $\mathbf{x}(t)$. In these cases, numerical methods can be used to instead *approximate* $\mathbf{x}(t)$.

As an example, consider the initial value problem

$$\begin{aligned} x'(t) &= \sin(x(t)), \\ x(0) &= x_0. \end{aligned} \tag{3.2}$$

The solution $x(t)$ is defined implicitly by

$$t = \ln \left| \frac{\cos(x_0) + \cot(x_0)}{\csc(x(t)) + \cot(x(t))} \right|.$$

This equation cannot be solved for $x(t)$, so it is difficult to understand what solutions to (3.2) look like. Since $sin(n\pi) = 0$, there are constant solutions $x_n(t) = n\pi$, $n \in \mathbb{Z}$. Using a numerical IVP solver, solutions for different values of x_0 can be approximated. Figure 3.1 shows several of these approximate solutions, along with some of the constant, or *equilibrium*, solutions.

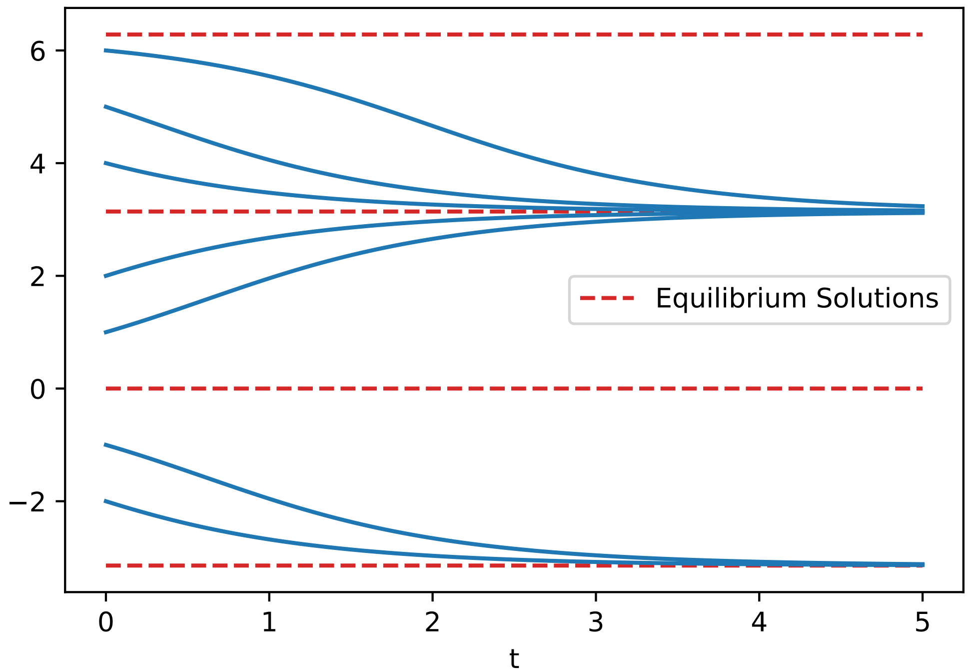


Figure 3.1: Several solutions of (3.2), using `scipy.integrate.odeint`.

Numerical Methods

For the numerical methods that follow, the key idea is to seek an approximation for the values of $\mathbf{x}(t)$ only on a finite set of values $t_0 < t_1 < \ldots < t_{n-1} < t_n$ $(= t_f)$. In other words, these methods try to solve for $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n$ such that $\mathbf{x}_i \approx \mathbf{x}(t_i)$.

Euler's Method

For simplicity, assume that each of the n subintervals $[t_{i-1}, t_i]$ has equal length $h = (t_f - t_0)/n$. h is called the *step size*. Assuming $\mathbf{x}(t)$ is twice-differentiable, for each component function $x_j(t)$ of $\mathbf{x}(t)$ and for each i, Taylor's Theorem says that

$$x_j(t_{i+1}) = x_j(t_i) + hx_j'(t_i) + \frac{h^2}{2}x_j''(c) \text{ for some } c \in [t_i, t_{i+1}].$$

The quantity $\frac{h^2}{2}x_j''(c)$ is negligible when h is sufficiently small, and thus $x_j(t_{i+1}) \approx x_j(t_i) + hx_j'(t_i)$. Therefore, bringing the component functions of $\mathbf{x}(t)$ back together gives

$$\begin{aligned}\mathbf{x}(t_{i+1}) &\approx \mathbf{x}(t_i) + h\mathbf{x}'(t_i),\\ &\approx \mathbf{x}(t_i) + hf(\mathbf{x}(t_i), t_i).\end{aligned}$$

This approximation leads to the *Euler method*: Starting with $\mathbf{x}_0 = \mathbf{x}(t_0)$, $\mathbf{x}_{i+1} = \mathbf{x}_i + hf(\mathbf{x}_i, t_i)$ for $i = 0, 1, \ldots, n-1$. Euler's method can be understood as starting with the point at $\mathbf{x}_0$, then calculating the derivative of $\mathbf{x}(t)$ at t_0 using $f(\mathbf{x}_0, t_0)$, followed by taking a step in the direction of the derivative scaled by h. Set that new point as $\mathbf{x}_1$ and continue.

It is important to consider how the choice of step size h affects the accuracy of the approximation. Note that at each step of the algorithm, the *local truncation error*, which comes from neglecting the $x''_j(c)$ term in the Taylor expansion, is proportional to h^2. The error $||\mathbf{x}(t_i) - \mathbf{x}_i||$ at the *ith* step comes from $i = \frac{t_i - t_0}{h}$ steps, which is proportional to h^{-1}, each contributing h^2 error. Thus the *global truncation error* is proportional to h. Therefore, the Euler method is called a *first-order method*, or a $\mathcal{O}(h)$ method. This means that as h gets small, the approximation of $\mathbf{x}(t)$ improves in two ways. First, $\mathbf{x}(t)$ is approximated at more values of t (more information about the solution), and second, the accuracy of the approximation at any t_i is improved proportional to h (better information about the solution).

Problem 1. Write a function which implements Euler's method for an IVP of the form (3.1). Test your function on the IVP:

$$\begin{aligned} x'(t) &= x(t) - 2t + 4, \quad 0 \leq t \leq 2, \\ x(0) &= 0, \end{aligned} \tag{3.3}$$

where the analytic solution is $x(t) = -2 + 2t + 2e^t$. Use the Euler method to numerically approximate the solution with step sizes $h = 0.2, 0.1$, and 0.05. Plot the true solution alongside the three approximations, and compare your results with Figure 3.2.

Midpoint Method

The midpoint method is very similar to Euler's method. For small h, use the approximation

$$\mathbf{x}(t_{i+1}) \approx \mathbf{x}(t_i) + hf(\mathbf{x}(t_i) + \frac{h}{2}f(\mathbf{x}(t_i), t_i), t_i + \frac{h}{2},).$$

In this approximation, first set $\hat{\mathbf{x}}_i = \mathbf{x}_i + \frac{h}{2}f(\mathbf{x}_i, t_i)$, which is an Euler method step of size $h/2$. Then evaluate $f(\hat{\mathbf{x}}_i, t_i + \frac{h}{2})$, which is a more accurate approximation to the derivative $\mathbf{x}'(t)$ in the interval $[t_i, t_{i+1}]$. Finally, a step is taken in that direction, scaled by h. It can be shown that the local truncation error for the midpoint method is $\mathcal{O}(h^3)$, giving global truncation error of $\mathcal{O}(h^2)$. This is a significant improvement over the Euler method. However, it comes at the cost of additional evaluations of f and a handful of extra floating point operations on the side. This tradeoff will be considered later in the lab.

Runge-Kutta Methods

The Euler method and the midpoint method belong to a family called *Runge-Kutta methods*. There are many Runge-Kutta methods with varying orders of accuracy. Methods of order four or higher are most commonly used. A fourth-order Runge-Kutta method (RK4) iterates as follows:

$$\begin{aligned} K_1 &= f(\mathbf{x}_i, t_i), \\ K_2 &= f(\mathbf{x}_i + \frac{h}{2}K_1, t_i + \frac{h}{2}), \\ K_3 &= f(\mathbf{x}_i + \frac{h}{2}K_2, t_i + \frac{h}{2}), \\ K_4 &= f(\mathbf{x}_i + hK_3, t_{i+1}), \\ \mathbf{x}_{i+1} &= \mathbf{x}_i + \frac{h}{6}(K_1 + 2K_2 + 2K_3 + K_4). \end{aligned}$$

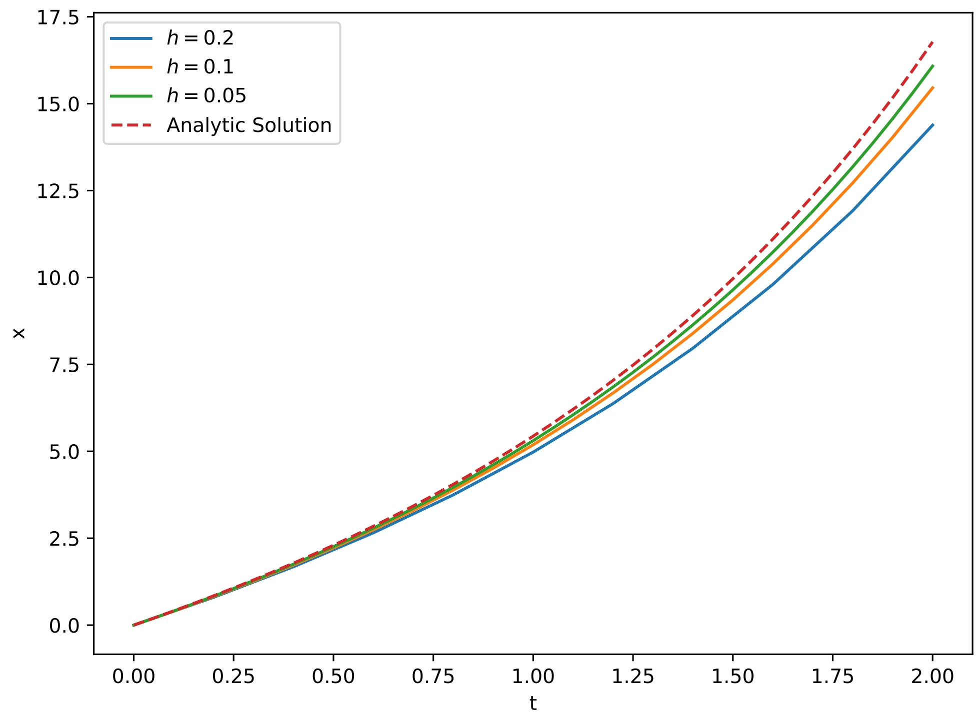


Figure 3.2: The solution of (3.3), alongside several approximations using Euler's method.

Runge-Kutta methods can be understood as a generalization of quadrature methods for approximating integrals, where the integrand is evaluated at specific points, and then the resulting values are combined in a weighted sum. For example, consider a differential equation

$$x'(t) = f(t)$$

Since the function f has no x dependence, this is a simple integration problem. In this case, Euler's method corresponds to the left-hand rule, the midpoint method becomes the midpoint rule, and RK4 reduces to Simpson's rule.

Advantages of Higher-Order Methods

It can be useful to visualize the order of accuracy of a numerical method. A method of order p has relative error of the form

$$E(h) = Ch^p$$

taking the logarithm of both sides yields

$$log(E(h)) = p \cdot log(h) + log(C)$$

Therefore, on a log-log plot against h, $E(h)$ is a line with slope p and intercept $log(C)$.

Problem 2. Write functions that implement the midpoint and fourth-order Runge-Kutta methods. Use the Euler, Midpoint, and RK4 methods to approximate the value of the solution for the IVP (3.3) from Problem 1 for step sizes of $h = 0.2$, 0.1, 0.05, 0.025, and 0.0125. Plot the true solution alongside the approximation obtained from each method when $h = 0.2$. Use `plt.loglog` to create a log-log plot of the relative error $|x(2) - x_n|/|x(2)|$ as a function of h for each approximation. Compare your results with Figure 3.3.

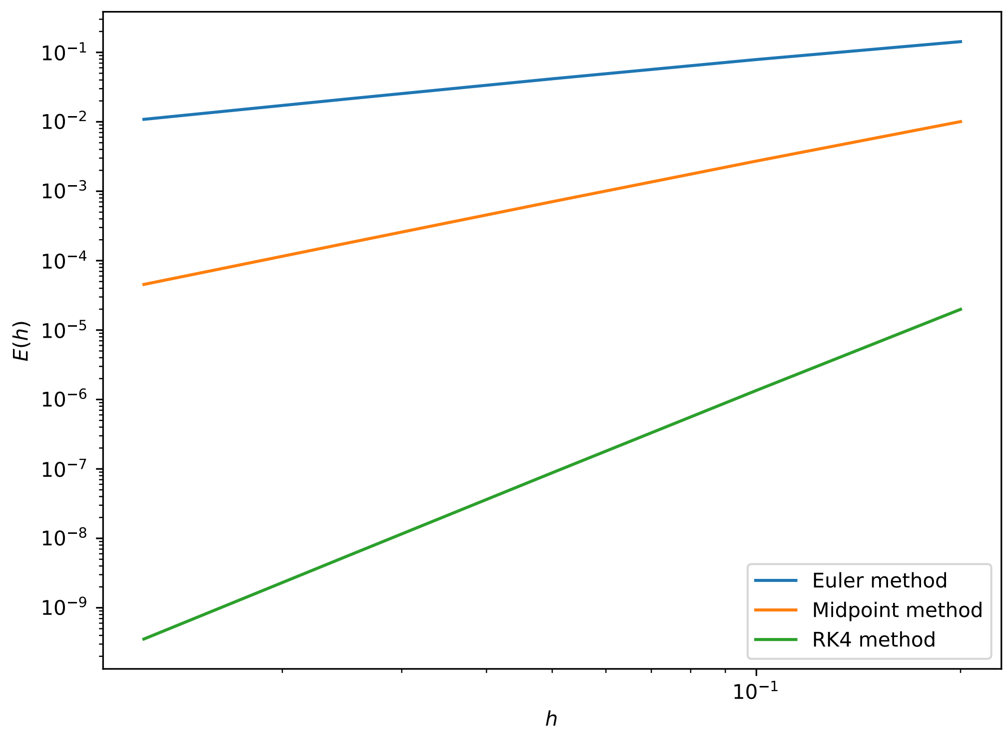


Figure 3.3: Loglog plot of the relative error in approximating $x(2)$, using step sizes $h = 0.2$, 0.1, 0.05, 0.025, and 0.0125. The slope of each line demonstrates the first, second, and fourth order convergence of the Euler, Midpoint, and RK4 methods, respectively.

The Euler, midpoint, and RK4 methods help illustrate the potential trade-off between order of accuracy and computational expense. To increase the order of accuracy, more evaluations of f must be performed at each step. It is possible that this trade-off could make higher-order methods undesirable, as (in theory) one could use a lower-order method with a smaller step size h. However, this is not generally the case. Assuming efficiency is measured in terms of the number of f-evaluations required to reach a certain threshold of accuracy, higher-order methods turn out to be much more efficient. For example, consider the IVP

$$\begin{aligned} x'(t) &= x(t)\cos(t), \quad t \in [0,8], \\ x(0) &= 1. \end{aligned} \tag{3.4}$$

Figure 3.4 illustrates the comparative efficiency of the Euler, Midpoint, and RK4 methods applied to (3.4). The higher-order RK4 method requires fewer f-evaluations to reach the same level of relative error as the lower-order methods. As h becomes small, which corresponds to increasing functional evaluations, each method reaches a point where the relative error $|x(8) - x_n|/|x(8)|$ stops improving. This occurs when h is so small that floating point round-off error overwhelms local truncation error. Notice that the higher-order methods are able to reach a better level of relative error before this phenomena occurs.

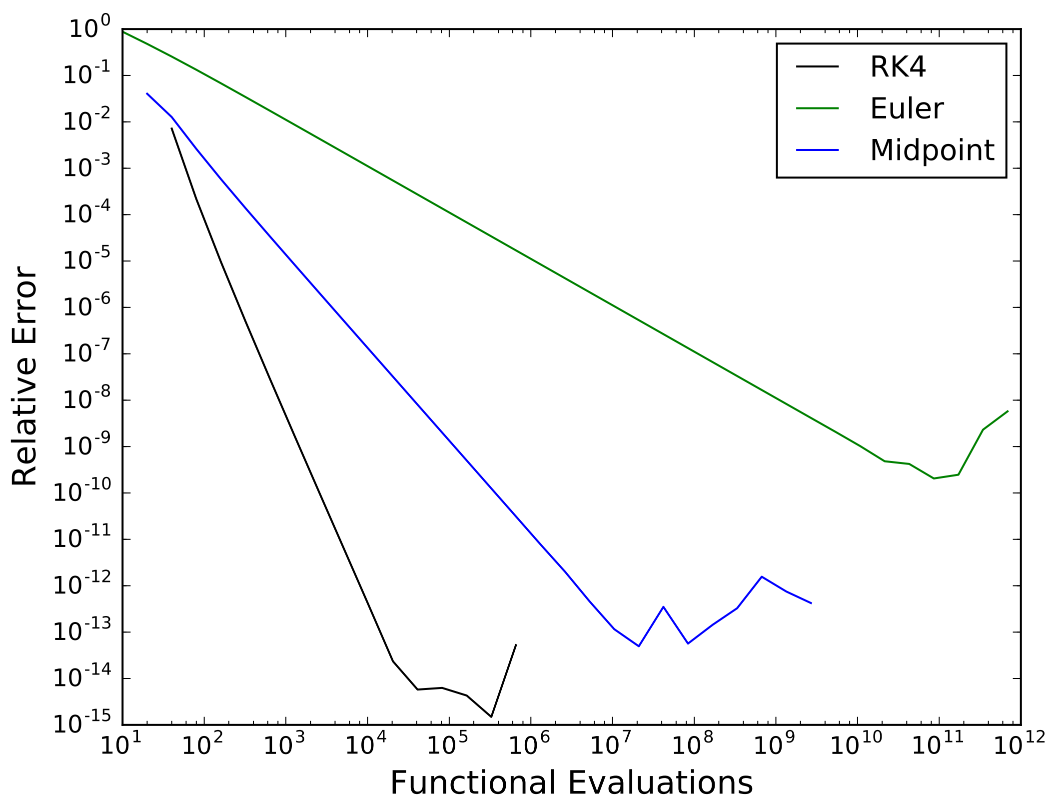


Figure 3.4: The relative error in computing the solution of (3.4) at $x = 8$ versus the number of times the right-hand side of (3.4) must be evaluated.

Harmonic Oscillators and Resonance

Harmonic oscillators are common in classical mechanics. A few examples include the pendulum (with small displacement), spring-mass systems, and the flow of electric current through various types of circuits. A harmonic oscillator $y(t)$ is a solution to an initial value problem of the form [1]

$$\begin{aligned} &my'' + \gamma y' + ky = f(t), \\ &y(0) = y_0, \quad y'(0) = y_0'. \end{aligned}$$

Here, m represents the mass on the end of a spring, γ represents the effect of damping on the motion, k is the spring constant, and $f(t)$ is the external force applied.

Simple harmonic oscillators

A simple harmonic oscillator is a harmonic oscillator that is not damped, $\gamma = 0$, and is free, $f = 0$, rather than forced, $f \neq 0$. A simple harmonic oscillator can described by the IVP

$$\begin{aligned} &my'' + ky = 0, \\ &y(0) = y_0, \quad y'(0) = y_0'. \end{aligned}$$

The solution of this IVP is $y = c_1 \cos(\omega_0 t) + c_2 \sin(\omega_0 t)$, where $\omega_0 = \sqrt{k/m}$ is the natural frequency of the oscillator and c_1 and c_2 are determined by applying the initial conditions.

To solve this IVP using a Runge-Kutta method, it must be written in the form

$$\mathbf{x}'(t) = f(\mathbf{x}(t), t)$$

This can be done by setting $x_1 = y$ and $x_2 = y'$. Then we have

$$\mathbf{x}' = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}' = \begin{bmatrix} x_2 \\ \frac{-k}{m} x_1 \end{bmatrix}$$

Therefore

$$f(\mathbf{x}(t), t) = \begin{bmatrix} x_2 \\ \frac{-k}{m} x_1 \end{bmatrix}$$

Problem 3. Use the RK4 method to solve the simple harmonic oscillator satisfying

$$\begin{aligned} &my'' + ky = 0, \quad 0 \leq t \leq 20, \\ &y(0) = 2, \quad y'(0) = -1, \end{aligned} \tag{3.5}$$

for $m = 1$ and $k = 1$.

Plot your numerical approximation of $y(t)$. Compare this with the numerical approximation when $m = 3$ and $k = 1$. Consider: Why does the difference in solutions make sense physically?

[1] It is customary to write y instead of $y(t)$ when it is unambiguous that y denotes the dependent variable.

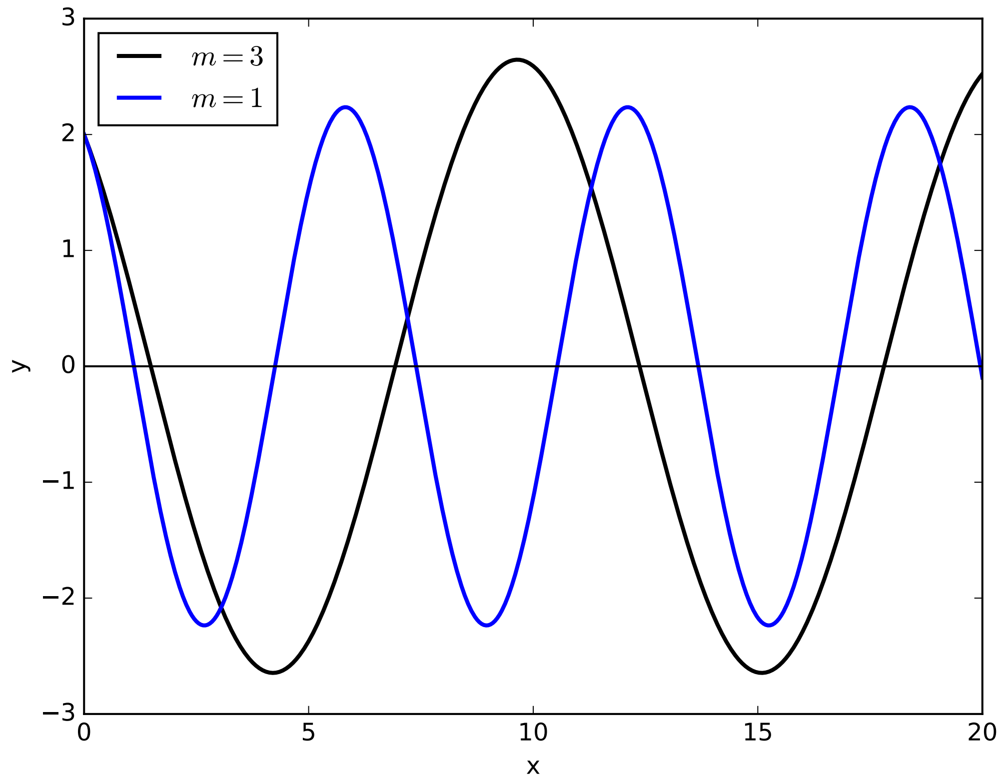


Figure 3.5: Solutions of (3.5) for several values of m.

Damped free harmonic oscillators

A damped free harmonic oscillator $y(t)$ satisfies the IVP

$$\begin{aligned} &my'' + \gamma y' + ky = 0, \\ &y(0) = y_0, \quad y'(0) = y_0'. \end{aligned}$$

The roots of the characteristic equation are

$$r_1, r_2 = \frac{-\gamma \pm \sqrt{\gamma^2 - 4km}}{2m}.$$

Note that the real parts of r_1 and r_2 are always negative, and so any solution $y(t)$ will decay over time due to a dissipation of the system energy. There are several cases to consider for the general solution of this equation:

1. If $\gamma^2 > 4km$, then the general solution is $y(t) = c_1 e^{r_1 t} + c_2 e^{r_2 t}$. Here the system is said to be *overdamped*. Notice from the general solution that there is no oscillation in this case.

2. If $\gamma^2 = 4km$, then the general solution is $y(t) = c_1 e^{\gamma t/2m} + c_2 t e^{\gamma t/2m}$. Here the system is said to be *critically damped*.

3. If $\gamma^2 < 4km$, then the general solution is

$$\begin{aligned} y(t) &= e^{-\gamma t/2m}\left[c_1\cos(\mu t) + c_2\sin(\mu t)\right], \\ &= Re^{-\gamma t/2m}\sin(\mu t + \delta), \end{aligned}$$

where R and δ are fixed, and $\mu = \sqrt{4km - \gamma^2}/2m$. This system does oscillate.

Problem 4. Use the RK4 method to solve for the damped free harmonic oscillator satisfying

$$\begin{aligned} &y'' + \gamma y' + y = 0, \quad 0 \le t \le 20, \\ &y(0) = 1, \quad y'(0) = -1. \end{aligned}$$

For $\gamma = 1/2$, and $\gamma = 1$, simultaneously plot your numerical approximations of y.

Forced harmonic oscillators without damping

Consider the systems described by the differential equation

$$my''(t) + ky(t) = F(t). \tag{3.6}$$

In many instances, the external force $F(t)$ is periodic, so assume that $F(t) = F_0\cos(\omega t)$. If $\omega_0 = \sqrt{k/m} \neq \omega$, then the general solution of 3.6 is given by

$$y(t) = c_1\cos(\omega_0 t) + c_2\sin(\omega_0 t) + \frac{F_0}{m(\omega_0^2 - \omega^2)}\cos(\omega t).$$

If $\omega_0 = \omega$, then the general solution is

$$y(t) = c_1\cos(\omega_0 t) + c_2\sin(\omega_0 t) + \frac{F_0}{2m\omega_0}t\sin(\omega_0 t).$$

When $\omega_0 = \omega$, the solution contains a term that grows arbitrarily large as $t \to \infty$. If we included damping, then the solution would be bounded but large for small γ and ω close to ω_0.

Consider a physical spring-mass system. Equation 3.6 holds only for small oscillations; this is where Hooke's law is applicable. However, the fact that the equation predicts large oscillations suggests the spring-mass system could fall apart as a result of the external force. This mechanical resonance has been known to cause failure of bridges, buildings, and airplanes.

Problem 5. Use the RK4 method to solve the damped and forced harmonic oscillator satisfying

$$\begin{aligned} &2y'' + \gamma y' + 2y = 2\cos(\omega t), \quad 0 \le t \le 40, \\ &y(0) = 2, \quad y'(0) = -1. \end{aligned} \tag{3.7}$$

For the following values of γ and ω, plot your numerical approximations of $y(t)$: $(\gamma, \omega) = (0.5, 1.5)$, $(0.1, 1.1)$, and $(0, 1)$. Compare your results with Figure3.7.

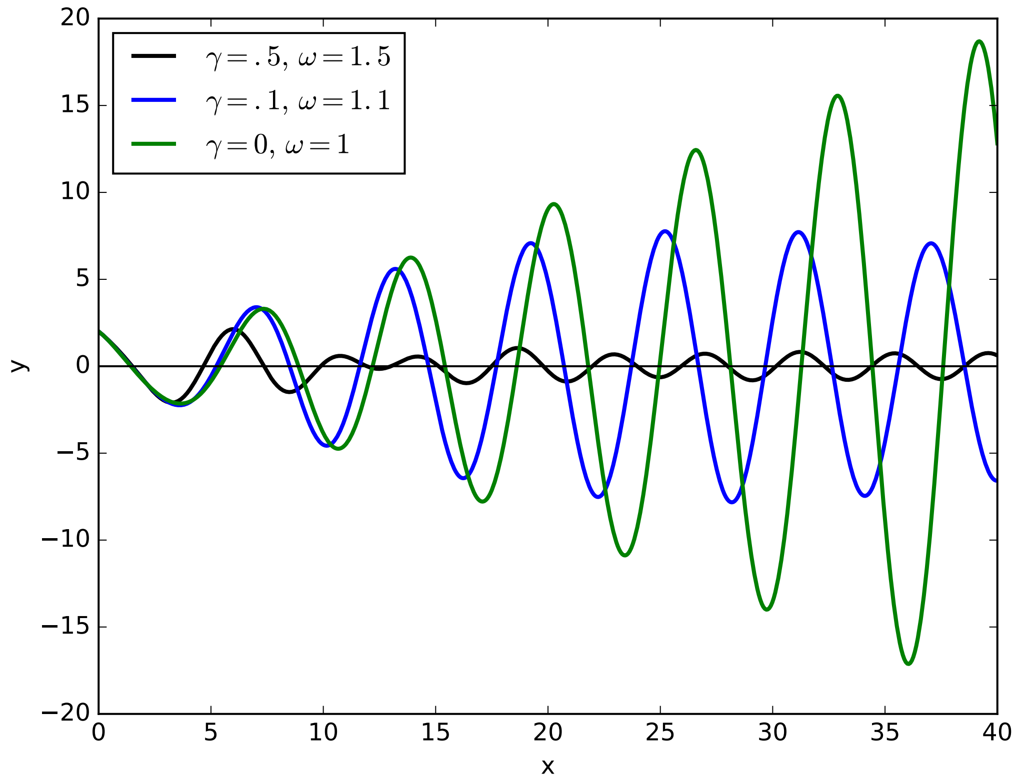


Figure 3.6: Solutions of (3.7) for several values of ω and γ.

4 Predator-Prey and Weight Change Models

Lab Objective: *We introduce built-in methods for solving Initial Value Problems and apply the methods to two dynamical systems. The first system looks at the relationship between a predator and its prey. The second model is a weight change model based on thermodynamics and kinematics.*

ODE Solvers

Initial Value Problems (IVPs) are a systems of one or more ordinary differential equations (ODEs) with defined initial conditions. In some cases, these can be solved by hand, but in real life it is more practical to use numerical solvers. For this lab you will use the `solve_ivp` solver from the `scipy.integrate` library.

`solve_ivp` solves a system of ODEs given by $dy/dt = f(t, y), \quad y(t_0) = y_0$, where y can be a vector. The solver takes as parameters the callable function f, the time boundaries `(t0,tf)`, the initial condition `y_0`, and an optional keyword argument `t_eval` that designates the times at which the solver will store the solution. Then `solve_ivp` returns a bunch object containing an array `y` with shape `(len(y_0), len(t))`, where each column gives the `y` values for one time point. The syntax for `solve_ivp` is shown below.

```python
from scipy.integrate import solve_ivp
sol = solve_ivp(f, (t0,tf), y0, t_eval=t)
```

Assuming that f, $y0$, t_0, t_f, and t are previously defined as explained above, `sol.y` is a vector containing the solution to the IVP and can be visualized by plotting each row of `sol.y` against the time domain or by plotting the rows against each other.

Predator-Prey Model

ODEs are commonly used to model relationships between predator and prey populations. For example, consider the populations of wolves, the predator, and rabbits, the prey), in Yellowstone National Park. Let $r(t)$ and $w(t)$ represent the rabbit and wolf populations respectively at time t, measured in years. We will make a few assumptions to simplify our model:

- In the absence of wolves, the rabbit population grows at a positive rate proportional to the current population. Thus when $w(t) = 0$, $dr/dt = \alpha r(t)$, where $\alpha > 0$.

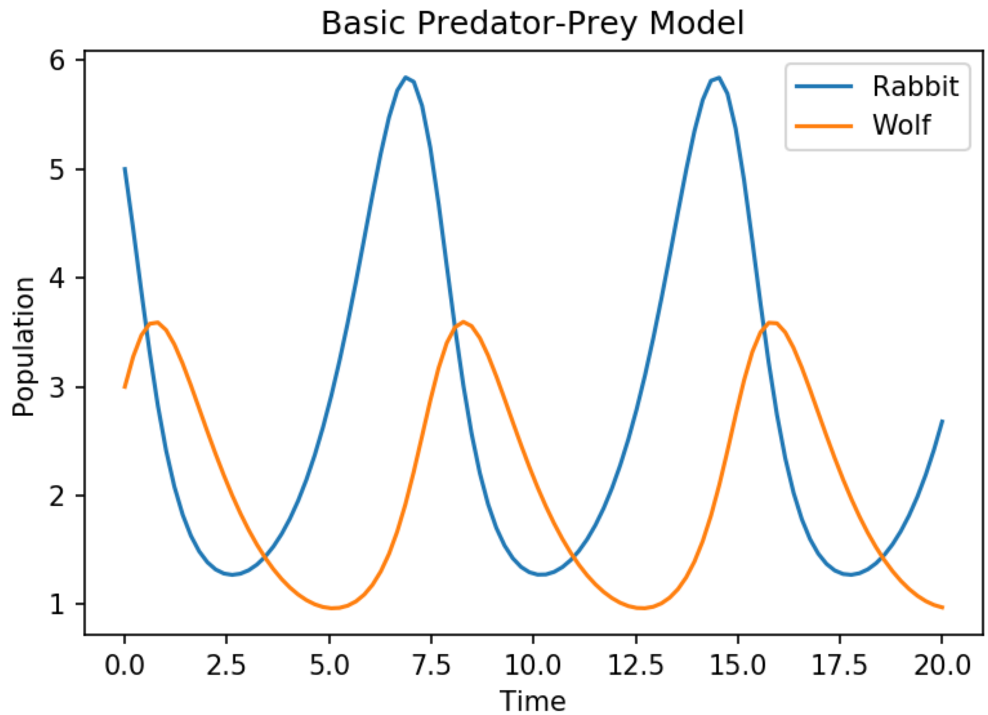


Figure 4.1: The solution to the system found in (4.1)

- In the absence of rabbits, the wolves die out. Thus when $r(t) = 0$, $dw/dt = -\delta w(t)$, where $\delta > 0$.
- The number of encounters between rabbits and wolves is proportional to the product of their populations. The wolf population grows proportional to the number of encounters by $\beta r(t)w(t)$ (where $\beta > 0$), and the rabbit population decreases proportional to the number of encounters by $-\gamma r(t)w(t)$ (where $\gamma > 0$).

This leads to the following system of ODEs:

$$\begin{aligned}\frac{dr}{dt} &= \alpha r - \beta r w = r(\alpha - \beta w)\\ \frac{dw}{dt} &= -\delta w + \gamma r w = w(-\delta + \gamma r)\end{aligned} \tag{4.1}$$

Problem 1. As mentioned above, the `solve_ivp` solver requires a callable function representing the right hand side of the IVP. Define the function `predator_prey()` that accepts the current $r(t)$ and $w(t)$ values as a 1d array y, and the current time t, and returns the right hand side of (4.1) as an ndarray. Use $\alpha = 1.0$, $\beta = 0.5$, $\delta = 0.75$, and $\gamma = 0.25$ as your growth parameters.

Problem 2. Use `solve_ivp` to solve (4.1) with initial conditions $(r_0, w_0) = (5, 3)$ and time ranging from 0 to 20 years. Display the resulting rabbit and wolf populations over time (stored as rows in the attribute `y` of the output of `solve_ivp`) on the same plot. Your graph should match the graph in figure 4.1.

Variations on the Predator-Prey

The Lotka-Volterra model

The representation of the predator-prey relationship found in (4.1) is called the Lotka-Volterra predator-prey model and is typically given by

$$\frac{du}{dt} = \alpha u - \beta uv,$$
$$\frac{dv}{dt} = -\delta v + \gamma uv.$$

where u and v represent the prey and predator populations, respectively. Here α, β, δ, and γ are the same as before but now for an arbitrary prey and predator.

The equlibria (fixed points) of a system occur when the derivatives are zero. In this example, that occurs at $(u, v) = (0, 0)$ and $(u, v) = (\frac{c}{d}, \frac{a}{b})$. Visualizing the phase portrait helps to give more insight into the dynamics of a system. We will do this by first nondimensionalzing our system to reduce the number of parameters. Let $U = \frac{\gamma}{\delta}u$, $V = \frac{\beta}{\alpha}v$, $\bar{t} = \alpha t$, and $\eta = \frac{\gamma}{\alpha}$. Substituting into the original ODEs we obtain the nondimensional system of equations

$$\begin{aligned}\frac{dU}{d\bar{t}} &= U(1 - V),\\ \frac{dV}{d\bar{t}} &= \eta V(U - 1).\end{aligned} \tag{4.2}$$

Problem 3. Similar to problem 1, define the function `Lotka_volterra()` that takes in the current predator and prey populations as a 1d array y and the current time as a float t and returns the right hand side of the system (4.2) with $\eta = 1/3$.

The following three lines of code plot the phase portrait of (4.2). For more documentation on quiver plots see the documentation.

```
Y1, Y2 = np.meshgrid(np.linspace(0, 4.5, 25), np.linspace(0, 4.5, 25))
dU, dV = Lotka_Volterra(0, (Y1, Y2))
Q = plt.quiver(Y1[::3, ::3], Y2[::3, ::3], U[::3, ::3], V[::3, ::3])
```

Using `solve_ivp`, solve (4.2) with three different initial conditions $y_0 = (1/2, 1/3)$, $y_0 = (1/2, 3/4)$, and $y_0 = (1/16, 3/4)$ and time domain $t = [0, 13]$. Plot these three solutions on the same graph as the phase portrait and the equilibria $(0, 0)$ and $(1, 1)$.

Since your solutions are being plotted with the phase portrait, plot the two populations against each other (instead of both individually against time). Your plot should match 4.2.

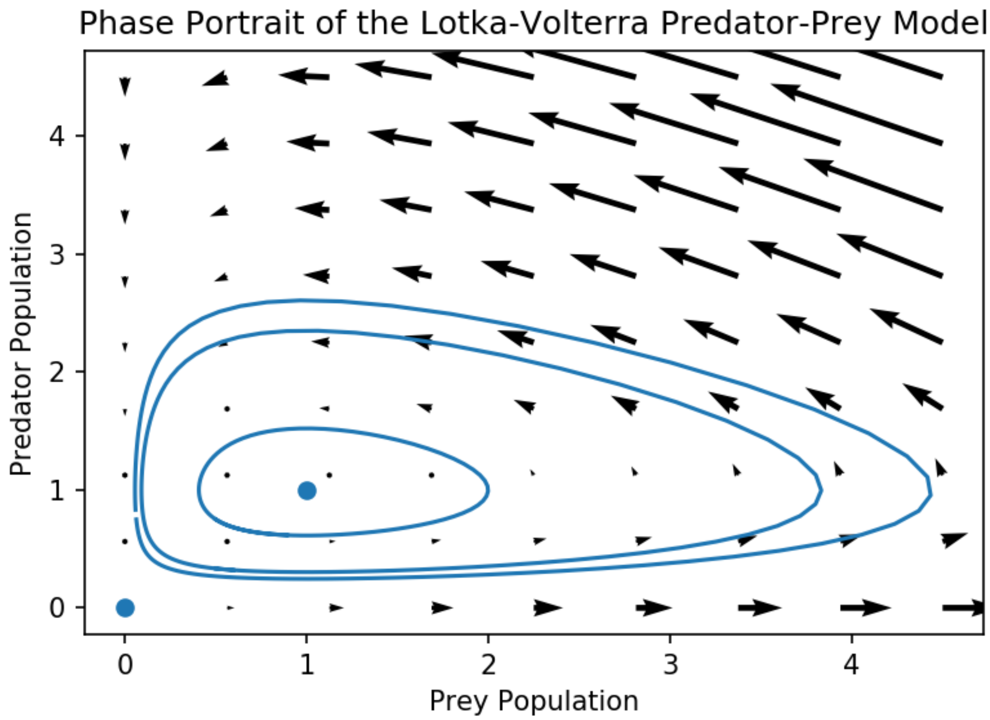


Figure 4.2: The phase portrait for the nondimensionalized Lotka-Volterra predator-prey equations with parameters $\eta = 1/3$.

The Logistic model

Notice that the Lotka-Volterra equations predict prey populations will grow exponentially in the absence of predators. The logistic predator-prey equations change this dynamic by adding a carrying capacity K to the prey population:

$$\frac{du}{dt} = \alpha u \left(1 - \frac{u}{K}\right) - \beta uv,$$
$$\frac{dv}{dt} = -\delta v + \gamma uv.$$

We can again do dimensional analysis on this system to simplify parameters. Let $U = \frac{u}{K}$, $V = \frac{\beta}{\alpha}v$, $\bar{t} = \alpha t$, $\eta = \frac{\gamma K}{\alpha}$, and $\rho = \frac{\delta}{\gamma K}$. Then the nondimensional logistic equations are

$$\begin{aligned} \frac{dU}{d\bar{t}} &= U(1 - U - V), \\ \frac{dV}{d\bar{t}} &= \eta V(U - \rho). \end{aligned} \tag{4.3}$$

Problem 4. Define a new function `Logistic_Model()` that takes in the current predator and prey populations y and the current time t and returns the right hand side of (4.3) as a tuple. Use `solve_ivp` to compute solutions (U, V) of (4.3) for initial conditions $(1/3, 1/3)$ and $(1/2, 1/5)$. Do this for parameter values η, $\rho = 1$, 0.3 and also for values η, $\rho = 1$, 1.1.

Create a phase portrait for the logistic equations using both sets of parameter values. Plot the direction field, all equilibrium points, and both solution orbits on the same plot for each set of parameter values.

A Weight Change Model

The main idea behind weight change is simple. If a person takes in more energy than they expend, they gain weight. If they take in less than they expend, they lose weight. Let *energy balance* EB be the difference between *energy intake* EI and *energy expenditure* EE, so that

$$EB = EI - EE.$$

If the balance is positive, weight is gained and similarly if the balance is negative, weight is lost.

A person's body weight at a time t can be expressed as the sum of the weight of their fat tissue $F(t)$ and the weight of their lean tissue $L(t)$; that is, $BW(t) = F(t) + L(t)$. Using this, the change in body weight can be expressed as the following system of ODEs:

$$\begin{aligned} \frac{dF}{dt} &= \frac{(1-p(t))EB(t)}{\rho_F}, \\ \frac{dL}{dt} &= \frac{p(t)EB(t)}{\rho_L}, \end{aligned} \tag{4.4}$$

where $(1 - p(t))$ and $p(t)$ represent the proportion of the energy balance ($EB(t)$) that results in a change in the quantity of fatty or lean tissue, respectively. The constants ρ_F and ρ_L represent the energy density of fatty and lean tissue, approximated as $\rho_F = 9400$ kcal/kg and $\rho_L = 1800$ kcal/kg.

To solve this system, we first need to express $p(t)$ and $EB(t)$ in terms of F and L. These functions will also depend on physical activity level, PAL, and energy intake, EI, which vary among individuals.

We will find an expression for $p(t)$ using Forbes' Law[1] which states that

$$\frac{dF}{dL} = \frac{F}{10.4}.$$

Notice

$$\frac{F}{10.4} = \frac{dF}{dL} = \frac{dF/dt}{dL/dt} = \frac{\dfrac{(1-p(t))EB(t)}{\rho_F}}{\dfrac{p(t)EB(t)}{\rho_L}} = \frac{\rho_L}{\rho_F}\frac{1-p(t)}{p(t)}.$$

Solving for $p(t)$ gives Forbes' equation

$$p(t) = \frac{C}{C + F(t)} \quad \text{where} \quad C = 10.4\frac{\rho_L}{\rho_F}. \tag{4.5}$$

[1] *Lean body mass-body fat interrelationships in humans*, Forbes, G.B.; *Nutrition reviews*, pgs 225-231, 1987.

We will now find an expression for $EB(t)$. Recall $EB(t) = EI - EE$. We will use the following expression for energy expenditure (EE) to define $EB(t)$.

$$EE = PAL \times RMR \tag{4.6}$$

where PAL is physical activity level (as previously mentioned) and RMR is resting metabolic rate. Physical activity level can be determined using the table above.

1.40–1.69	People who are sedentary and do not exercise regularly, spend most of their time sitting, standing, with little body displacement
1.70–1.99	People who are active, with frequent body displacement throughout the day or who exercise frequently
2.00–2.40	People who engage regularly in strenuous work or exercise for several hours each day

Table 4.1: This is a rough guide for physical activity level (PAL).

We will use the following equation for computing RMR,

$$RMR = K + \gamma_F F(t) + \gamma_L L(t) + \eta_F \frac{dF}{dt} + \eta_L \frac{dL}{dt} + \beta_{at} EI, \tag{4.7}$$

where $\gamma_F = 3.2$ kcal/kg/d, $\gamma_L = 22$ kcal/kg/d, $\eta_F = 180$ kcal/kg, and $\eta_L = 230$ kcal/kg [2] [3]. Further, we let $\beta_{at} = 0.14$ denote the coefficient for adaptive thermogenesis. Finally, we remark that the constant K can be tuned to an individual's body type directly through RMR and fat measurement, and is assumed to remain constant over time.

Thus, since the input EI is assumed to be known, we can use (4.6), (4.7) and (4.5) to write (4.4) in terms of F and L, thus allowing us to close the system of ODEs.

Specifically, we have

$$\begin{aligned}
RMR = \frac{EE}{PAL} &= K + \gamma_F F(t) + \gamma_L L(t) + \eta_F \frac{dF}{dt} + \eta_L \frac{dL}{dt} + \beta_{at} EI \\
\frac{1}{PAL}(EE - EI + EI) &= K + \gamma_F F(t) + \gamma_L L(t) \\
&\quad + \left(\frac{\eta_F}{\rho_F}(1 - p(t)) + \frac{\eta_L}{\rho_L} p(t) \right) EB(t) + \beta_{at} EI. \\
\left(\frac{1}{PAL} - \beta_{at} \right) EI &= K + \gamma_F F(t) + \gamma_L L(t) \\
&\quad + \left(\frac{\eta_F}{\rho_F}(1 - p(t)) + \frac{\eta_L}{\rho_L} p(t) + \frac{1}{PAL} \right) EB(t).
\end{aligned}$$

Solving for $EB(t)$ in the last equation yields

$$EB(t) = \frac{\left(\frac{1}{PAL} - \beta_{at} \right) EI - K - \gamma_F F(t) - \gamma_L L(t)}{\frac{\eta_F}{\rho_F}(1 - p(t)) + \frac{\eta_L}{\rho_L} p(t) + \frac{1}{PAL}}. \tag{4.8}$$

[2] *Modeling weight-loss maintenance to help prevent body weight regain*; Hall, K.D. and Jordan, P.N.; *The American journal of clinical nutrition*, pg 1495, 2008

[3] *Quantification of the effect of energy imbalance on bodyweight*; Hall, K.D. et al.; *The Lancet*, pgs 826-837, 2011

In equilibrium ($EB = 0$), this gives us

$$K = \left(\frac{1}{PAL} - \beta_{at}\right) EI - \gamma_F F - \gamma_L L. \tag{4.9}$$

Thus, for a subject who has maintained the same weight for a while, one can determine K by using (4.9), if they know their average caloric intake and amount of fat (assume $L = BW - F$).

Problem 5. Write a function `forbes()` which takes as input `F`, the weight of fat tissue at a given time (i.e. the function $F(t)$ evaluated at a certain time), and returns Forbe's equation given in (4.5). Also write the function `energy_balance()` which takes as input `F`, `L`, `PAL`, and `EI` and returns the energy balance as given in (4.8). In `energy_balance()` we also have that `F` is the fat tissue weight at a given time, and `L` is the lean tissue weight at a given time.

Using `forbes()` and `energy_balance()`, define the function `weight_odesystem()` which takes as input the current time as a float t and the current fat and lean weights as an array y and returns the right hand side of (4.4) as a tuple.

Use $\rho_F = 9400$, $\rho_L = 1800$, $\gamma_F = 3.2$, $\gamma_L = 22$, $\eta_F = 180$, $\eta_L = 230$, $K = 0$ and $\beta_{AT} = 0.14$.

Hint: The functions `forbes()` and `energy_balance()` are not time dependent in the same way equations (4.5) and (4.8) are. The time dependent portions of these functions, $F(t)$ and $L(t)$, are determined by what will be input from the `y` argument of `weight_odesystem()`.

Problem 6. Consider the initial value problem corresponding to (4.4).

$$\begin{aligned}
\frac{dF(t)}{dt} &= \frac{(1-p(t))EB(t)}{\rho_F}, \\
\frac{dL(t)}{dt} &= \frac{p(t)EB(t)}{\rho_L}, \\
F(0) &= F_0, \\
L(0) &= L_0.
\end{aligned} \tag{4.10}$$

The following function returns the fat mass of an individual based on body weight (kg), age (years), height (meters), and sex. Use this function to define initial conditions F_0 and L_0 for the IVP above: $F_0 = fat\_mass(args^*)$, $L_0 = BW - F_0$.

```python
def fat_mass(BW, age, H, sex):
    BMI = BW / H**2.
    if sex == 'male':
        return BW * (-103.91 + 37.31 * log(BMI) + 0.14 * age) / 100
    else:
        return BW * (-102.01 + 39.96 * log(BMI) + 0.14 * age) / 100
```

Suppose a 38 year old female, standing 5'8" and weighing 160 lbs, reduces her intake from 2143 to 2025 calories/day, and increases her physical activity from little to no exercise (PAL=1.4) to exercising to 2-3 days per week (PAL=1.5).

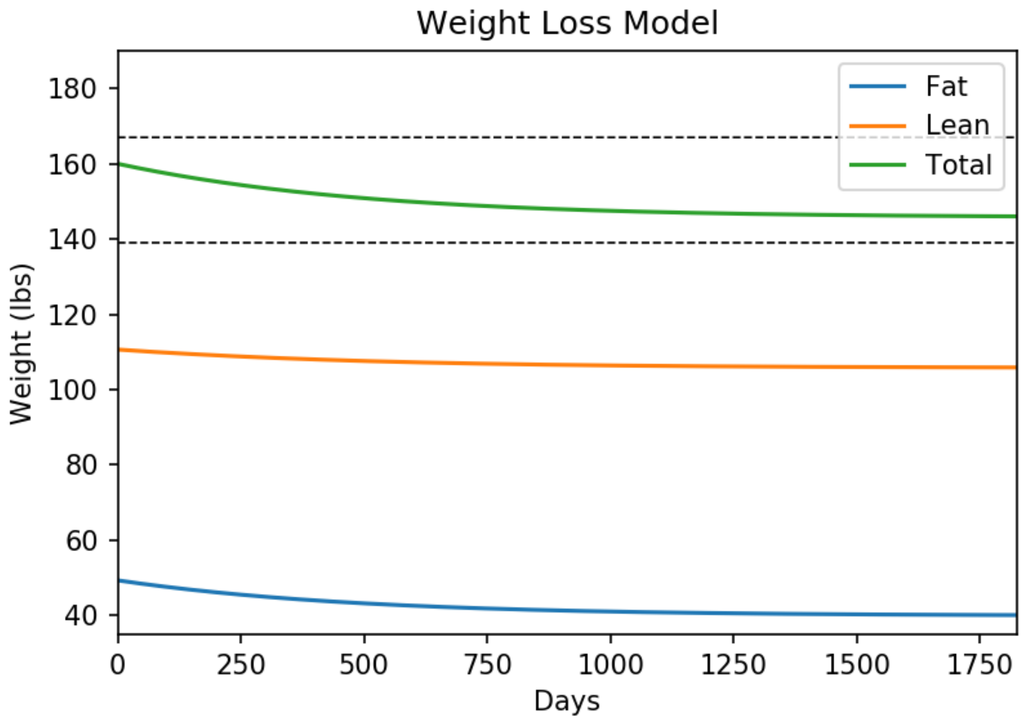


Figure 4.3: The solution of the weight change model for problem 6.

Use (4.9) and the original intake and phyical activity levels to compute K for this system. Then use `solve_ivp` to solve the IVP. Graph the solution curve for this single-stage weightloss intervention over a period of 5 years. Your plot should match figure 4.3.

Note the provided code requires quantities in metric units (kilograms, meters, days) while our graph is converted to units of pounds and days.

Problem 7. Modify the preceding problem to handle a two stage weightloss intervention: Suppose for the first 16 weeks intake is reduced from 2143 to 1600 calories/day and physical activity is increased from little to no exercise (PAL=1.4) to an hour of exercise 5 days per week (PAL=1.7). The following 16 weeks intake is increased from 1600 to 2025 calories/day, and exercise is limited to only 2-3 days per week (PAL=1.5).

You will need to recompute F_0, and L_0 at the end of the first 16 weeks, but K will stay the same. Find and graph the solution curve over the 32 week period.

5 Bifurcations and Hysteresis

Recall that any ordinary differential equation can be written as a first order system of ODEs,

$$\dot{x} = F(x), \quad \dot{x} := \frac{d}{dt}x(t). \tag{5.1}$$

Many interesting applications and physical phenomena can be modeled using ODEs. Given a mathematical model of the form (5.1), it is important to understand geometrically how its solutions behave. This information can then be conveyed in a phase portrait, a graph describing solutions of (5.1) with differential initial conditions. The first step in constructing a phase portrait is to find the equilibrium solutions of the equation, i.e., the zeros of $F(x)$, and to determine their stability.

It is often the case that the mathematical model we study depends on some parameter or set of parameters λ. Thus the ODE becomes

$$\dot{x} = F(x, \lambda). \tag{5.2}$$

The parameter λ can then be tuned to better fit the physical application. As λ varies, the equilibrium solutions and other geometric features of (5.2) may suddenly change. A value of λ where the phase portrait changes is called a *bifurcation point*; the study of how these changes occur is called *bifurcation theory*. The parameter values and corresponding equilibrium solutions are often graphed together in a bifurcation diagram.

As an example, consider the scalar differential equation

$$\dot{x} = x^2 + \lambda. \tag{5.3}$$

For $\lambda > 0$ equation (5.3) has no equilibrium solutions. At $\lambda = 0$ the equilibrium point $x = 0$ appears, and for $\lambda < 0$ it splits into two equilibrium points. For this system, a bifurcation occurs at $\lambda = 0$. This is an example of a saddle-node bifurcation. The bifurcation diagram is shown in Figure 5.1

Suppose that $F(x_0, \lambda_0) = 0$. We use a method called natural embedding to find zeros (x, λ) of F for nearby values of λ. Specifically, we step forward in λ by letting $\lambda_1 = \lambda_0 + \triangle\lambda$, and use Newton's method to find the value x_1 that satisfies $F(x_1, \lambda_1) = 0$. This method works well except when λ is near a bifurcation point λ^*.

The following code implements the natural embedding algorithm, and then uses that algorithm to find the curves in the bifurcation diagram for (5.3). Notice that this algorithm needs a good initial guess for x_0 to get started.

```
import numpy as np
```

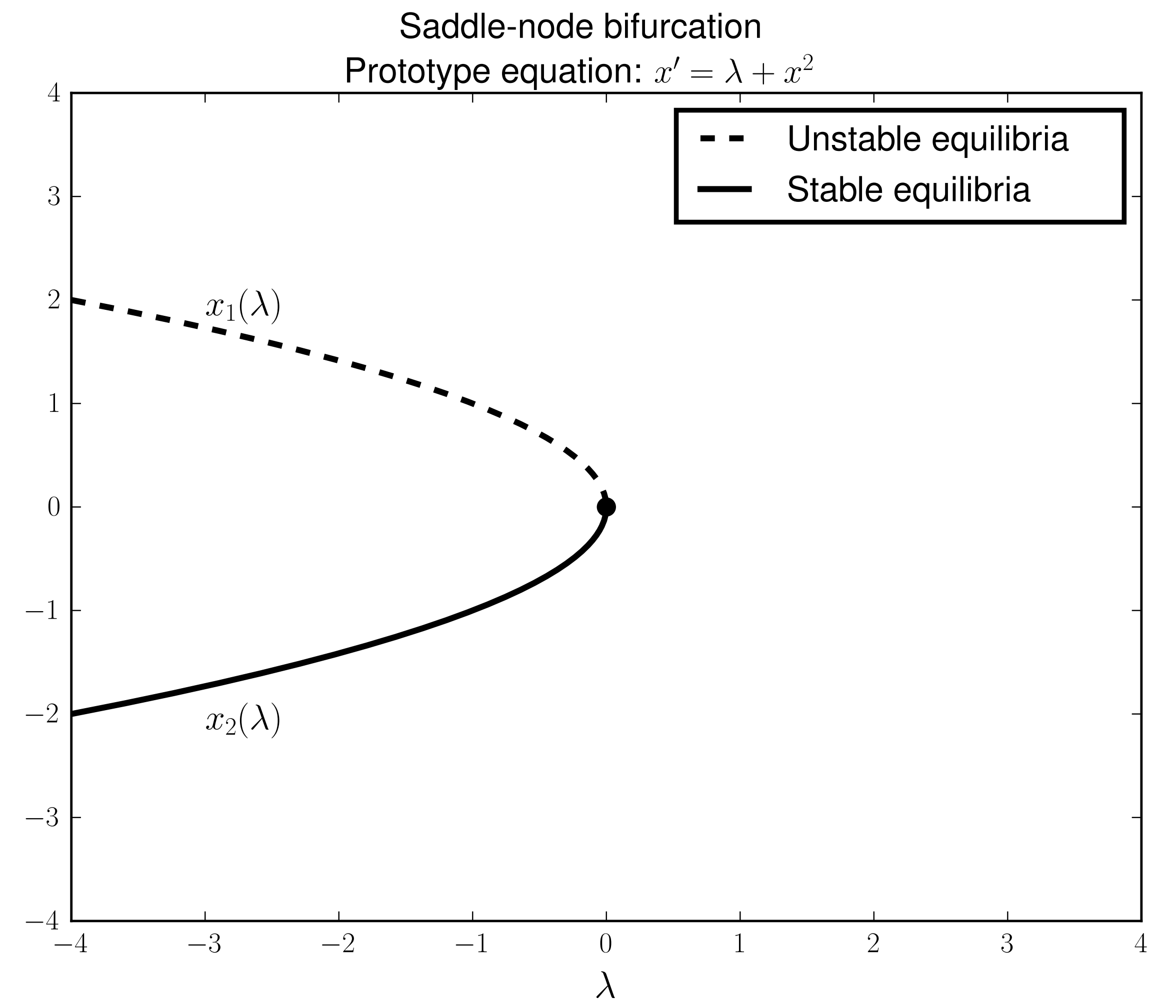


Figure 5.1: Bifurcation diagram for the equation $\dot{x} = \lambda + x^2$.

```
import matplotlib.pyplot as plt
from scipy.optimize import newton

def EmbeddingAlg(param_list, guess, F):
    X = []
    for param in param_list:
        try:
            # Solve for x_value making F(x_value, param) = 0.
            x_value = newton(F, guess, fprime=None, args=(param,), tol=1E-7, ↩
                maxiter=50)
            # Record the solution and update guess for the next iteration.
            X.append(x_value)
            guess = x_value
        except RuntimeError:
            # If Newton's method fails, return a truncated list of parameters
```

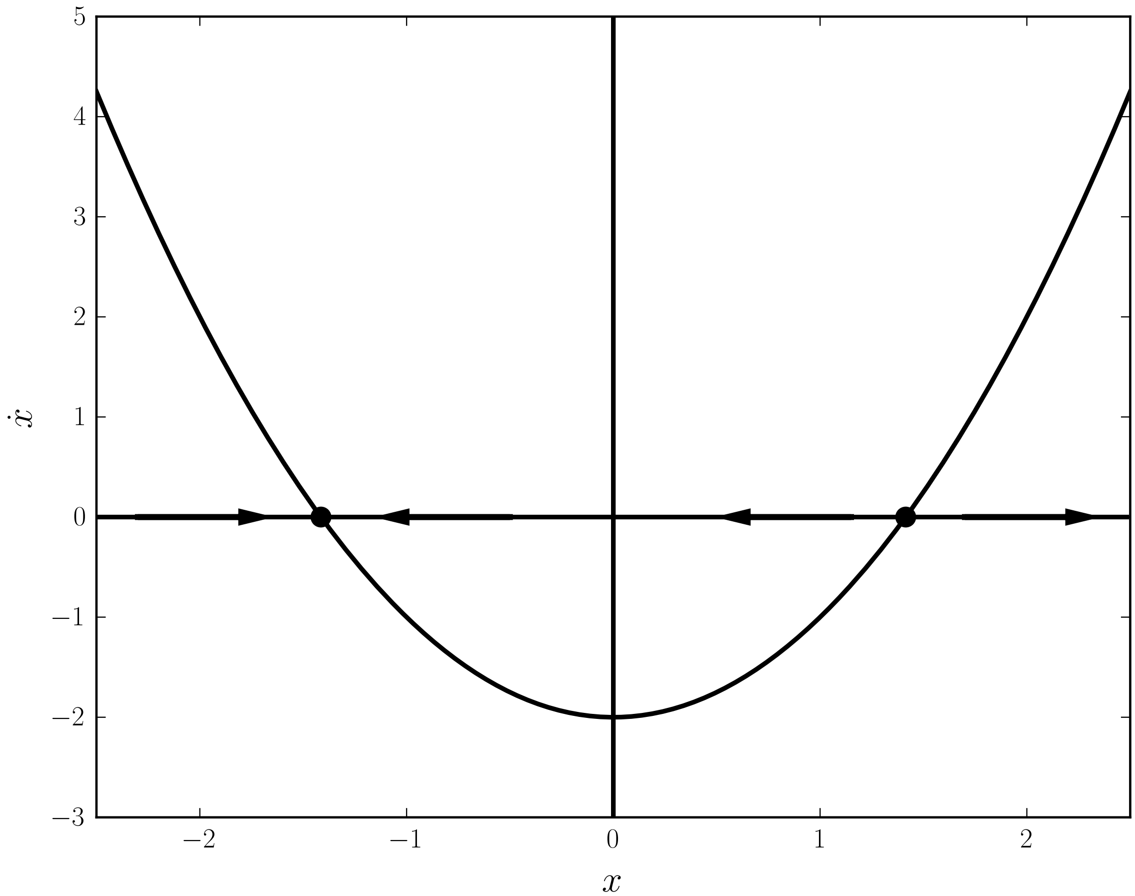


Figure 5.2: Phase Portrait for the equation $\dot{x} = -2 + x^2$.

```
            # with the corresponding x values.
            return param_list[:len(X)], X
    # Return the list of parameters and the corresponding x values.
    return param_list, X

def F(x, lmbda):
    return x**2 + lmbda

# Top curve shown in the bifurcation diagram
C1, X1 = EmbeddingAlg(np.linspace(-5, 0, 200), np.sqrt(5), F)
# The bottom curve
C2, X2 = EmbeddingAlg(np.linspace(-5, 0, 200), -np.sqrt(5), F)
```

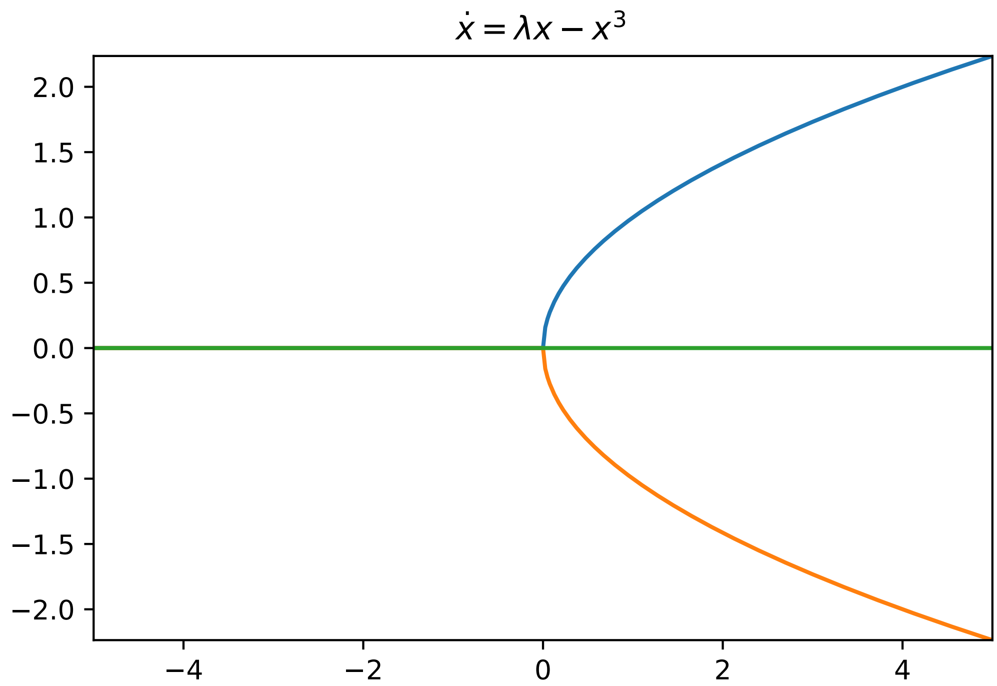


Figure 5.3: Bifurcation diagram for the equation $\dot{x} = \lambda x - x^3$.

Problem 1. Use the natural embedding algorithm to create a bifurcation diagram for the differential equation

$$\dot{x} = \lambda x - x^3.$$

This type of bifurcation is called a pitchfork bifurcation (you should see a pitchfork in your diagram).

Hints: Essentially this amounts to running the same code as the example, but with different parameters and function calls so that you are tracing through the right curves for this problem. To make this first problem work, you will want to have your 'linspace' run from high to low instead of from low to high. There will be three different lines in this image. See Figure 5.3.

Problem 2. Create bifurcation diagrams for the differential equation

$$\dot{x} = \eta + \lambda x - x^3,$$

where $\eta = -1, -.2, .2$ and 1. Notice that when $\eta = 0$ you can see the pitchfork bifurcation of the previous problem. There should be four different images, one for each value of η. Each image will be built of 3 pieces. See Figure 5.4.

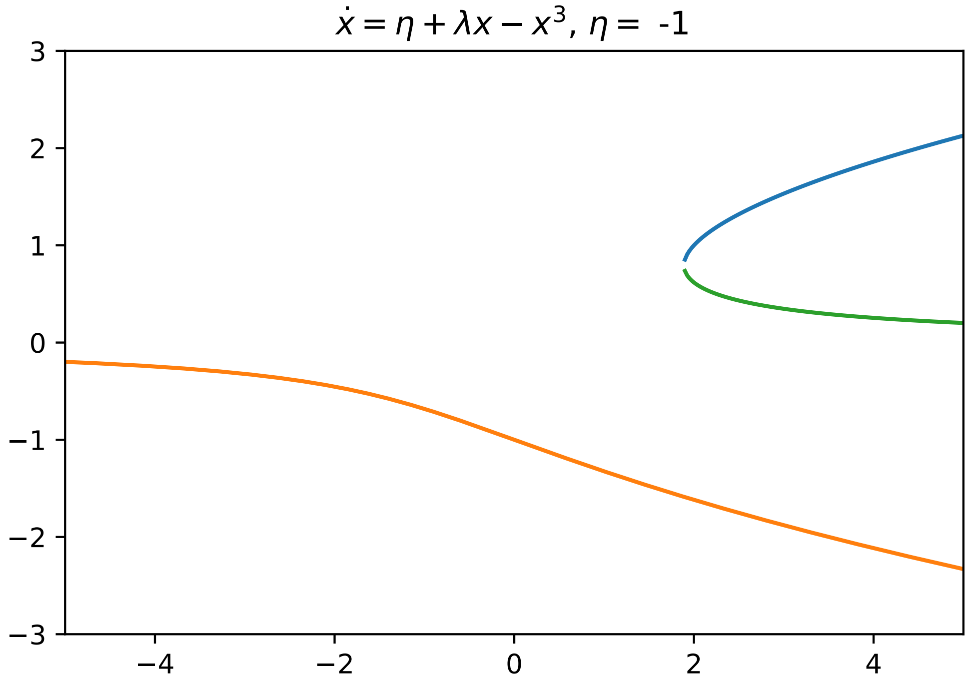


Figure 5.4: Bifurcation diagram for the equation $\dot{x} = \eta + \lambda x - x^3$ with $\eta = -1$.

Hysteresis

The following ODE exhibits an interesting bifurcation phenomenon called hysteresis:

$$x' = \lambda + x - x^3.$$

This system has a bifurcation diagram containing what is known as a hysteresis loop, shown in Figure 5.5. In the hysteresis loop, when the parameter λ moves beyond the bifurcation point the equilibrium solution makes a sudden jump to the other stable branch. When this occurs the system cannot reach its previous equilibrium by simply rewinding the parameter slightly. The next section discusses a model with a hysteresis loop.

Budworm Population Dynamics

Here we study a mathematical model describing the population dynamics of an insect called the spruce budworm. In eastern Canada, an outbreak in the budworm population can destroy most of the trees in a forest of balsam fir trees in about 4 years. The mathematical model is given by

$$\dot{N} = RN\left(1 - \frac{N}{K}\right) - p(N). \tag{5.4}$$

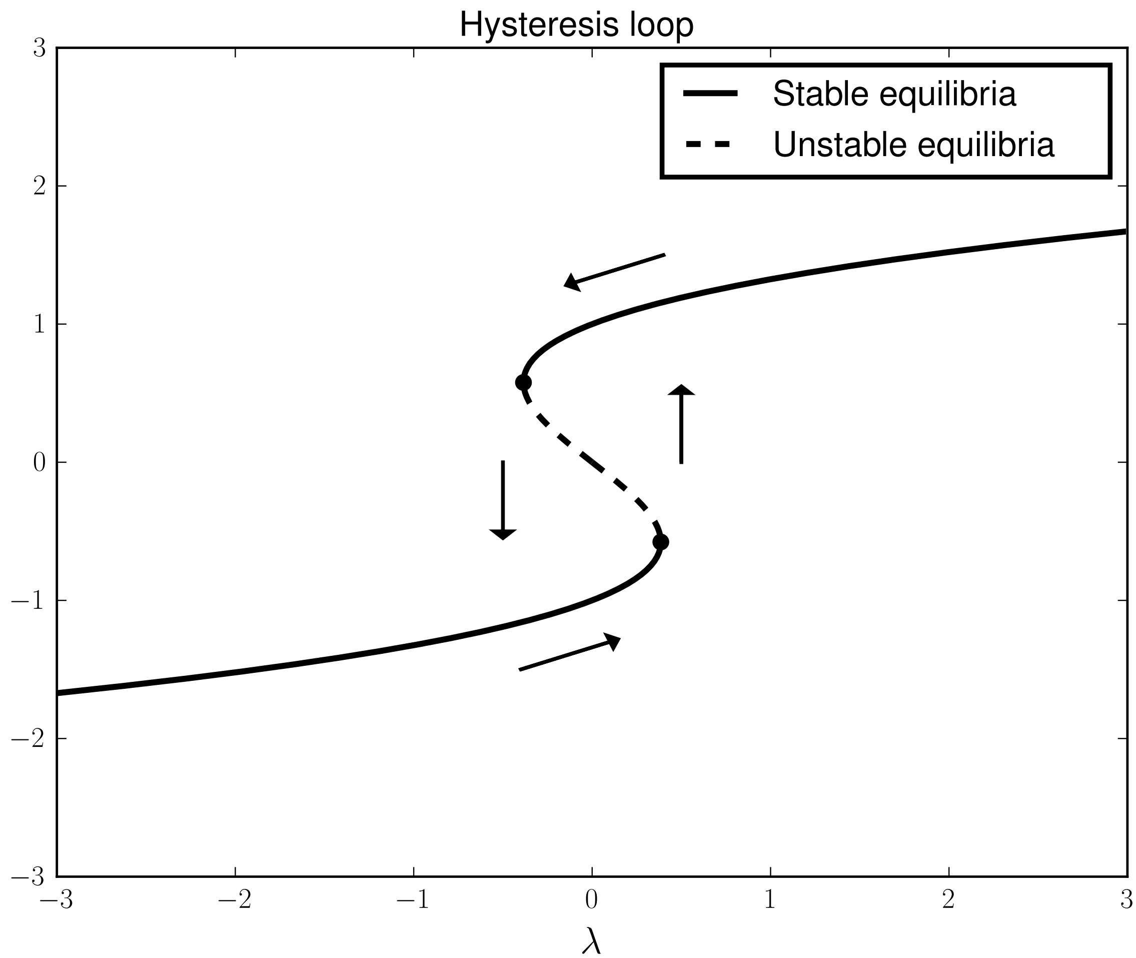


Figure 5.5: Bifurcation diagram for the ODE $x' = \lambda + x - x^3$.

This model was studied by Ludwig et al (1978), and is described well in Strogatz's text *Nonlinear Dynamics and Chaos*. Here $N(t)$ represents the budworm population at time t, R is the growth rate of the budworm population and K represents the carrying capacity of the environment. We could interpret K to represent the amount of food available to the budworms. $p(N)$ represents the death rate of budworms due to predators (birds); we assume specifically that $p(N)$ has the form $P(N) = \frac{BN^2}{A^2+N^2}$.

Before studying the equilibrium points of (5.4) it is important to reduce the number of parameters in the system by nondimensionalizing. Thus, we make the coordinate change $x = N/A$, $\tau = Bt/A$, $r = RA/B$, and $k = K/A$, obtaining finally the system

$$\frac{dx}{d\tau} = rx(1 - x/k) - \frac{x^2}{1 + x^2}. \tag{5.5}$$

Note that $x = 0$ is always an equilibrium solution. To find other equilibrium solutions we study the equation $r(1-x/k)-x/(1+x^2) = 0$. Fix $r = .56$, and consider Figure (5.6) ($k = 8$ in the figure).

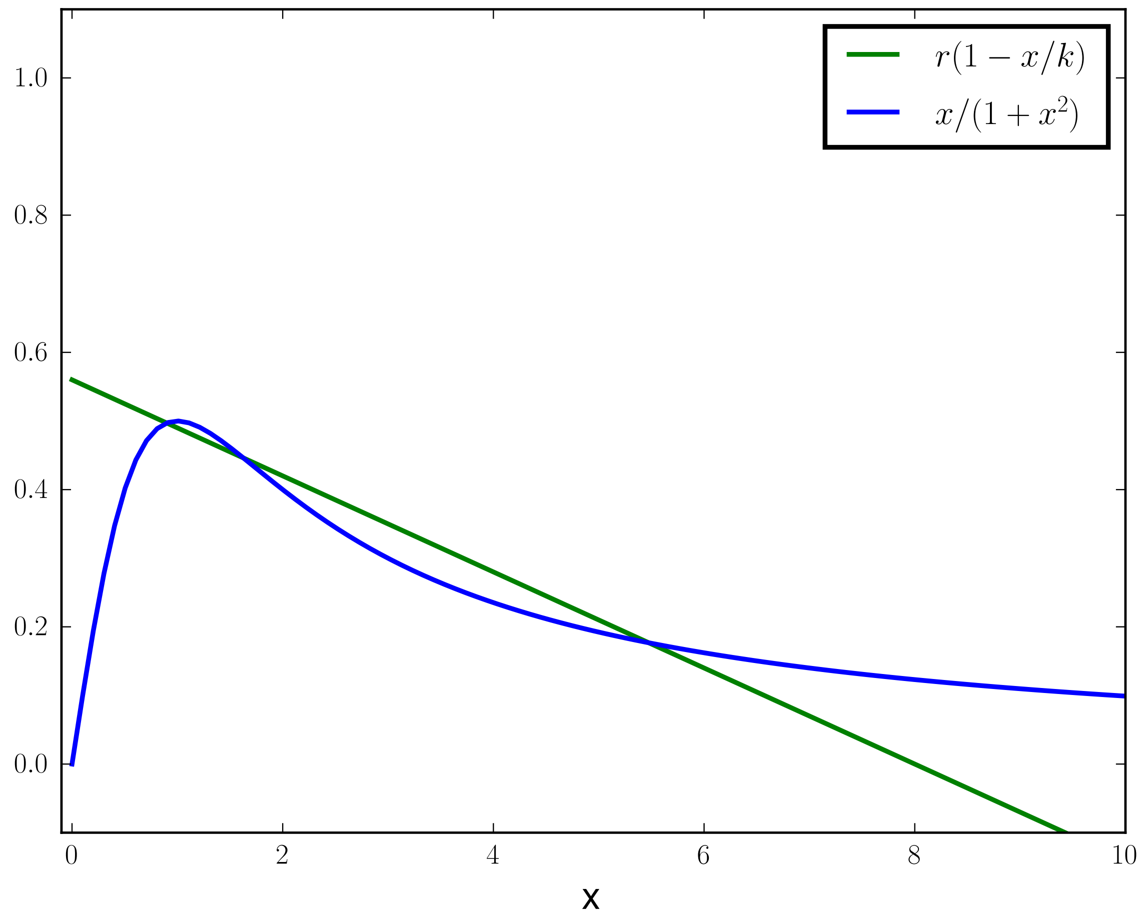


Figure 5.6: Graphical demonstration of nonzero equilibrium solutions for the budworm population (here $r = .56,\ k = 8$); equilibrium solutions occur where the curves cross. As k increases, the line $y = r(1 - x/k)$ gets more shallow and the number of solutions goes from one to three and then back to one.

Problem 3 (Budworm Population). Reproduce the bifurcation diagram for the differential equation

$$\frac{dx}{d\tau} = rx(1 - x/k) - \frac{x^2}{1+x^2},$$

where $r = 0.56$.

Hint: Find a value for k that you know is in the middle of the plot (i.e. where there are three possible solutions), then use the code above to expand along each contour till you obtain the desired curve. Now find the proper initial guesses that give you the right bifurcation curve. The final plot will look like the one in Figure 5.7, but you will have to run the embedding algorithm 4-6 times to get every part of the plot.

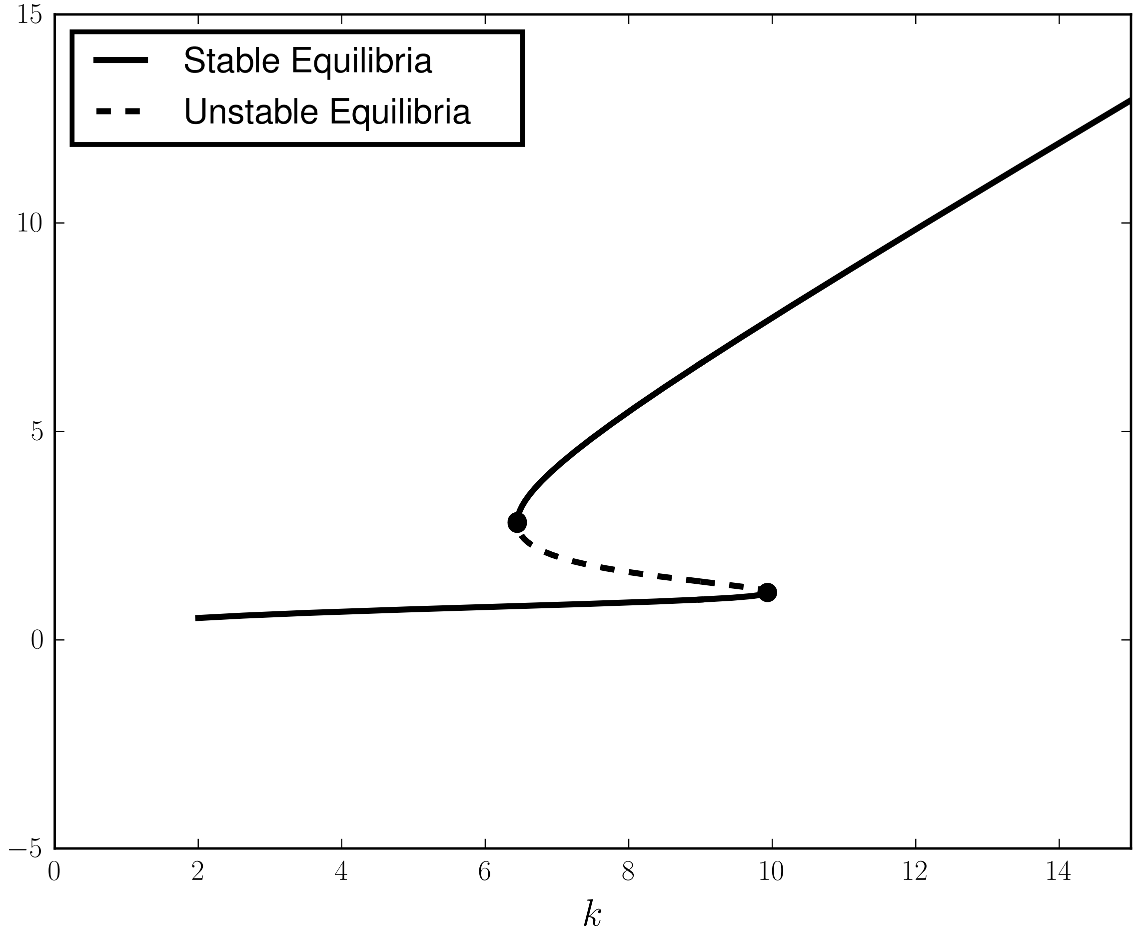


Figure 5.7: Bifurcation diagram for the budworm population model. The parameter r is fixed at 0.56. The lower stable branch is known as the refuge level of the bundworm population, while the upper stable branch is known as the outbreak level. Once the budworm population reaches an outbreak level, the available food (foliage of the balsam fir trees) in the system must be reduced drastically to jump back down to refuge level. Thus many of the balsam fir trees die before the budworm population returns to refuge level.

6 Lorenz Equations

Lab Objective: *Investigate the behavior of a system that exhibits chaotic behavior. Demonstrate methods for visualizing the evolution of a system.*

Chaos is everywhere. It can crop up in unexpected places and in remarkably simple systems, and a great deal of work has been done to describe the behavior of chaotic systems. One primary characteristic of chaos is that small changes in initial conditions result in large changes over time in the solution curves.

The Lorenz System

One of the earlier examples of chaotic behavior was discovered by Edward Lorenz. In 1963, while working to study atmospheric dynamics, he derived the simple system of equations

$$\begin{aligned}\frac{\partial x}{\partial t} &= \sigma\,(y - x)\\ \frac{\partial y}{\partial t} &= \rho x - y - xz\\ \frac{\partial z}{\partial t} &= xy - \beta z\end{aligned}$$

where σ, ρ, and β are all constants. After deriving these equations, he plotted the solutions and observed some unexpected behavior. For appropriately chosen values of σ, ρ, and β, the solutions did not tend toward any steady fixed points, nor did the system permit any stable cycles. The solutions did not tend off toward infinity either. With further work, he began the study of what was called a *strange attractor*. This system, though relatively simple, exhibits chaotic behavior.

Problem 1. Write a function that implements the Lorenz equations. Let $\sigma = 10$, $\rho = 28$, $\beta = \frac{8}{3}$. Make a 3D plot of a solution to the Lorenz equations, where the initial conditions x_0, y_0, z_0 are each drawn randomly from a uniform distribution on $[-15, 15]$. As usual, use `scipy.integrate.odeint` to compute an approximate solution. Compare your results with Figure 6.1.

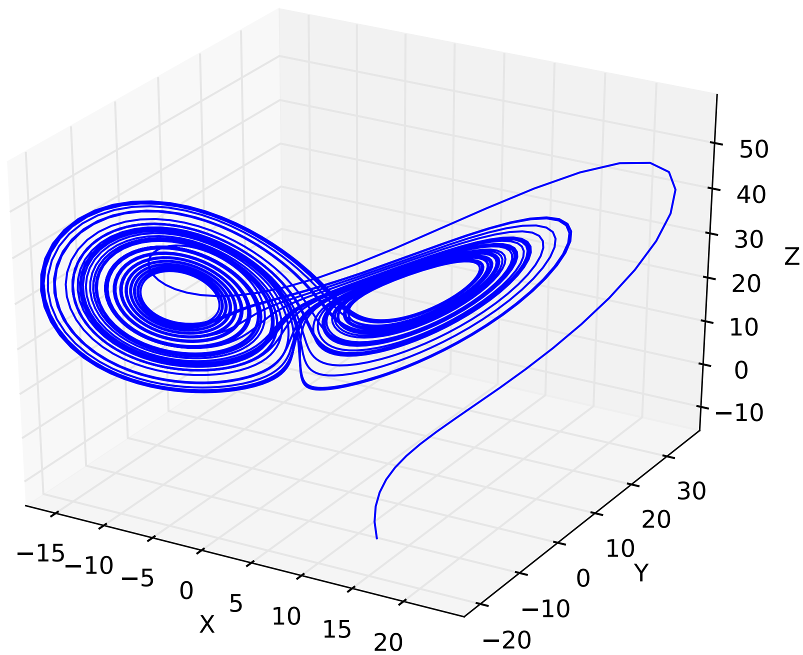


Figure 6.1: Approximate solution to the Lorenz equation with random initial conditions

Basin of Attraction

Notice in the first problem that the solution tended to a 'nice' region. This region is a basin of attraction, and the set of numerical values towards which a system will converge to is an **attractor**. Consider what happens when we change up the initial conditions.

Problem 2. To better visualize the Lorenz attractor, produce a single 3D plot displaying three solutions to the Lorenz equations, each with random initial conditions (as before). Compare your results with Figure 6.2.

Chaos

Chaotic systems exhibit high sensitivity to initial conditions. This means that a small difference in initial conditions may result in solutions that diverge significantly from each other. However, chaotic systems are not *random*. According to Lorenz, chaos is "when the present determines the future, but the approximate present does not approximately determine the future."

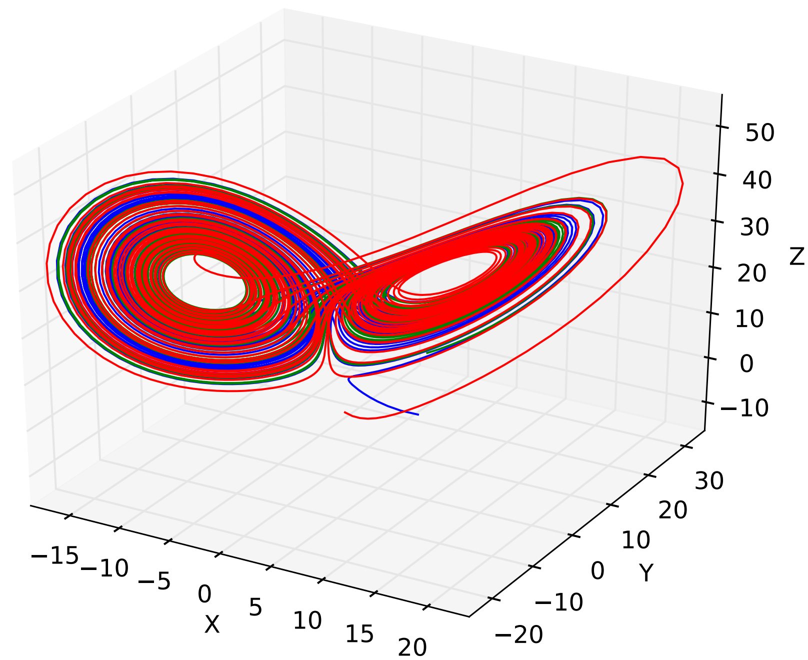


Figure 6.2: Multiple solutions to the Lorenz equation with random initial conditions

Problem 3. Use `matplotlib.animation.FuncAnimation` to produce a 3D animation of two solutions to the Lorenz equations with nearly identical initial conditions. To make the initial conditions, draw x_0, y_0, z_0 as before, and then make a second initial condition by adding a small perturbation to the first (Hint: try using `np.random.randn(3)*(1e-10)` for the perturbation). Note that it may take several seconds before the separation between the two solutions will be noticeable.

The animation should display a point marker as well as the past trajectory curve for each solution. Save your animation as `lorenz_animation.mp4`.

In a chaotic system, round-off error implicit in a numerical method can also cause divergent solutions. For example, using a Runge-Kutta method with two different values for the stepsize h on identical initial conditions will still result in approximations that differ in a chaotic fashion.

Problem 4. The `odeint` function allows user to specify error tolerances (similar to setting a value of h in a Runge-Kutta method). Using a single initial condition, produce two approximations by using the `odeint` arguments (`atol=1e-15, rtol=1e-13`) for the first approximation and (`atol=1e-12, rtol=1e-10`) for the second.

As in the previous problem, use `FuncAnimation` to animation both solutions. Save the animation as `lorenz_animation2.mp4`.

Lyapunov Exponents

The *Lyapunov exponent* of a dynamical system is one measure of how chaotic a system is. While there are more conditions for a system to be considered chaotic, one of the primary indicators of a chaotic system is *extreme sensitivity to initial conditions*. Strictly speaking, this is saying that a chaotic system is poorly conditioned. In a chaotic system, the sensitivity to changes in initial conditions depends expoentially on the time the system is allowed to evolve. If $\delta(t)$ represents the difference between two solution curves, when $\delta(t)$ is small, the following approximation holds.

$$\|\delta(t)\| \sim \|\delta(0)\|e^{\lambda t}$$

where λ is a constant called the Lyapunov exponent. In other words, $\log(\|\delta(t)\|)$ is approximately linear as a function of time, with slope λ. For the Lorenz system (and for the parameter values specified in this lab), experimentally it can be verified that $\lambda \approx .9$.

Problem 5. Estimate the Lyapunov exponent of the Lorenz equations by doing the following:

- Produce an initial condition that already lies in the attractor. This can be done by using a random "dummy" initial condition, approximating the resulting solution to the Lorenz system for a short time, and then using the endpoint of that solution (which is now in the attractor) as the desired initial condition.
- Produce a second initial condition by adding a small perturbation to the first (as before).
- For both initial conditions, use `odeint` to produce approximate solutions for $0 \leq t \leq 10$
- Compute $\|\delta(t)\|$ by taking the norm of the vector difference between the two solutions for each value of t.
- Use `scipy.stats.linregress` to calculate a best-fit line for $\log(\|\delta(t)\|)$ against t.
- The slope of the best-fit line is an approximation for the Lyapunov exponent λ

Produce a plot similar to Figure 6.3 by using `plt.semilogy`.

Hint: Remember that the best-fit line you calculated corresponds to a best-fit exponential for $\|\delta(t)\|$. If `a` and `b` are the slope and intercept of the best-fit line, the best-fit exponential can be plotted using `plt.semilogy(t,np.exp(a*t+b)`.

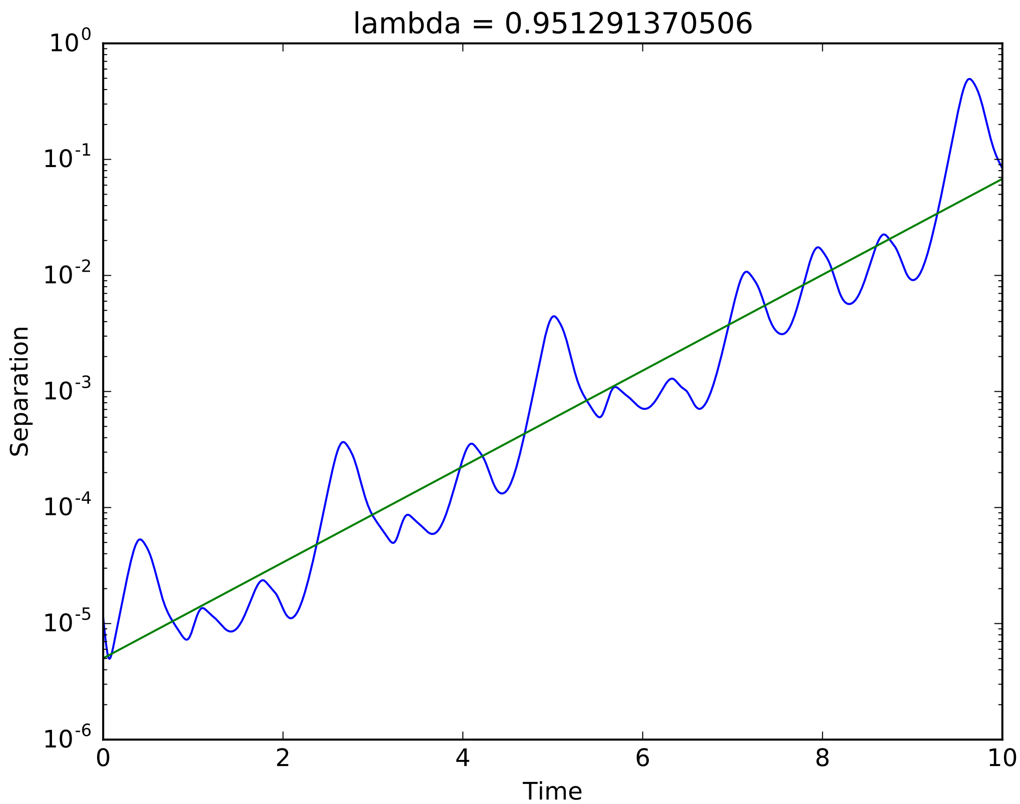


Figure 6.3: A semilog plot of the separation between two solutions to the Lorenz equations together with a fitted line that gives a rough estimate of the Lyapunov exponent of the system.

7 The Finite Difference Method

A **finite difference** for a function $f(x)$ is an expression of the form $f(x+s) - f(x+t)$. Finite differences can give a good approximation of derivatives.

Suppose we have a function $u(x)$, defined on an interval $[a, b]$. Let $a = x_0, x_1, \ldots x_{n-1}, x_n = b$ be a grid of $n+1$ evenly spaced points, with $x_{i+1} - x_i = h$, where $h = (b-a)/n$.

You are used to seeing the derivative $u'(x)$, which can written in centered-difference form as:

$$u'(x) = \lim_{h \to \infty} \frac{u(x+h) - u(x-h)}{2h}.$$

Suppose we are interested in knowing the value of the derivative at the points $\{x_i\}$. Even if we don't have a formula for $u'(x)$, we can approximate it using finite differences. We first write the Taylor polynomial expansion of $u(x+h)$ and $u(x-h)$ centered at x. This gives

$$u(x+h) = u(x) + u'(x)h + \frac{1}{2}u''(x)h^2 + \frac{1}{6}u'''(x)h^3 + \mathcal{O}(h^4) \tag{7.1}$$

$$u(x-h) = u(x) - u'(x)h + \frac{1}{2}u''(x)h^2 - \frac{1}{6}u'''(x)h^3 + \mathcal{O}(h^4) \tag{7.2}$$

Subtracting (7.2) from (7.1) and rearranging gives

$$u'(x) = \frac{u(x+h) - u(x-h)}{2h} + \mathcal{O}(h^2).$$

In terms of our grid points $\{x_i\}$, we have:

$$u'(x_i) \approx \frac{u(x_i + h) - u(x_i - h)}{2h} = \frac{u(x_{i+1}) - u(x_{i-1})}{2h}.$$

We won't worry about the derivative at the endpoints, $u'(x_0)$ and $u'(x_n)$. This allows us to approximate the values $\{u'(x_i)\}$ as the solution to a system of equations:

$$\frac{1}{2h} \underbrace{\begin{bmatrix} -1 & 0 & 1 & & & & \\ & -1 & 0 & 1 & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & -1 & 0 & 1 & \\ & & & & -1 & 0 & 1 \end{bmatrix}}_{(n-1)\times(n+1)} \cdot \underbrace{\begin{bmatrix} u(x_0) \\ u(x_1) \\ \vdots \\ u(x_{n-1}) \\ u(x_n) \end{bmatrix}}_{(n+1)\times 1} \approx \underbrace{\begin{bmatrix} u'(x_1) \\ u'(x_2) \\ \vdots \\ u'(x_{n-2}) \\ u'(x_{n-1}) \end{bmatrix}}_{(n-1)\times 1}. \tag{7.3}$$

This can be rewritten with a $(n-1)\times(n-1)$ tridiagonal matrix instead:

$$\frac{1}{2h}\underbrace{\begin{bmatrix} 0 & 1 & & & \\ -1 & 0 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 0 & 1 \\ & & & -1 & 0 \end{bmatrix}}_{(n-1)\times(n-1)} \cdot \underbrace{\begin{bmatrix} u(x_1) \\ u(x_2) \\ \vdots \\ u(x_{n-2}) \\ u(x_{n-1}) \end{bmatrix}}_{(n-1)\times 1} + \underbrace{\begin{bmatrix} -u(x_0)/(2h) \\ 0 \\ \vdots \\ 0 \\ u(x_n)/(2h) \end{bmatrix}}_{(n-1)\times 1} \approx \underbrace{\begin{bmatrix} u'(x_1) \\ u'(x_2) \\ \vdots \\ u'(x_{n-2}) \\ u'(x_{n-1}) \end{bmatrix}}_{(n-1)\times 1}. \tag{7.4}$$

Next, we will consider the approximation for $u''(x)$. If we let

$$u'(x) \approx \frac{u(x+\frac{h}{2}) - u(x-\frac{h}{2})}{h}$$

then

$$u''(x) \approx \frac{u'(x+\frac{h}{2}) - u'(x-\frac{h}{2})}{h} \approx \frac{\frac{u((x+\frac{h}{2})+\frac{h}{2}) - u((x+\frac{h}{2})-\frac{h}{2})}{h} - \frac{u((x-\frac{h}{2})+\frac{h}{2}) - u((x-\frac{h}{2})-\frac{h}{2})}{h}}{h}$$

$$= \frac{u(x+h) - 2u(x) + u(x-h)}{h^2}$$

You can achieve the same result by again consider the Taylor polynomial expansion and adding (7.1) and (7.2) and rearranging. Thus

$$u''(x_i) \approx \frac{u(x_i+h) - 2u(x_i) + u(x_i-h)}{h^2} = \frac{u(x_{i+1}) - 2u(x_i) + u(x_{i-1})}{h^2}$$

Again ignoring the second derivative at the endpoints, this can be written in matrix form as

$$\frac{1}{h^2}\underbrace{\begin{bmatrix} 1 & -2 & 1 & & & & \\ & 1 & -2 & 1 & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & 1 & -2 & 1 & \\ & & & & 1 & -2 & 1 \end{bmatrix}}_{(n-1)\times(n+1)} \cdot \underbrace{\begin{bmatrix} u(x_0) \\ u(x_1) \\ \vdots \\ u(x_{n-1}) \\ u(x_n) \end{bmatrix}}_{(n+1)\times 1} \approx \underbrace{\begin{bmatrix} u''(x_1) \\ u''(x_2) \\ \vdots \\ u''(x_{n-2}) \\ u''(x_{n-1}) \end{bmatrix}}_{(n-1)\times 1}. \tag{7.5}$$

This can also be written with a $(n-1)\times(n-1)$ tridiagonal matrix:

$$\frac{1}{h^2}\underbrace{\begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{bmatrix}}_{(n-1)\times(n-1)} \cdot \underbrace{\begin{bmatrix} u(x_1) \\ u(x_2) \\ \vdots \\ u(x_{n-2}) \\ u(x_{n-1}) \end{bmatrix}}_{(n-1)\times 1} + \underbrace{\begin{bmatrix} u(x_0)/h^2 \\ 0 \\ \vdots \\ 0 \\ u(x_n)/h^2 \end{bmatrix}}_{(n-1)\times 1} = \underbrace{\begin{bmatrix} u''(x_1) \\ u''(x_2) \\ \vdots \\ u''(x_{n-2}) \\ u''(x_{n-1}) \end{bmatrix}}_{(n-1)\times 1} \tag{7.6}$$

Problem 1. Let $u(x) = \sin((x+\pi)^2 - 1)$. Use (7.3) - (7.6) to approximate $\frac{1}{2}u'' - u'$ at the grid points where $a = 0$, $b = 1$, and $n = 10$. Graph the result.

The previous equations are not only useful for approximating derivatives, but they can be also used to solve differential equations. Suppose that instead of knowing the function $u(x)$, we know that $\frac{1}{2}u'' - u' = f$, where the function $f(x)$ is given. How do we solve for $u(x)$?

Finite Difference Methods

Numerical methods for differential equations seek to approximate the exact solution $u(x)$ at some finite collection of points in the domain of the problem. Instead of analytically solving the original differential equation, defined over an infinite-dimensional function space, they use a well-chosen finite system of algebraic equations to approximate the original problem.

Consider the following differential equation:

$$
\begin{aligned}
&\varepsilon u''(x) - u(x)' = f(x), \quad x \in (0,1), \\
&u(0) = \alpha, \quad u(1) = \beta.
\end{aligned} \tag{7.7}
$$

Equation (7.7) can be written $Du = f$, where $D = \varepsilon \frac{d^2}{dx^2} - \frac{d}{dx}$ is a differential operator defined on the infinite-dimensional space of functions that are twice continuously differentiable on $[0,1]$ and satisfy $u(0) = \alpha$, $u(1) = \beta$.

We look for an approximate solution $\{U_i\}$, where

$$
U_i \approx u(x_i)
$$

on an evenly spaced grid of points, $a = x_0, x_1, \ldots, x_n = b$,. Our finite difference method will replace the differential operator $D = \varepsilon \frac{d^2}{dx^2} - \frac{d}{dx}$, (which is defined on an infinite-dimensional space), with finite difference operators (defined on a finite dimensional space). To do this, we replace derivative terms in the differential equation with appropriate difference expressions.

Recalling that

$$
\begin{aligned}
\frac{d^2}{dx^2} u(x_i) &= \frac{u(x_{i+1}) - 2u(x_i) + u(x_{i-1})}{h^2} + \mathcal{O}(h^2), \\
\frac{d}{dx} u(x_i) &= \frac{u(x_{i+1}) - u(x_{i-1})}{2h} + \mathcal{O}(h^2).
\end{aligned}
$$

we define the finite difference operator D_h by

$$
D_h U_i = \varepsilon \frac{1}{h^2} \left(U_{i+1} - 2U_i + U_{i-1} \right) - \frac{1}{2h} \left(U_{i+1} - U_{i-1} \right). \tag{7.8}
$$

Thus we discretize equation (7.7) using the equations

$$
\frac{\varepsilon}{h^2} (U_{i+1} - 2U_i + U_{i-1}) - \frac{1}{2h} \left(U_{i+1} - U_{i-1} \right) = f(x_i), \quad i = 1, \ldots, n-1,
$$

along with boundary conditions $U_0 = \alpha$, $U_n = \beta$.

This gives $n+1$ equations and $n+1$ unknowns, and can be written in matrix form as

$$
\frac{1}{h^2}
\underbrace{\begin{bmatrix}
h^2 & 0 & 0 & \ldots & 0 \\
(\varepsilon + h/2) & -2\varepsilon & (\varepsilon - h/2) & \ldots & 0 \\
\vdots & & \ddots & & \vdots \\
0 & \ldots & (\varepsilon + h/2) & -2\varepsilon & (\varepsilon - h/2) \\
0 & \ldots & & 0 & h^2
\end{bmatrix}}_{(n+1)\times(n+1)}
\cdot
\underbrace{\begin{bmatrix}
U_0 \\ U_1 \\ \vdots \\ U_{n-1} \\ U_n
\end{bmatrix}}_{(n+1)\times 1}
=
\underbrace{\begin{bmatrix}
\alpha \\ f(x_1) \\ \vdots \\ f(x_{n-1}) \\ \beta
\end{bmatrix}}_{(n+1)\times 1}
.
$$

As before, we can remove two equations to modify the system to obtain an $(n-1)\times(n-1)$ tridiagonal system:

$$\frac{1}{h^2}\underset{(n-1)\times(n-1)}{\begin{bmatrix} -2\varepsilon & (\varepsilon-h/2) & 0 & \dots & 0 \\ (\varepsilon+h/2) & -2\varepsilon & (\varepsilon-h/2) & \dots & 0 \\ \vdots & & \ddots & & \vdots \\ 0 & \dots & (\varepsilon+h/2) & -2\varepsilon & (\varepsilon-h/2) \\ 0 & \dots & & (\varepsilon+h/2) & -2\varepsilon \end{bmatrix}} \cdot \underset{(n-1)\times 1}{\begin{bmatrix} U_1 \\ U_2 \\ \vdots \\ U_{n-2} \\ U_{n-1} \end{bmatrix}} = \underset{(n-1)\times 1}{\begin{bmatrix} f(x_1)-\alpha(\varepsilon+h/2)/h^2 \\ f(x_2) \\ \vdots \\ f(x_{n-2}) \\ f(x_{n-1})-\beta(\varepsilon-h/2)/h^2 \end{bmatrix}}. \tag{7.9}$$

Problem 2. Use equation (7.9) to solve the singularly perturbed BVP (7.7) with $\varepsilon = 1/10$, $f(x) = -1$, $\alpha = 1$, and $\beta = 3$ on a grid with $n = 30$ subintervals. Graph the solution. This BVP is called singularly perturbed because of the location of the parameter ε. For $\varepsilon = 0$ the ODE has a drastically different character - it then becomes first order, and can no longer support two boundary conditions.

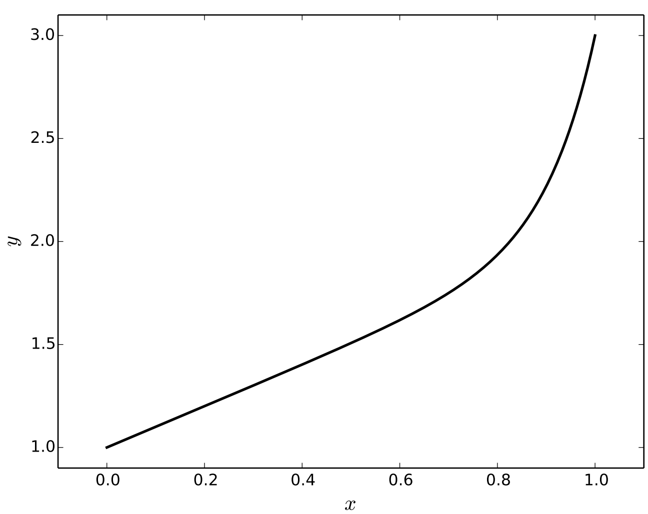


Figure 7.1: The solution to Problem 2. The solution gets steeper near $x = 1$ as ε gets small.

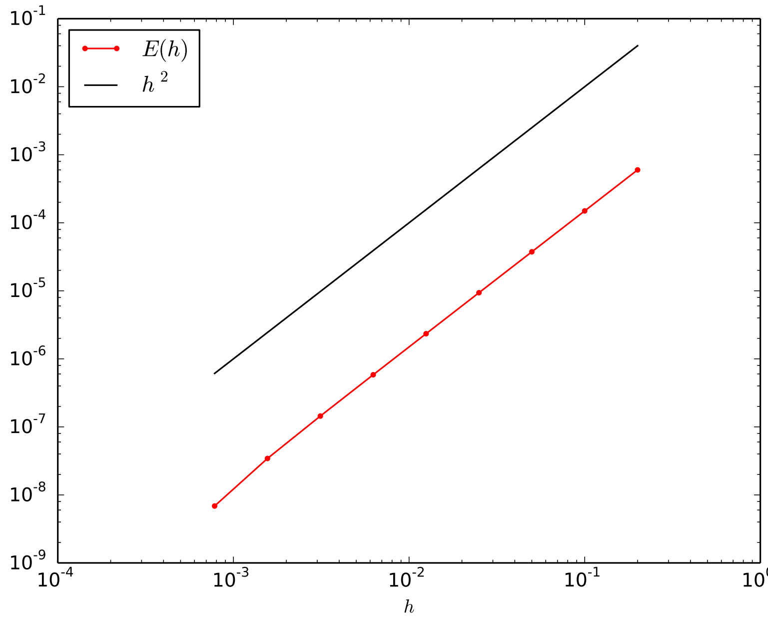


Figure 7.2: Demonstration of second order convergence for the finite difference approximation (7.8) of the BVP given in (7.7) with $\varepsilon = .5$.

A heuristic test for convergence

The finite differences used above are second order approximations of the first and second derivatives of a function. It seems reasonable to expect that the numerical solution would converge at a rate of about $\mathcal{O}(h^2)$. How can we check that a numerical approximation is reasonable?

Suppose a finite difference method is $\mathcal{O}(h^p)$ accurate. This means that the error $E(h) \approx Ch^p$ for some constant C as $h \to 0$ (in other words, for $h > 0$ small enough).

So compute the approximation y_k for each stepsize h_k, $h_1 > h_2 > \ldots > h_m$. y_m should be the most accurate approximation, and will be thought of as the true solution. Then the error of the approximation for stepsize $h_k, k < m$, is

$$\begin{aligned} E(h_k) &= \max(|y_k - y_m|) \approx Ch_k^p, \\ \log(E(h_k)) &= \log(C) + p\log(h_k). \end{aligned}$$

Thus on a log-log plot of $E(h)$ vs. h, these values should be on a straight line with slope p when h is small enough to start getting convergence. We should note that demonstrating second-order convergence does NOT imply that the numerical approximation is converging to the correct solution.

Problem 3. Visualize the $\mathcal{O}(h^2)$ convergence of this finite difference method by producing a loglog plot similar to Figure 7.2, except in the case $\varepsilon = .1$. Implement a function `singular_bvp` to compute the finite difference solution to 7.7. Using $n = 5 \times 2^0, 5 \times 2^1, \ldots, 5 \times 2^9$ subintervals, compute 10 approximate solutions.

To produce the plot, treat the approximation with $n = 5 \times 2^9$ subintervals as the "true solution", and measure the error for the other approximations against it. Note that, since the number of subintervals for each approximation is a multiple of 2, we can compute the L_∞ error for the $n = 5 \times 2^j$ approximation by using the `step` argument in the array slicing syntax:

```
# best approximation
sol_best = singular_bvp(eps,alpha,beta,f,5*(2**9))

# approximation with 5*(2^j) intervals
sol_approx = singular_bvp(eps,alpha,beta,f,5*(2**j))

# approximation error
error = np.max(np.abs(sol_approx - sol_best[::2**(9-j)]))
```

Problem 4. Extend your finite difference code to the case of a general second order linear BVP with boundary conditions:

$$\begin{aligned} &a_1(x)y'' + a_2(x)y' + a_3(x)y = f(x), \quad x \in (a, b), \\ &y(a) = \alpha, \quad y(b) = \beta. \end{aligned}$$

Use your code to solve the boundary value problem

$$\begin{aligned} \varepsilon y'' - 4(\pi - x^2)y &= \cos x, \\ y(0) = 0, \quad y(\pi/2) &= 1, \end{aligned}$$

for $\varepsilon = 0.1$ on a grid with $n = 30$ subintervals. Be sure to modify the finite difference operator D_h in (7.8) correctly.

The next few problems will help you test your finite difference code.

Problem 5. Numerically solve the boundary value problem

$$\begin{aligned} \varepsilon y'' + xy' &= -\varepsilon\pi^2 \cos(\pi x) - \pi x \sin(\pi x), \\ y(-1) &= -2, \quad y(1) = 0, \end{aligned}$$

for $\varepsilon = 0.1, 0.01$, and 0.001. Use a grid with $n = 150$ subintervals.

Problem 6. Numerically solve the boundary value problem

$$\begin{aligned} (\varepsilon + x^2)y'' + 4xy' + 2y &= 0, \\ y(-1) = 1/(1+\varepsilon), \quad y(1) &= 1/(1+\varepsilon), \end{aligned}$$

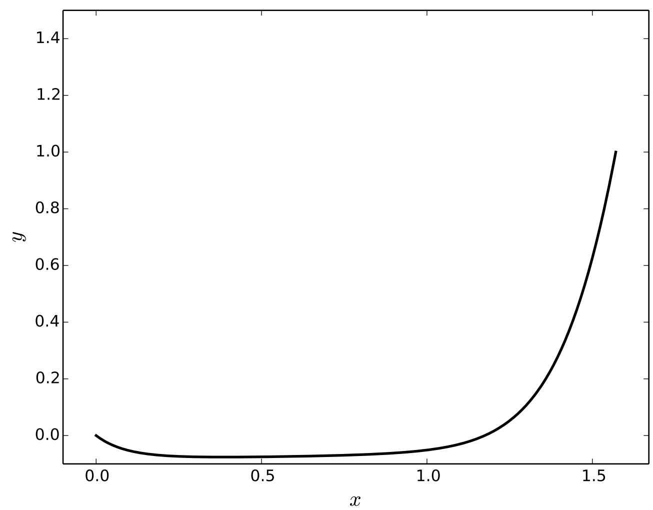


Figure 7.3: The solution to Problem 4.

for $\varepsilon = 0.05, 0.02$. Use a grid with $n = 150$ subintervals.

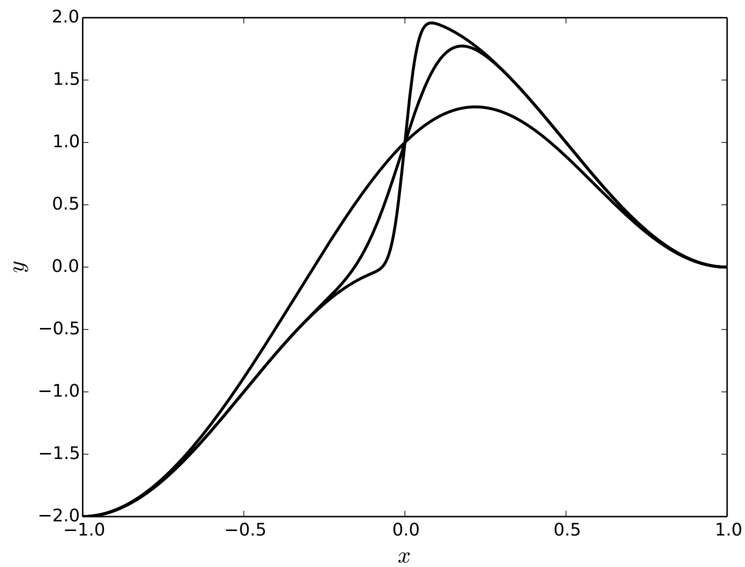


Figure 7.4: The solution to Problem 5.

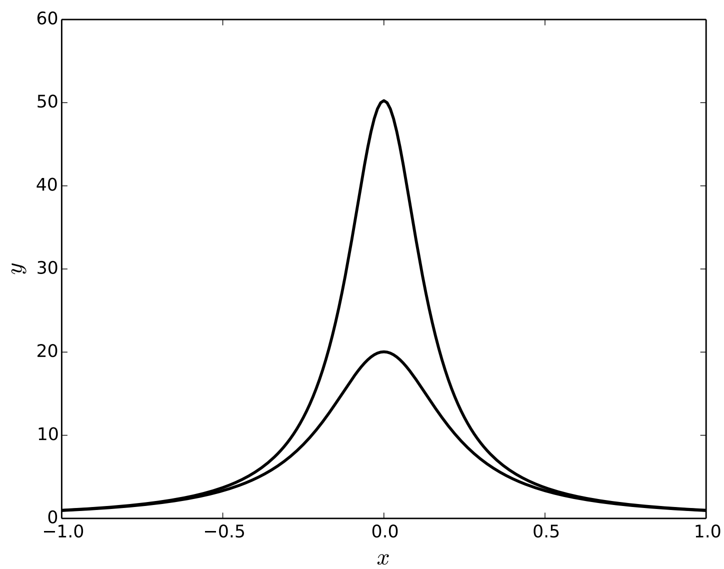


Figure 7.5: The solution to Problem 6.

8 Conservation laws and heat flow

A conservation law is a balance law, and corresponds to an equation that describes how a quantity is balanced in some system throughout a given process. (Consider how this is related to conservation laws in physics.) For example, suppose we are keeping track of some measurable quantity in a physical system (e.g. heat, water, etc). The fundamental conservation law then states that the rate of change of the total quantity in the system is equal to the rate of the quantity flowing into the system plus the rate at which the quantity is produced by sources inside the system.

Derivation of the Conservation equation in multiple dimensions

Suppose Ω is a region in $\mathbb{R}^n$, and $V \subset \Omega$ is bounded with a reasonably well-behaved boundary ∂V. Let $u(\vec{x}, t)$ represent the density (concentration) of some quantity throughout Ω. Let $\vec{n}(x)$ represent the normal direction to V at $x \in \partial V$, and let $\vec{J}(\vec{x}, t)$ be the flux vector for the quantity, so that $\vec{J}(\vec{x}, t) \cdot \vec{n}(x)\, dA$ represents the rate at which the quantity leaves V by crossing a boundary element with area dA. Note that the total amount of the quantity in V is

$$\int_V u(\vec{x}, t)\, dt,$$

and the rate at which the quantity enters V is

$$-\int_{\partial V} \vec{J}(\vec{x}, t) \cdot \vec{n}(x)\, dA.$$

We let the source term be given by $g(\vec{x}, t, u)$; we may interpret this to mean that the rate at which the quantity is produced in V is

$$\int_V g(\vec{x}, t, u)\, dt.$$

Then the integral form of the conservation law for u is expressed as

$$\frac{d}{dt}\int_V u(\vec{x}, t)\, d\vec{x} = -\int_{\partial V} \vec{J} \cdot \vec{n}\, dA + \int_V g(\vec{x}, t, u)\, d\vec{x}.$$

If u and J are sufficiently smooth functions, then we have

$$\frac{d}{dt}\int_V u\, d\vec{x} = \int_V u_t\, d\vec{x},$$

and

$$\int_{\partial V} \vec{J} \cdot \vec{n}\, dA = \int_V \nabla \cdot \vec{J}\, d\vec{x}.$$

Since this holds for all nice subsets $V \subset \Omega$ with V arbitrarily small, we obtain the differential form of the conservation law for u:

$$u_t + \nabla \cdot \vec{J} = g(\vec{x}, t, u),$$

where ∇ is the gradient function and $\nabla \cdot \vec{J} = \frac{\partial J_1}{\partial x_1} + \cdots + \frac{\partial J_n}{\partial x_n}$

Constitutive Relations

Currently our conservation law appears in the form

$$u_t + \nabla \cdot \vec{J} = g(\vec{x}, t, u).$$

Thus the conservation law consists of one equation and 2 unknowns (u and J). To this equation we add other equations, called constitutive relations, which are used to fully determine the system.

For example, suppose we wish to describe the flow of heat. Since heat flows from warmer regions to colder regions, and the rate of heat flow depends on the difference in temperature between regions, we usually assume that the flux vector $\vec{J}$ is given by

$$\vec{J}(x, t) = -\nu \nabla u(x, t),$$

where ν is a diffusion constant and $\nabla u(x,t) = [\partial_{x_1} u \ldots \partial_{x_n} u]^T$. This constitutive relation is called Fick's law, and is the basic model for any diffusive process. Substituting into the conservation law we obtain

$$u_t - \nu \Delta u(x, t) = g(\vec{x}, t, u)$$

where Δ is the Laplacian operator, and $\Delta u(x,t) = \frac{\partial^2 u}{\partial x_1^2} + \cdots + \frac{\partial^2 u}{\partial x_n^2}$. The function g represents heat sources/sinks within the region.

Numerically modeling heat flow

Consider the heat flow equation in one dimension together with appropriate initial conditions and homogeneous Dirichlet boundary conditions:

$$\begin{aligned}
&u_t = \nu u_{xx}, \quad x \in [a, b], \quad t \in [0, T], \\
&u(a, t) = 0, \quad u(b, t) = 0, \\
&u(x, 0) = f(x).
\end{aligned}$$

We will look for an approximation U_i^j to $u(x_i, t_j)$ on the grid $x_i = a + hi$, $t_j = kj$, where h and k are small changes in x and t respectively and i and j are indices. Note that the index i ranges over different spacial grid points and the index j ranges over different time steps. We will denote the approximate value of u at the i'th grid point and the j'th time step as U_i^j.

A common method for modeling ordinary and partial differential equations is the finite difference method, so-named because equations containing derivatives are replaced with equations containing difference schemes. These difference schemes can often be found using Taylor's theorem. For example, the equation

$$u(x, t_j + k) = u(x, t_j) + u_t(x, t_j)k + \mathcal{O}(k^2)$$

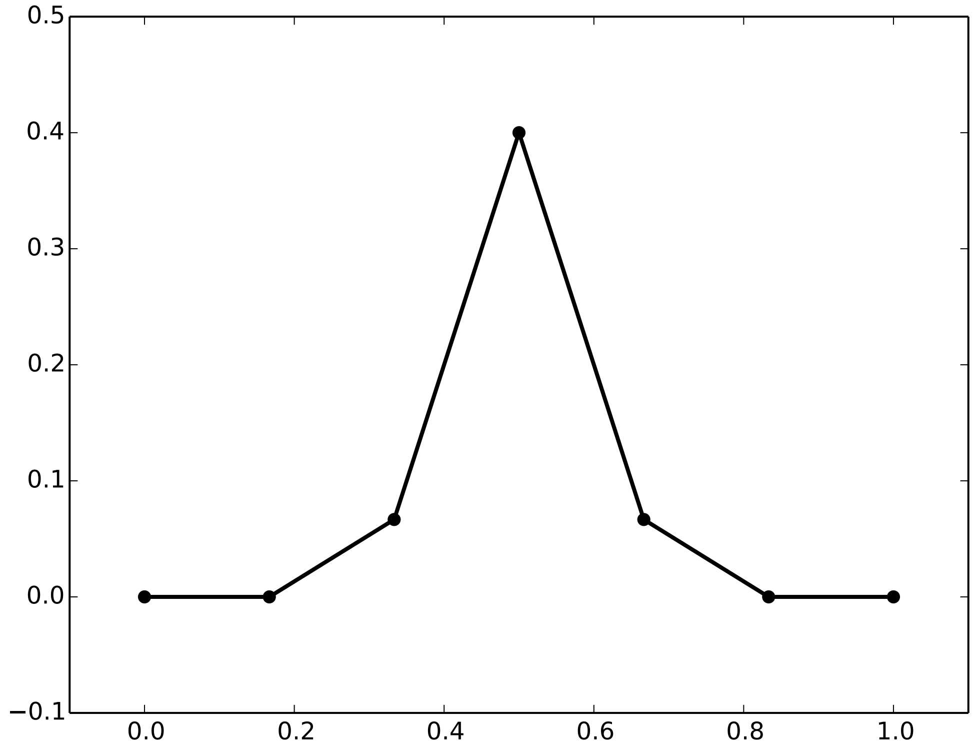


Figure 8.1: The graph of U^0, the approximation to the solution $u(x, t = 0)$ for Problem 1.

yields a first-order forward difference approximation to $u_t(x, t_j)$, namely,

$$u_t(x, t_j) = \frac{u(x, t_j + k) - u(x, t_j)}{k} + \mathcal{O}(k).$$

Similarly, by adding the equations

$$u(x_i + h, t) = u(x_i, t) + u_x(x_i, t)h + u_{xx}(x_i, t)\frac{h^2}{2} + u_{xxx}(x_i, t)h^3 + \mathcal{O}(h^4),$$
$$u(x_i - h, t) = u(x_i, t) + u_x(x_i, t)(-h) + u_{xx}(x_i, t)\frac{(-h)^2}{2} + u_{xxx}(x_i, t)(-h)^3 + \mathcal{O}(h^4),$$

we obtain a second-order centered difference approximation to $u_{xx}(x_i, t)$:

$$u_{xx}(x_i, t_j) = \frac{u(x_i + h, t_j) - 2u(x_i, t_j) - u(x_i - h, t_j)}{h^2} + \mathcal{O}(h^2).$$

These difference approximations give us the $\mathcal{O}(h^2 + k)$ explicit method

$$\begin{aligned} \frac{U_i^{j+1} - U_i^j}{k} &= \nu \frac{U_{i+1}^j - 2U_i^j + U_{i-1}^j}{h^2}, \\ U_i^{j+1} &= U_i^j + \frac{\nu k}{h^2}(U_{i+1}^j - 2U_i^j + U_{i-1}^j). \end{aligned} \tag{8.1}$$

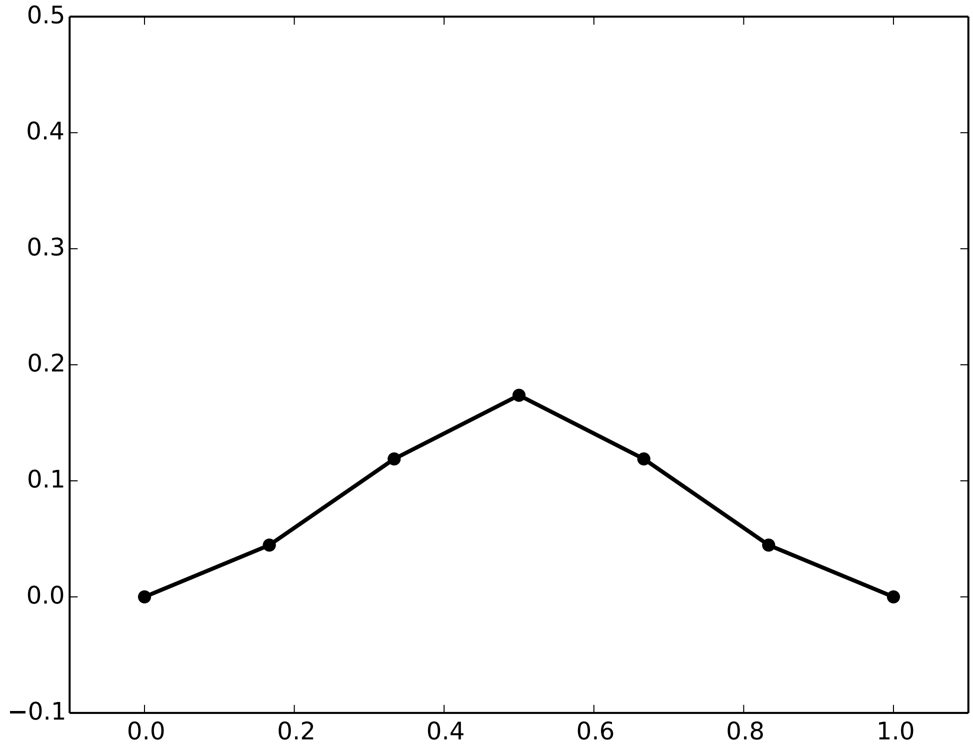


Figure 8.2: The graph of U^4, the approximation to the solution $u(x, t = .4)$ for Problem 1.

This method can be written in matrix form as

$$U^{j+1} = AU^j,$$

where A is the tridiagonal matrix given by

$$A = \begin{bmatrix} 1 & 0 & & & \\ \lambda & 1-2\lambda & \lambda & & \\ & \ddots & \ddots & \ddots & \\ & & \lambda & 1-2\lambda & \lambda \\ & & & 0 & 1 \end{bmatrix},$$

$\lambda = \nu k/h^2$, and U^j represents the approximation at time t_j. We can get this method started by using the initial condition given in our problem, so that $U_i^0 = f(x_i)$.

Note

Finite difference schemes, though they can be *represented* using matrix multiplication, should not be *implemented* using raw matrix multiplication. Using NumPy, it is best to vectorize the difference scheme so that you do not have to loop over the spatial indices. If you are using a language with faster loops (like C, C++, Fortran, or Cython), it could work well to loop directly through the indices in both time and space.

To account for boundary conditions using this differencing scheme, simply set the boundary points to the appropriate values in the initial conditions, then avoid modifying them as you update for each time step. This would be the equivalent of replacing the first and last rows of the matrix representation of the differencing scheme with the first and last rows of the identity matrix.

Problem 1. Consider the initial/boundary value problem

$$\begin{aligned}&u_t = .05u_{xx}, \quad x \in [0,1], \quad t \in [0,1]\\&u(0,t) = 0, \quad u(1,t) = 0,\\&u(x,0) = 2\max\{.2 - |x - .5|, 0\}.\end{aligned} \tag{8.2}$$

Approximate the solution $u(x,t)$ at time $t = .4$ by taking 6 subintervals in the x dimension and 10 subintervals in time. The graphs for U^0 and U^4 are given in Figures 8.1 and 8.2.

Problem 2. Solve the initial/boundary value problem

$$\begin{aligned}&u_t = u_{xx}, \quad x \in [-12,12], \quad t \in [0,1],\\&u(-12,t) = 0, \quad u(12,t) = 0,\\&u(x,0) = \max\{1 - x^2, 0\}\end{aligned} \tag{8.3}$$

using the first order explicit method 8.1. Use 140 subintervals in the x dimension and 70 subintervals in time. The initial and final states are shown in Figure 8.3. Animate your results.

Explicit methods usually have a stability condition, called a CFL condition (for Courant-Friedrichs-Lewy). For method 8.1 the CFL condition that must be satisfied is that

$$\lambda \leq \frac{1}{2}.$$

Repeat your computations using 140 subintervals in the x dimension and 66 subintervals in time. Animate the results. For these values the CFL condition is broken; you should easily see the result of this instability in the approximation U^{66}.

Implicit methods often have better stability properties than explicit methods. The Crank-Nicolson method, for example, is unconditionally stable and has order $\mathcal{O}(h^2 + k^2)$. To derive the Crank-Nicolson method, we use the following approximations:

$$\begin{aligned}u_t(x_i, t_{j+1/2}) &= \frac{u(x_i, t_{j+1}) - u(x_i, t_j)}{k} + \mathcal{O}(k^2),\\u_{xx}(x_i, t_{j+1/2}) &= \frac{u_{xx}(x_i, t_{j+1}) + u_{xx}(x_i, t_j)}{2} + \mathcal{O}(k^2).\end{aligned}$$

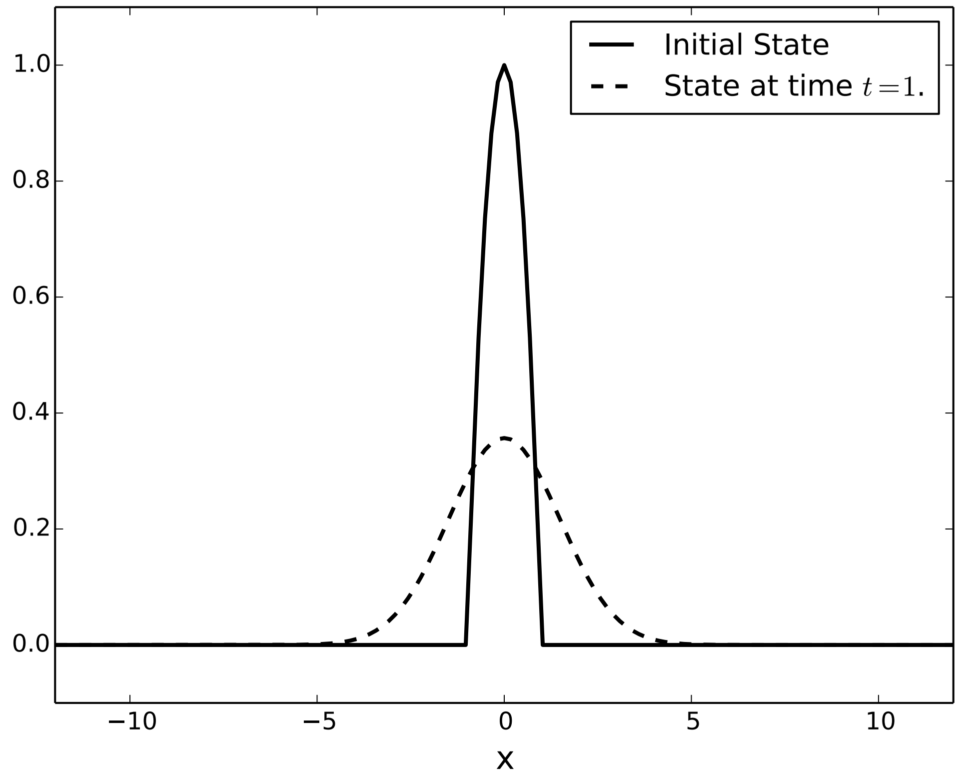


Figure 8.3: The initial and final states for equation Problem 2.

The first equation is a Finite Difference approximation, and the second is a midpoint approximation. These approximations give the method

$$\begin{aligned} \frac{U_i^{j+1} - U_i^j}{k} &= \frac{1}{2}\left(\frac{U_{i+1}^j - 2U_i^j + U_{i-1}^j}{h^2} + \frac{U_{i+1}^{j+1} - 2U_i^{j+1} + U_{i-1}^{j+1}}{h^2}\right), \\ U_i^{j+1} &= U_i^j + \frac{k}{2h^2}\left(U_{i+1}^j - 2U_i^j + U_{i-1}^j + U_{i+1}^{j+1} - 2U_i^{j+1} + U_{i-1}^{j+1}\right). \end{aligned} \tag{8.4}$$

This method can be written in matrix form as

$$BU^{j+1} = AU^j,$$

where A and B are tridiagonal matrices given by

$$B = \begin{bmatrix} 1 & 0 & & & \\ -\lambda & 1+2\lambda & -\lambda & & \\ & \ddots & \ddots & \ddots & \\ & & -\lambda & 1+2\lambda & -\lambda \\ & & & 0 & 1 \end{bmatrix},$$

$$A = \begin{bmatrix} 1 & 0 & & & \\ \lambda & 1-2\lambda & \lambda & & \\ & \ddots & \ddots & \ddots & \\ & & \lambda & 1-2\lambda & \lambda \\ & & & 0 & 1 \end{bmatrix},$$

where $\lambda = \nu k/(2h^2)$, and U^j represents the approximation at time t_j. Note that here we have defined λ differently than we did before!

How do we know if a numerical approximation is reasonable? One way to determine this is to compute solutions for various step sizes h and see if the solutions are converging to something. To be more specific, suppose our finite difference method is $\mathcal{O}(h^p)$ accurate. This means that the error $E(h) \approx Ch^p$ for some constant C as $h \to 0$ (i.e., for $h > 0$ small enough).

So compute the approximation y_k for each stepsize h_k, $h_1 > h_2 > \ldots > h_m$. We will think of y_m as the true solution. Then the error of the approximation for stepsize $h_k, k < m$, is

$$\begin{aligned} E(h_k) &= \max(|y_k - y_m|) \approx Ch_k^p, \\ \log(E(h_k)) &= \log(C) + p\log(h_k). \end{aligned}$$

Thus on a log-log plot of $E(h)$ vs. h, these values should be on a straight line with slope p when h is small enough to start getting convergence.

Problem 3. Using the Crank Nicolson method, numerically approximate the solution $u(x,t)$ of the problem

$$\begin{aligned} &u_t = u_{xx}, \quad x \in [-12, 12], \quad t \in [0,1], \\ &u(-12,t) = 0, \quad u(12,t) = 0, \\ &u(x,0) = \max\{1 - x^2, 0\}. \end{aligned} \tag{8.5}$$

Demonstrate that the numerical approximation at $t = 1$ converges to $u(x, t = 1)$. Do this by computing U at $t = 1$ using $20, 40, 80, 160, 320$, and 640 steps. Use the same number of steps in both time and space. Reproduce the loglog plot shown in Figure 8.4. The slope of the line there shows the proper rate of convergence.

To measure the error, use the solution with the smallest h (largest number of intervals) as if it were the exact solution, then sample each solution only at the x-values that are represented in the solution with the largest h (smallest number of intervals). Use the ∞-norm on the arrays of values at those points to measure the error.

Notice that, since the Crank-Nicolson method is unconditionally stable, there is no CFL condition and we can use the same number of intervals in time and space.

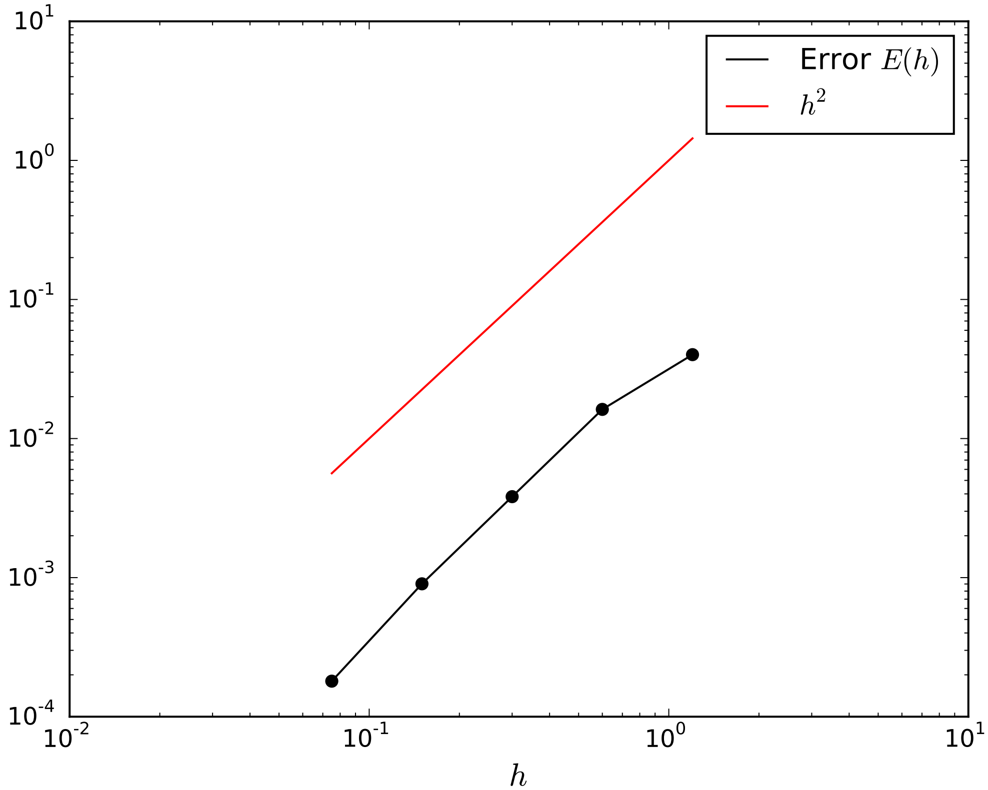


Figure 8.4: $E(h)$ represents the (approximate) maximum error in the numerical solution U to Problem 3 at time $t = 1$, using a stepsize of h.

9 Wave Phenomena

Advection Equation

The advection equation (or transport equation) is given by $u_t + su_x = 0$, where s is a nonzero constant. Consider the Cauchy problem

$$\begin{aligned} u_t + su_x &= 0, \quad -\infty < x < \infty, \\ u(x, 0) &= f(x). \end{aligned}$$

The function $f(x)$ may be thought of as an initial wave or signal. The general solution of this initial boundary value problem is $u(x, t) = f(x - st)$ (check this!). The solution $u(x, t)$ is a travelling wave that takes the signal $f(x)$ and moves it along at a constant speed s - to the right if $s > 0$, and to the left if $s < 0$.

Wave Equation

Many different wave phenomena can be described using a hyperbolic PDE called the wave equation. These wave phenomena occur in fields such as electromagnetics, fluid dynamics, and acoustics. This equation is given by

$$u_{tt} = s^2 \triangle u. \tag{9.1}$$

The 1D equation can be derived in the context of many physical models; a common derivation describes the motion of a string vibrating in a plane. Another nice derivation uses Hooke's law from the theory of elasticity.

After making the change of variables $(\xi, \eta) = (x - st, x + st)$ and using the chain rule, we find that the 1D wave equation $u_{tt} = s^2 u_{xx}$ is equivalent to $u_{\xi\eta} = 0$. The general solution of this last equation is

$$u(\xi, \eta) = F(\xi) + G(\eta)$$

for some scalar functions F and G. In (x, t) coordinates the solution is

$$u(x, t) = F(x - st) + G(x + st)$$

Thus the general solution of the wave equation is the sum of two parts: one is a signal travelling to the right with constant speed $|s|$, and the other is a signal travelling to the left with speed $|s|$.

The wave equation is usually seen in the context of an initial boundary value problem. This takes the form

$$
\begin{aligned}
u_{tt} &= s^2 u_{xx}, \quad 0 < x < l, \quad t > 0,\\
u(0,t) &= u(l,t) = 0,\\
u(x,0) &= f(x),\\
u_t(x,0) &= g(x).
\end{aligned}
$$

Numerical solution of the wave equation

We look to approximate $u(x,t)$ on a grid of points $(x_j, t_m)_{j=0,m=0}^{J,M}$. Denote the approximation to $u(x_j, t_m)$ by U_j^m. Recall that the centered approximations in space and time are

$$
\begin{aligned}
D_{tt}U_j^m &= \frac{U_j^{m+1} - 2U_j^m + U_j^{m-1}}{(\triangle t)^2},\\
D_{xx}U_j^m &= \frac{U_{j+1}^m - 2U_j^m + U_{j-1}^m}{(\triangle x)^2}.
\end{aligned}
$$

The resulting method is given by

$$
\begin{aligned}
\frac{U_j^{m+1} - 2U_j^m + U_j^{m-1}}{(\triangle t)^2} &= s^2 \frac{U_{j+1}^m - 2U_j^m + U_{j-1}^m}{(\triangle x)^2},\\
U_j^{m+1} &= -U_j^{m-1} + 2(1-\lambda^2)U_j^m + \lambda^2(U_{j+1}^m + U_{j-1}^m),
\end{aligned}
$$

where $\lambda = s(\triangle t)/(\triangle x)$. This method may be written in matrix form as

$$
U^{m+1} = AU^m - U^{m-1}
$$

where

$$
A = \begin{bmatrix}
2(1-\lambda^2) & \lambda^2 & & & \\
\lambda^2 & 2(1-\lambda^2) & \lambda^2 & & \\
\ddots & \ddots & \ddots & & \\
 & \lambda^2 & 2(1-\lambda^2) & \lambda^2 \\
 & & \lambda^2 & 2(1-\lambda^2)
\end{bmatrix}
$$

and

$$
U^m = \begin{bmatrix} U_1^m \\ U_2^m \\ \vdots \\ U_{J-1}^m \end{bmatrix}
$$

In the matrix equation above, we have already used the boundary conditions to determine that $U_0^m = U_J^m = 0$ at each time t_m. Note that, to obtain the approximation U_j^{m+1} of $u(x_j, t_{m+1})$, the method uses the value of the approximation at *the previous two time steps.* We can find the solution for the first two time steps by using the initial conditions. Using the initial conditions directly gives an approximation at $t = t_0 = 0$:

$$
U_j^0 = f(x_j), \quad 1 \le j \le J-1
$$

To obtain an approximation at the second time step, we consider the Taylor expansion

$$u(x_j, t_1) = u(x_j, 0) + u_t(x_j, 0)\triangle t + u_{tt}(x_j, 0)\frac{\triangle t^2}{2} + u_{ttt}(x_j, t_1^*)\frac{\triangle t^3}{6}.$$

Recalling that the solution $u(x,t)$ satisfies the wave equation, we substitute in expressions from our initial conditions:

$$u(x_j, t_1) = u(x_j, 0) + g(x_j)\triangle t + s^2 f''(x_j)\frac{\triangle t^2}{2} + u_{ttt}(x_j, t_1^*)\frac{\triangle t^3}{6}.$$

Ignoring the third order term, we obtain a second order approximation for the second time step:

$$U_j^1 = U_j^0 + g(x_j)\triangle t + s^2 f''(x_j)\frac{\triangle t^2}{2}, \quad 1 \leq j \leq J-1$$

or if f is not readily differentiable,

$$U_j^1 = U_j^0 + g(x_j)\triangle t + \frac{\lambda^2}{2}(U_{j-1}^0 - 2U_j^0 + U_{j+1}^0)$$

This method is conditionally stable; the CFL condition is that $\lambda \leq 1$.

Problem 1. Consider the initial boundary value problem

$$\begin{aligned} u_{tt} &= u_{xx}, \\ u(0,t) &= u(1,t) = 0, \\ u(x,0) &= \sin(2\pi x), \\ u_t(x,0) &= 0. \end{aligned}$$

Numerically approximate the solution $u(x,t)$ for $t \in [0, .5]$. Use $J = 50$ subintervals in the x dimension and $M = 50$ subintervals in the t dimension. Animate the results. Compare your results with the analytic solution $u(x,t) = \sin(2\pi x)\cos(2\pi t)$. This function is known as a standing wave. See Figure 9.1.

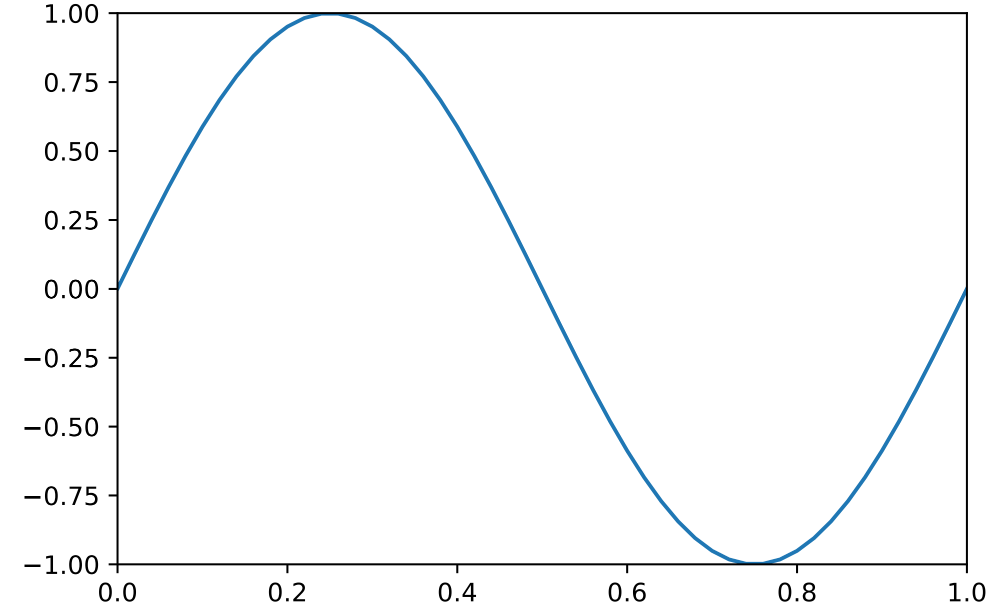


Figure 9.1: $u(x, t = 0)$.

Problem 2. Consider the initial boundary value problem

$$\begin{aligned} u_{tt} &= u_{xx}, \\ u(0,t) &= u(1,t) = 0, \\ u(x,0) &= .2e^{-m^2(x-1/2)^2} \\ u_t(x,0) &= .4m^2(x-1/2)e^{-m^2(x-1/2)^2}. \end{aligned}$$

The solution of this problem is a Gaussian pulse. It travels to the right at a constant speed. This solution models, for example, a wave pulse in a stretched string. Note that the fixed boundary conditions reflect the pulse back when it meets the boundary.

Numerically approximate the solution $u(x,t)$ for $t \in [0,1]$. Set $m = 20$. Use 200 subintervals in space and 220 in time, and animate your results. Then use 200 subintervals in space and 180 in time, and animate your results. Note that the stability condition is not satisfied for the second mesh. See 13.2.

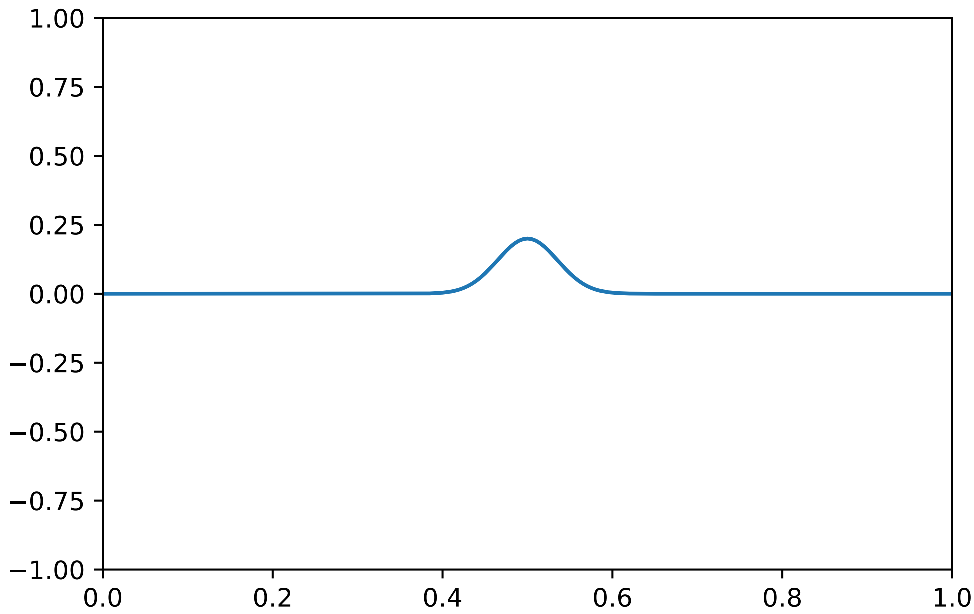


Figure 9.2: $u(x, t = 0)$.

Problem 3. Consider the initial boundary value problem

$$u_{tt} = u_{xx},$$
$$u(0,t) = u(1,t) = 0,$$
$$u(x,0) = .2e^{-m^2(x-1/2)^2}$$
$$u_t(x,0) = 0.$$

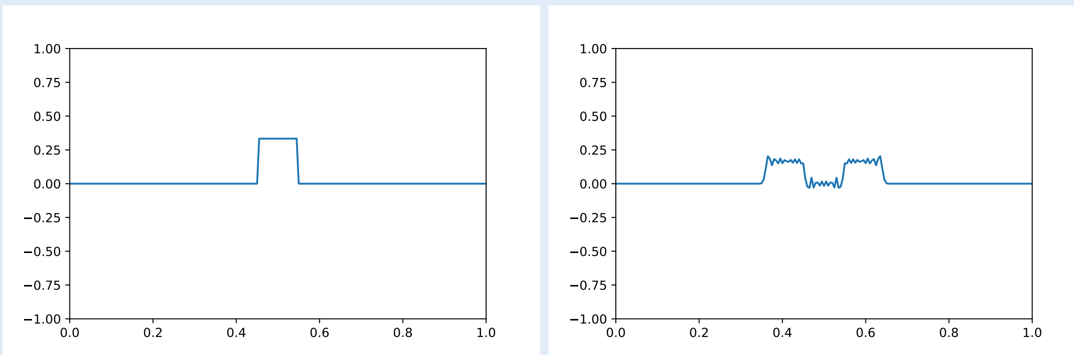
The initial condition separates into two smaller, slower-moving pulses, one travelling to the right and the other to the left. This solution models, for example, a plucked guitar string

Numerically approximate the solution $u(x,t)$ for $t \in [0,2]$. Set $m = 20$. Use 200 subintervals in space and 440 in time, and animate your results. It is rather easy to see that the solution to this problem is the sum of two travelling waves, one travelling to the left and the other to the right, as described earlier.

Problem 4. Consider the initial boundary value problem

$$
\begin{aligned}
u_{tt} &= u_{xx}, \\
u(0,t) &= u(1,t) = 0, \\
u(x,0) &= \begin{cases} 1/3 & \text{if } 5/11 < x < 6/11, \\ 0 & \text{otherwise} \end{cases} \\
u_t(x,0) &= 0.
\end{aligned}
$$

Numerically approximate the solution $u(x,t)$ for $t \in [0,2]$. Use 200 subintervals in space and 440 in time, and animate your results. Even though the method is second order and stable for this discretization, since the initial condition is discontinuous there are large dispersive errors. See Figure 9.3.



(a) $u(x,t=0)$.

(b) $u(x,t=.1)$.

Figure 9.3: The graphs for Problem 4 at various times t.

Travelling Wave Solutions of an Evolution Equation

Recall that the advection (transport) equation with initial conditions, given by

$$
\begin{aligned}
u_t + s u_x &= 0, \quad -\infty < x < \infty, \\
u(x,0) &= f(x),
\end{aligned}
$$

has as its general solution $u(x,t) = f(x - st)$. Consider a general evolutionary PDE of the form

$$u_t = G(u, u_x, u_{xx}, \ldots) \tag{9.2}$$

An interesting question to ask is whether (9.2) has travelling wave solutions: is there a signal or wave profile $f(x)$, so that $u(x,t) = f(x - st)$ is a solution of (9.2) that carries the signal at a constant speed s? These travelling waves are often significant physically. For example, in a PDE modeling insect population dynamics a travelling wave could represent a swarm of locusts; in a PDE describing a combustion process a travelling wave could represent an explosion or detonation.

Burgers' equation

We will examine the process of studying travelling wave solutions using Burgers' equation, a nonlinear PDE from gas dynamics. It is given by

$$u_t + \left(\frac{u^2}{2}\right)_x = \nu u_{xx}, \tag{9.3}$$

where u and ν represent the velocity and viscosity of the gas, respectively. It models both the process of transport with the nonlinear advection term $(u^2/2)_x = uu_x$, as well as diffusion due to the viscosity of the gas (νu_{xx}).

Let us look for a travelling wave solution $u(x,t) = \hat{u}(x-st)$ for Burgers equation. We transform (9.3) into the moving frame $(x,t) \to (\bar{x},\bar{t}) = (x-st,t)$. In this frame (9.3) becomes

$$u_{\bar{t}} - su_{\bar{x}} + \left(\frac{u^2}{2}\right)_{\bar{x}} = \nu u_{\bar{x}\bar{x}} \tag{9.4}$$

This new frame of reference corresponds to an observer moving along with the wave, so that the wave appears stationary as the observer studies it. Thus, $\hat{u}_{\bar{t}} = 0$, so that the wave profile $\hat{u}$ satisfies the ordinary differential equation

$$-su_{\bar{x}} + \left(\frac{u^2}{2}\right)_{\bar{x}} = \nu u_{\bar{x}\bar{x}}. \tag{9.5}$$

From here on we will drop the bar notation for simplicity. We seek a travelling wave solution with asymptotically constant boundary conditions; that is, $\lim_{x\to\pm\infty} \hat{u}(x) = u_\pm$

both exist, and $\lim_{x\to\pm\infty} \hat{u}'(x) = 0$. We will suppose that $u_- > u_+ > 0$.

Note that to this point we still don't know the speed of the travelling wave. Integrating both sides of this differential equation, and then taking the limit as $x \to +\infty$, we obtain

$$\begin{aligned}
-s\int_{-\infty}^{x} u' + \int_{-\infty}^{x}\left(\frac{u^2}{2}\right)' &= \nu\int_{-\infty}^{x} u'', \\
-s(u(x)-u_-) + \frac{u^2(x)}{2} - \frac{u_-^2}{2} &= \nu(u'(x) - u'(-\infty)), \\
-s(u_+ - u_-) + \frac{u_+^2}{2} - \frac{u_-^2}{2} &= 0.
\end{aligned}$$

Thus given boundary conditions $u_\pm$ at $\pm\infty$, the speed of the travelling wave must be $s = \frac{u_-+u_+}{2}$.

Usually at this point, the travelling wave must be numerically solved using the profile ODE ((9.5) for Burgers equation). However, the profile ODE for Burgers is simple enough that it is possible to obtain an analytic solution. The travelling wave is given by

$$\hat{u}(x) = s - a\tanh\left(\frac{ax}{2\nu} + \delta\right)$$

where $a = (u_- - u_+)/2$ and δ is fixed real number. We get a family of solutions because any translation of a travelling wave solution is also a travelling wave solution.

Stability of travelling waves

Suppose that an evolutionary PDE

$$u_t = G(u, u_x, u_{xx}, \ldots). \tag{9.6}$$

has a travelling wave solution $u(x,t) = \hat{u}(x - st)$. An interesting question to consider is whether the mathematical solution, $\hat{u}$, has a physical analogue. In other words, does the travelling wave show up in real life? This question is the start of the mathematical study of stability of travelling waves.

We begin by translating (9.6) into the moving frame $(x,t) \to (\bar{x}, \bar{t}) = (x - st, t)$. In this frame the PDE becomes

$$u_t - su_x = G(u, u_x, u_{xx}, \ldots).$$

In these coordinates the travelling wave is stationary. Thus, the solution of

$$\begin{aligned} u_t - su_x &= G(u, u_x, u_{xx}, \ldots), \\ u(x, t = 0) &= \hat{u}(x), \end{aligned}$$

is given by $u(x,t) = \hat{u}(x)$. We say that the travelling wave $\hat{u}$ is asymptotically orbitally stable if whenever $v(x)$ is a small perturbation of $\hat{u}(x)$, the general solution of

$$\begin{aligned} u_t - su_x &= G(u, u_x, u_{xx}, \ldots), \\ u(x, t = 0) &= v(x), \end{aligned}$$

converges to some translation of $\hat{u}$ as $t \to \infty$. Using this definition to prove stability of a travelling wave is a nontrivial task.

Visualizing stability of the travelling wave solution of Burgers' equation

The travelling wave solution of Burgers' equation is a stable wave. To view this numerically, we discretize the PDE

$$u_t - su_x + uu_x = u_{xx}$$

using the second order centered approximations

$$D_t U_j^{n+1/2} = \frac{U_j^{n+1} - U_j^n}{\triangle t}, \quad D_{xx} U_j^{n+1/2} = \frac{1}{2}\left(\frac{U_{j+1}^{n+1} - U_{j-1}^{n+1}}{2\triangle x} + \frac{U_{j+1}^{n} - U_{j-1}^{n}}{2\triangle x}\right),$$

$$D_{xx} U_j^{n+1/2} = \frac{1}{2}\left(\frac{U_{j+1}^{n+1} - U_j^{n+1} + U_{j-1}^{n+1}}{(\triangle x)^2} + \frac{U_{j+1}^{n} - U_j^{n} + U_{j-1}^{n}}{(\triangle x)^2}\right)$$

Substituting these expressions into the PDE we obtain a second-order, implicit Crank-Nicolson method

$$\begin{aligned} U_j^{n+1} - U_j^n = K_1 &\big[(s - U_j^{n+1})(U_{j+1}^{n+1} - U_{j-1}^{n+1}) + (s - U_j^n)(U_{j+1}^n - U_{j-1}^n)\big] \\ &+ K_2\big[(U_{j+1}^{n+1} - 2U_j^{n+1} + U_{j-1}^{n+1}) + (U_{j+1}^n - 2U_j^n + U_{j-1}^n)\big], \end{aligned}$$

where $K_1 = \frac{\triangle t}{4\triangle x}$ and $K_2 = \frac{\triangle t}{2(\triangle x)^2}$.

Problem 5. Numerically solve the initial value problem

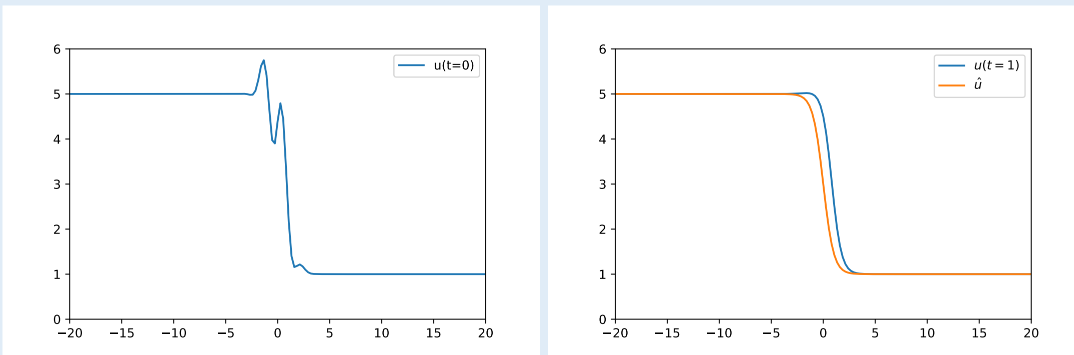
$$\begin{aligned} &u_t - su_x + uu_x = u_{xx}, \quad x \in (-\infty, \infty), \\ &u(x, 0) = v(x), \end{aligned}$$

for $t \in [0, 1]$. Let the perturbation $v(x)$ be given by

$$v(x) = 3.5(\sin(3x) + 1)\frac{1}{\sqrt{2\pi}}\exp(-x^2/2)$$

And let the initial condition be $u(x, 0) = \hat{u}(x) + v(x)$ Approximate the x domain,$(-\infty, \infty)$, numerically by the finite interval $[-20, 20]$, and fix $u(-20) = u_-$, $u(20) = u_+$. Let $u_- = 5$, $u_+ = 1$. Use 150 intervals in space and 350 steps in time. Animate your results. You should see the solution converge to a translate of the travelling wave $\hat{u}$. See Figure 9.4.

Hint: This difference scheme is no longer a linear equation. We have a nonlinear equation in U^{n+1}. We can still solve this function using Newton's method or some other similar solver. In this case, use `scipy.optimize.fsolve`.



(a) $u(x, t = 0)$.

(b) $u(x, t = 1)$ vs $\hat{u}$.

Figure 9.4: The graphs for Problem 5

10 Anisotropic Diffusion

Lab Objective: *Demonstrate the use of finite difference schemes in image analysis.*

A common task in image processing is to remove extra static from an image. This is most easily done by simply blurring the image, which can be accomplished by treating the image as a rectangular domain and applying the diffusion (heat) equation:

$$u_t = c\Delta u$$

where c is some diffusion constant and Δ is the Laplace operator. Unfortunately, this also blurs the boundary lines between distinct elements of the image.

A more general form of the diffusion equation in two dimensions is:

$$u_t = \nabla \cdot (c(x, y, t)\nabla u)$$

where c is a function representing the diffusion coefficient at each given point and time. In this case, $\nabla\cdot$ is the divergence operator and ∇ is the gradient.

To blur a picture uniformly, choose c to be a constant function. Since c controls how much diffusion is allowed at each point, it can be modified so that diffusion is minimized across edges in the image. In this way we attempt to limit diffusion near the boundaries between different features of the image, and allow smaller details of the image (such as static) to blur away. This method for image denoising is especially useful for denoising low quality images, and was first introduced by Pietro Perona and Jitendra Malik in 1987. It is known as Anisotropic Diffusion or Perona-Malik Diffusion.

A Finite Difference Scheme

Suppose we have some estimate E of the rate of change at a given point in an image. E will be largest at the boundaries in the image. We will then let $c(x, y, t) = g(E(x, y, t))$ where g is some function such that $g(0) = 1$ and $\lim_{x\to\infty} g(x) = 0$. Thus c will be small where E is large, so that little diffusion occurs near the boundaries of different portions of the image.

We will model this system using a finite differencing scheme with an array of values at a 2D grid of points, and iterate through time. Let $U^n_{l,m}$ be the discretized approximation of the function u, n be the index in time, l be the index along the x-axis, and m be the index along the y-axis.

The Laplace operator can be approximated with the finite difference scheme

$$\Delta u = u_{xx} + u_{yy} \approx \frac{U^n_{l-1,m} - 2U^n_{l,m} + U^n_{l+1,m}}{(\Delta x)^2} + \frac{U^n_{l,m-1} - 2U^n_{l,m} + U^n_{l,m+1}}{(\Delta y)^2}.$$

A good metric to use with images is to let the distance between each pixel be equal to one, so $\Delta x = \Delta y = 1$. Rearranging terms, we obtain

$$\Delta u \approx (U^n_{l-1,m} - U^n_{l,m}) + (U^n_{l+1,m} - U^n_{l,m}) + (U^n_{l,m-1} - U^n_{l,m}) + (U^n_{l,m+1} - U^n_{l,m}).$$

Again, since we are working with images and not some time based problem, we can without loss of generality let $\Delta t = 1$, so we obtain the finite difference scheme

$$U^{n+1}_{l,m} = U^n_{l,m} + (U^n_{l-1,m} - U^n_{l,m}) + (U^n_{l+1,m} - U^n_{l,m}) + (U^n_{l,m-1} - U^n_{l,m}) + (U^n_{l,m+1} - U^n_{l,m}).$$

We will now limit the diffusion near the edges of objects by making the modification

$$\begin{aligned} U^{n+1}_{l,m} = U^n_{l,m} + \lambda \Big(& g(|U^n_{l-1,m} - U^n_{l,m}|)(U^n_{l-1,m} - U^n_{l,m}) \\ & + g(|U^n_{l+1,m} - U^n_{l,m}|)(U^n_{l+1,m} - U^n_{l,m}) \\ & + g(|U^n_{l,m-1} - U^n_{l,m}|)(U^n_{l,m-1} - U^n_{l,m}) \\ & + g(|U^n_{l,m+1} - U^n_{l,m}|)(U^n_{l,m+1} - U^n_{l,m}) \Big), \end{aligned} \tag{10.1}$$

where $\lambda \leq \frac{1}{4}$ is the stability condition.

In this difference scheme, each term is affected most by nearby terms that are most similar to it, so less diffusion will happen anywhere there is a sharp difference between pixels. This scheme also has the useful property that it does not increase or decrease the total brightness of the image. Intuitively, this is because the effect of each point on its neighbors is exactly the opposite effect its neighbors have on it.

Two commonly used functions for g are $g(x) = e^{-\left(\frac{x}{\sigma}\right)^2}$ and $g(x) = \frac{1}{1+\left(\frac{x}{\sigma}\right)^2}$. The parameter σ allows us to control how much diffusion decreases across boundaries, with larger σ values allowing more diffusion. Note that $g(0) = 1$ and $\lim_{x\to\infty} g(x) = 0$ for both functions. In this lab we use $g(x) = e^{-\left(\frac{x}{\sigma}\right)^2}$.

It is worth noting that this particular difference scheme is *not* an accurate finite difference scheme for the version of the diffusion equation we discussed before, but it *does* accomplish the same thing in the same way. As it turns out, this particular scheme is the solution to a slightly different diffusion PDE, but can still be used the same way.

For this lab's examples we read in the image using the `imageio.imread` function, and normalized it so that the colors are represented as floating point values between 0 and 1. An image can converted to black and white when it is read by including the argument `as_gray=True`.

```python
from matplotlib import cm, pyplot as plt
from imageio import imread

# To read in an image, convert it to grayscale, and rescale it.
picture = imread('balloon.png', as_gray=True) * 1./255

# To display the picture as grayscale
plt.imshow(picture, cmap=cm.gray)
plt.show()
```

Simplifying Calculations

You will notice that the algorithm given in 10.1 does not describe what to do for the edges and corners of U^{n+1}. In these cases we will simply eliminate the undefined terms in the algorithm. For example, the top edge equation becomes

$$\begin{aligned}U^{n+1}_{l,m} = U^n_{l,m} + &\lambda(g(|U^n_{l+1,m} - U^n_{l,m}|)(U^n_{l+1,m} - U^n_{l,m})\\ &+ g(|U^n_{l,m+1} - U^n_{l,m}|)(U^n_{l,m+1} - U^n_{l,m}))\\ &+ g(|U^n_{l,m-1} - U^n_{l,m}|)(U^n_{l,m-1} - U^n_{l,m})),\end{aligned}$$

and top left corner equation becomes

$$\begin{aligned}U^{n+1}_{l,m} = U^n_{l,m} + &\lambda(g(|U^n_{l+1,m} - U^n_{l,m}|)(U^n_{l+1,m} - U^n_{l,m})\\ &+ g(|U^n_{l,m+1} - U^n_{l,m}|)(U^n_{l,m+1} - U^n_{l,m})).\end{aligned}$$

Essentially we are only using the terms of the difference scheme that are actually defined.

To help facilitate this we can create a larger "padded" matrix that will make these calculations easy to do. This padded matrix will have an extra row on the top and bottom, and an extra column on either side of the original matrix. These extra rows and columns will duplicate the outer edge of the original matrix.

So if our original array `X` has shape `m,n`, then our padded array `Y` has shape `m+2,n+2`. The top edge of `Y` will be defined so that `Y[0,1:-1] == X[0,:]` is true, and the rest of the edges of `Y` follow the same pattern.

Notice that this allows us to simply implement the algorithm found in 10.1 without having to make special cases for the edges and corners, since those previously undefined terms become zero when using the padded matrix.

Problem 1. Complete the following function, by implementing the anisotropic diffusion algorithm found in 10.1 for black and white images. Use the padded array technique found in the Simplifying Calculations section.

In your function, use

$$g(x) = e^{-\left(\frac{x}{\sigma}\right)^2}$$

```python
def anisdiff_bw(U, N, lambda_, g):
    """ Run the Anisotropic Diffusion differencing scheme
    on the array U of grayscale values for an image.
    Perform N iterations, use the function g
    to limit diffusion across boundaries in the image.
    Operate on U inplace to optimize performance. """
    pass
```

Run the function on `balloon.jpg`. Show the original image and the diffused image for $\sigma = .1$, $\lambda = .25$, $N = 5, 20, 100$.

original image

5 iterations with $\sigma = .1$ and $\lambda = .25$

20 iterations

100 iterations

Color Schemes

Colored images can be processed in a similar manner. Instead of being represented as a two-dimensional array, colored images are represented as three dimensional arrays. The third dimension is used to store the intensities of each of the standard 3 colors. This diffusion process can be carried out in the exact same way, on each of the arrays of intensities for each color, but instead of detecting edges just in one color, we need to detect edges in any color, so instead of using something of the form $g(|U^n_{l+1,m} - U^n_{l,m}|)$ as before, we will now use something of the form $g(||U^n_{l+1,m} - U^n_{l,m}||)$, where $U^n_{l+1,m}$ and $U^n_{l,m}$ are vectors now instead of scalars. The difference scheme can be treated as an equation on vectors in 3-space and now reads:

$$\begin{aligned}U^{n+1}_{l,m} = U^n_{l,m} + \lambda(&g(||U^n_{l-1,m} - U^n_{l,m}||)(U^n_{l-1,m} - U^n_{l,m})\\ &+ g(||U^n_{l+1,m} - U^n_{l,m}||)(U^n_{l+1,m} - U^n_{l,m})\\ &+ g(||U^n_{l,m-1} - U^n_{l,m}||)(U^n_{l,m-1} - U^n_{l,m})\\ &+ g(||U^n_{l,m+1} - U^n_{l,m}||)(U^n_{l,m+1} - U^n_{l,m}))\end{aligned}$$

When implementing this scheme for colored images, use the 2-norm on 3-space, i.e $||x|| = \sqrt{x_1^2 + x_2^2 + x_3^2}$ where x_1, x_2, and x_3 are the different coordinates of x.

Problem 2. Complete the following function to process a colored image. You may modify your code from the previous problem. Measure the difference between pixels using the 2-norm. Use the corresponding vector versions of the boundary conditions given in Problem 1.

```
def anisdiff_color(U, N, lambda_, sigma):
    """ Run the Anisotropic Diffusion differencing scheme
    on the array U of grayscale values for an image.
    Perform N iterations, use the function g = e^{-x^2/sigma^2}
    to limit diffusion across boundaries in the image.
    Operate on U inplace to optimize performance. """
    pass
```

Run the function on `balloons_color.jpg`. Show the original image and the diffused image for $\sigma = .1$, $\lambda = .25$, $N = 5, 20, 100$.

Hint: If you have an $m \times n \times 3$ matrix representing the RGB differences of each pixel, then to find a matrix representing the norm of the differences, you can use the following code. This code squares each value and sums along the last axis, and takes the square root. In order to keep the dimension size of the matrix and aid in broadcasting, you must use `keepdims=True`.

```
# x is mxnx3 matrix of pixel color values
norm = np.sqrt(np.sum(x**2, axis=2, keepdims=True))
```

original image after 50 iterations

Figure 10.1: Smearing of similar colors when using an anisotropic diffusion filter.

Noisy Images

Problem 3. Use the following code to add noise to your grayscale image.

```
from numpy.random import randint

image = imread('balloon.jpg', as_gray=True)
x, y = image.shape
for i in xrange(x*y//100):
    image[randint(x),randint(y)] = 127 + randint(127)
```

Run `anisdiff_bw()` on the noisy image with $\sigma = .1$, $\lambda = .25$, $N = 20$. Display the original image and the noisy image. Explain why anisotropic diffusion does not smooth out the noise.

Hint: Don't forget to rescale.

Minimum Bias (Optional)

This sort of anisotropic diffusion can be very effective, but, depending on the image, it may also smear out edges that do not have large differences between them. An example of this limitation can be seen in Figure 10.1

As we can see, after 100 iterations, some of the boundaries between similar shades of grey have smeared unevenly. You may still have to look closely to see it. This can be counteracted somewhat by further decreasing the σ value, but if we have random noise throughout the image, this will not remove it. If we have random static in the image, we can remove this using a modified version of the filter. Instead of measuring the rate of change in the picture in each direction, we change each point according to whether or not any of its adjacent points have roughly the same value it has. This is called a minimum-biased filter. This sort of trick is especially good for removing isolated pixels that are different from those around them. A very simple way to do this is by taking the average of the two smallest differences between each pixel and its eight neighbors and using that in place of g in the difference scheme above. Along the boundaries, we do not have 8 neighbors for each pixel, but we can get by by just using the pixels we have and eliminating the other terms in the difference scheme, just as we did before. This will make it so that points that neighbor points of similar value will not be changed, while points that do not match their surroundings will be faded to become more like the points surrounding them. This does not have the same symmetrical diffusion as the other scheme, i.e. if one pixel changes, it does not necessarily change its neighboring pixels by the same amount. As long as you leave $\lambda \leq \frac{1}{4}$ and you have scaled the pixels to have floating point values between 0 and 1, the scheme will still remain within its minimum and maximum bounds, since the tendency is always to move points closer to the values of their neighbors. To demonstrate the action of such a filter, we make changes to random pixels in the color version of the same photo and use both filters to remove the noise we have added. Below, we include an example where we have added noise to the color version of that same picture, then used a minimum-biased filter to diminish the noise and the original filter to smooth what remains.

***Problem 4.** (Optional)

Implement the minimum-biased finite difference scheme described above. Add noise to `balloons_color.jpg` using the provided code below, and clean it using your implementation. Show the original image, the noised image, and the cleaned image.

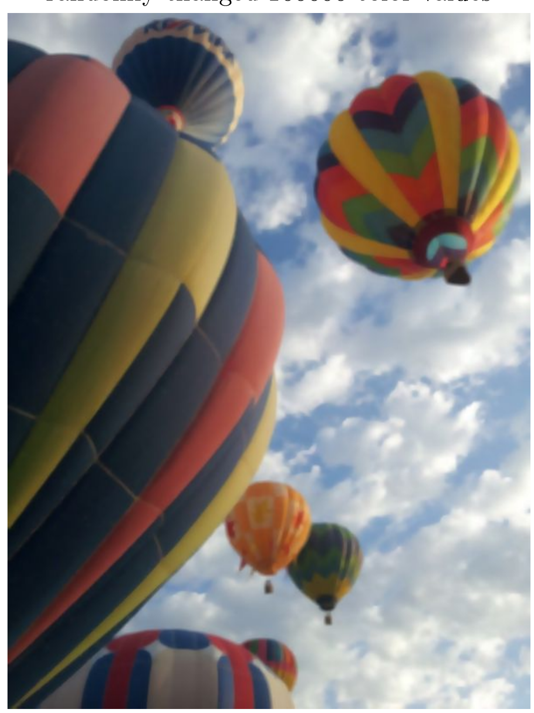
```
image = imread('balloons_color.jpg')
x,y,z = image.shape
for dim in xrange(z):
    for i in xrange(x*y//100):
        # Assign a random value to a random place
        image[randint(x),randint(y),dim] = 127 + randint(127)
```

Hint: Don't forget to rescale.

original image

randomly changed 100000 color values

300 iterations of a min-biased scheme



after 8 additional iterations of the first filter with $\lambda = .25$ and $\sigma = .04$.

11 Finite Volume Methods

When solving a PDE numerically, how do we deal with discontinuous initial data? The Finite Volume method has particular strength in this area. It is commonly used for hyperbolic PDEs whose solutions can spontaneously develop discontinuities as they evolve in time. These solutions are often called shock waves.

Conservation Laws

Consider the conservation law

$$u_t + f(u)_x = 0, \tag{11.1}$$

where u is a (spatially) one-dimensional conserved quantity, and $f(u)$ is the flux of u. The continuous integral formulation of (11.1) states that

$$\frac{d}{dt}\int_a^b u(x,t)dx + \int_a^b f(u)_x\, dx = 0.$$

$\frac{d}{dt}\int_a^b u(x,t)dx$ may be thought of as the time evolution of the total 'mass' of u across the domain $[a,b]$, and is dependent only on the flux through the boundaries, since

$$\frac{d}{dt}\int_a^b u(x,t)dx = f(u(a)) - f(u(b)).$$

This fact is an important idea utilized by finite volume methods, which generally consider the evolution of u not at a given point, but instead in volume-averaged regions. For example, let $\{x_i\}$ be a grid of equally spaced points with spacing Δx, and let C_i be the i-th 'volume' (subinterval) defined by $(x_{i-1/2}, x_{i+1/2})$. We are interested in the evolution of the volume average of u over this interval,

$$U_i^n = \frac{1}{\Delta x}\int_{C_i} u(x,t^n)dx,$$

where $\{t^n\}$ is the time discretization.

The evolution of these volume-averaged quantities will depend only on the flux through the cell edges, so that

$$\frac{d}{dt}\int_{C_i} u(x,t)dx = f(u(x_{i-1/2},t)) - f(u(x_{i+1/2},t)). \tag{11.2}$$

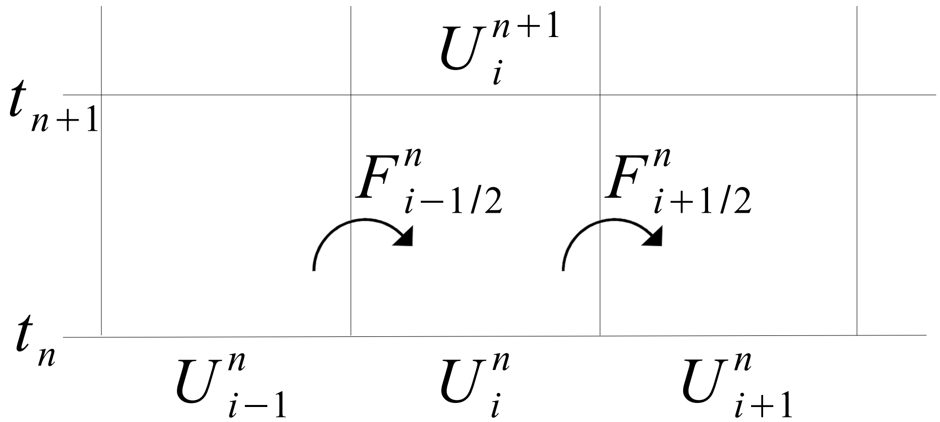


Figure 11.1: A schematic of the fluxes for the finite volume method as indicated by (11.3).

We can then construct a time-stepping method where $\sum_i U_i^n \Delta x$ (the total 'mass' of the system) is conserved from one time step n to the next.

Let $F_{i-1/2}^n = \frac{1}{\triangle t} \int_{t^n}^{t^{n+1}} f(u(x_{i-1/2}, t))\, dt$. Then

$$\begin{aligned} \int_{t^n}^{t^{n+1}} \left[\frac{d}{dt} \int_{C_i} u(x,t)\, dx \right] &= \int_{C_i} u(x, t^{n+1}) - u(x, t^n)\, dx, \\ &= \triangle t \left(F_{i-1/2}^n - F_{i+1/2}^n \right). \end{aligned}$$

Thus, by integrating (11.2) in time, we may approximate the evolution of the cell ('volume') averages with the method

$$U_i^{n+1} = U_i^n - \frac{\Delta t}{\Delta x} \left(F_{i+1/2}^n - F_{i-1/2}^n \right). \tag{11.3}$$

where $U_i^n = \frac{1}{\triangle x} \int_{C_i} u(x, t^n)\, dt$. This formulation guarantees the conservation properties that are so desirable for conservation laws, if the time-averaged fluxes $F_{i-1/2}^n$ can be discretized in a natural way.

The key contribution of finite volume methods is the computation of $F_{i-1/2}^n$. For a truly nonlinear $f(u)$ this can be rather complicated and messy, and typically will involve solving what is usually referred to as the Riemann problem for the conservation law. The interested student can look at [LeV02] for a very thorough introduction and discussion on the subject. We will consider the linear problem in one dimension. The analog to higher dimensions is obtained by considering the eigenvector decomposition of any linear system. Nonlinear equations complicate things further.

The linear advection equation and upwinding

The simplest conservation law describes the advection or transport of a quantity. The PDE is given by

$$u_t + a u_x = 0, \tag{11.4}$$

and describes the motion of a concentration of some constituent u by a constant velocity one-dimensional 'wind' $a > 0$. In higher dimensions this is an important problem in many fields, for example the transport of chemicals in the atmosphere and oceans, proper mixing of various properties in metallurgy, and the passing of information along a network.

Note that whenever $u(x,t)$ is a solution of the advection equation, then $u(x-at,t_0)$ (for any fixed t_0) is also a solution. Thus, if $u(x,0)=u_0(x)$ then the solution for all time can be represented by $u(x,t)=u_0(x-at)$. This is an important property of (11.4), and gives a new meaning to the term advection: this equation merely takes the initial conditions and passively transports them with velocity a.

For this equation the computation of the flux appears straightforward: $F^n_{i-1/2}=a\overline{U}^n_{i-1/2}$ where the $\overline{U}^n_{i-1/2}$ refers to the time average of $U_{i-1/2}$ over the interval t_n to t_{n+1}. Let us determine how to approximate this time average. Note from Figure 11.2 that when $a>0$ the flux that determines U^{n+1}_i will be dependent on the value of U^n_{i-1}. Thus, one possibility is to approximate the flux by $F^n_{i-1/2}=aU^n_{i-1}$. Using this approximation of the flux together with the flux differencing formula (11.3) yields the first order upwind method, given by

$$U^{n+1}_i = U^n_i - \frac{a\Delta t}{\Delta x}\left(U^n_i - U^n_{i-1}\right).$$

Another way to derive the upwind method is to instead suppose that what we want to do is reconstruct $u(x)$ at each time step n inside each cell $(x_{i-1/2},x_{i+1/2})$from the mean values in that cell and its surrounding neighbors. This reconstructed $\tilde{u}(x)^n$ is then defined piecewise for each cell i. The solution at the next time step can be found as $\tilde{u}^{n+1}(x)=\tilde{u}^n(x-a\triangle t)$ which allows us to determine the fluxes $F^n_{i-1/2}$ once we have settled on a method for determining $\tilde{u}^n(x)$ in each cell. The simplest approach is

$$\tilde{u}^n(x) = U^n_i \text{ for } x\in(x_{i-1/2},x_{i+1/2})$$

This leads to fluxes given by

$$\begin{aligned} F^n_{i-1/2} &= \frac{a}{\triangle t}\int_0^{t_{n+1}-t_n} \tilde{u}^n(x_{i-1/2},t)\,dt, && (11.5)\\ &= \frac{a}{\triangle t}\int_0^{\triangle t} \tilde{u}^n(x_{i-1/2}-at)\,dt, && (11.6)\\ &= aU^n_{i-1}. \end{aligned}$$

The following code solves the problem

$$\begin{aligned} u_t + au_x &= 0, \quad 0<x<1,\\ u(x,t) &= f(x), && (11.7)\\ u(0,t) &= u(1,t), \end{aligned}$$

where f represents a signal with two parts: one is smooth and the other is discontinuous. Notice that this PDE has periodic boundary conditions. Essentially we are evolving the signal around the unit circle. This allows us to evolve the signal much further to test our numerical methods, since we only have to discretize the interval $[0,1]$ instead of a much larger domain. To see how to implement the boundary conditions, consider a grid $0=x_0<x_1<\ldots<x_{N-1}<x_N=1$ of evenly spaced points. Since $u(x)$ is periodic then $u(x_N)=u(x_0)$, so it is sufficient to track $x_0,\ldots,x_{N-1}$.

```
import numpy as np
from matplotlib import pyplot as plt
from math import floor

def upwind(u0, a, xmin, xmax, t_final, nt):
    """ Solve the advection equation with periodic
    boundary conditions on the interval [xmin, xmax]
```

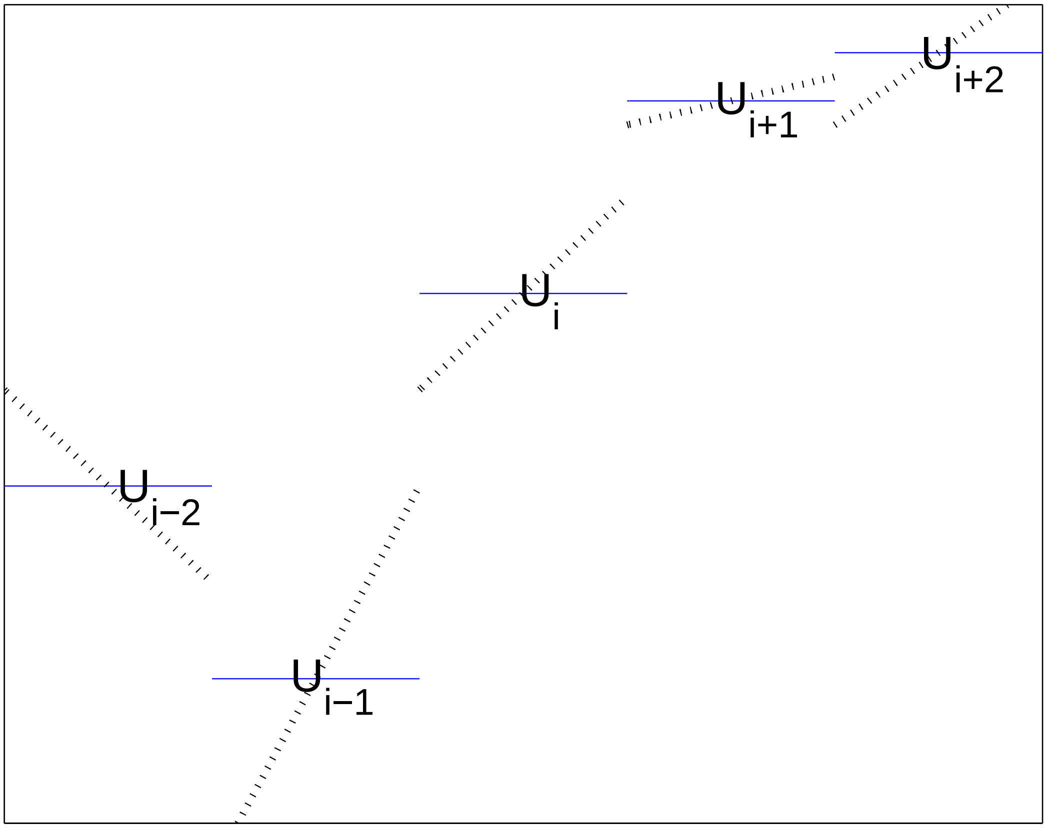


Figure 11.2: The piecewise linear reconstruction for the upwind and Lax-Wendroff methods. The solid lines represent the simplest reconstruction of the cell averages leading to the upwind method, and the dashed lines are those whose slope is obtained via the Lax-Wendroff method. Note that the LW method introduces a spurious maximum at $i + 3/2$ (the cell edge between U_{i+1} and U_{i+2}) and the minimum at $i - 3/2$ will be unphysical exaggerated. The upwind method avoids this difficulties, but clearly loses a significant amount of the available information. This provides the motivation for the slope limiters.

```
    using the upwind finite volume scheme.
    Use u0 as the initial conditions.
    a is the constant from the PDE.
    Use the size of u0 as the number of nodes in
    the spatial dimension.
    Let nt be the number of spaces in the time dimension
    (this is the same as the number of steps if you do
    not include the initial state).
    Plot and show the computed solution along
    with the exact solution. """
```

```
    dt = float(t_final) / nt
    # Since we are doing periodic boundary conditions,
    # we need to divide by u0.size instead of (u0.size - 1).
    dx = float(xmax - xmin) / u0.size
    lambda_ = a * dt / dx
    u = u0.copy()
    for j in xrange(nt):
        # The Upwind method. The np.roll function helps us
        # account for the periodic boundary conditions.
        u -= lambda_ * (u - np.roll(u, 1))
    # Get the x values for the plots.
    x = np.linspace(xmin, xmax, u0.size+1)[:-1]
    # Plot the computed solution.
    plt.plot(x, u, label='Upwind Method')
    # Find the exact solution and plot it.
    distance = a * t_final
    roll = int((distance - floor(distance)) * u0.size)
    plt.plot(x, np.roll(u0, roll), label='Exact solution')
    # Show the plot with the legend.
    plt.legend(loc='best')
    plt.show()

# Define the initial conditions.
# Leave off the last point since we're using periodic
# boundary conditions.
nx = 30
nt = nx * 3 // 2
x = np.linspace(0., 1., nx+1)[:-1]
u0 = np.exp(-(x - .3)**2 / .005)
arr = (.6 < x)  &  (x < .7 )
u0[arr] += 1.

# Run the simulation.
upwind(u0, 1.2, 0, 1, 1.2, nt)
```

Try running the previous code block with `nx` set to 30, 60, 120, and 240. You will notice that the numerical solution diffuses with time. It diffuses especially fast at the points of discontinuity.

Piecewise linear reconstruction and slope limiters

The upwind method is formally only first order, and actually does relatively poorly in terms of actually transporting the initial data with velocity a. You can notice from the example code that the upwind method has errors that are 'diffusive' meaning that the initial data is diffused as time evolves, losing the peaks and fine details. This is because the error for the upwind method is on the order of the second derivative of u which is of a diffusive nature. To get an improved method, consider a better reconstruction inside each cell, i.e.

$$\tilde{u}^n(x) = U_i^n + m_i^n(x - x_i) \text{ for } x \in (x_{i-1/2}, x_{i+1/2}) \tag{11.8}$$

where the slope of this linear reconstruction m_i^n is determined as a function of the neighboring cell averages at time n and U_i^n itself. Then the flux is given by

$$\begin{aligned} F_{i-1/2}^n &= \frac{a}{\triangle t}\int_0^{t_{n+1}-t_n} \tilde{u}^n(x_{i-1/2}-at)\,dt, \\ &= \frac{a}{\triangle t}\int_0^{\triangle t} U_{i-1}^n + m_i^n(x_{i-1/2}-at-x_i), \\ &= a\left(U_{i-1}^n + \frac{m_{i-1}^n}{2}(\triangle x - a\triangle t)\right). \end{aligned} \tag{11.9}$$

One of the most natural approaches is to just estimate the slope depending on the cell i and a neighboring cell $i+1$ or $i-1$. This leads to two popular methods, the Lax-Wendroff method and the Beam-Warming method (that really is the name). The Lax-Wendroff method has a slope chosen as

$$m_i^n = \frac{U_{i+1}^n - U_i^n}{\Delta x}. \tag{11.10}$$

which it turns out is formally second-order accurate. It turns out though that the errors for this method are dispersive, meaning that near very steep gradients, the method will generate very rapid oscillations (due to the third derivative of u not being approximated accurately). Another way to consider how these errors arise is to notice from Figure 11.2 that if the piecewise linear reconstruction is advocated by some positive wind a then there will be places where the discontinuous nature of the reconstruction will introduce spurious maxima or minima into the solution. These become the spurious waves seen in simulations using the Lax-Wendroff method.

A solution to this dilemma between balancing the diffusive and dispersive errors comes from constructing slopes m_i^n that ensure no such non-monotonic transport takes place. The basic idea is to constrain the slope so that the reconstructed piecewise linear function $\tilde{u}^n(x)$ will not generate unphysical extremal values when it is advocated by some finite wind a. The Minmod limiter chooses the slope as

$$m_i^n = minmod\left(\frac{U_i^n - U_{i-1}^n}{\Delta x}, \frac{U_{i+1}^n - U_i^n}{\Delta x}\right) \tag{11.11}$$

where

$$minmod(a,b) = \begin{cases} a \text{ if } |a| < |b| \text{ and } ab > 0 \\ b \text{ if } |b| < |a| \text{ and } ab > 0 \\ 0 \text{ if } ab < 0. \end{cases} \tag{11.12}$$

Problem 1. Implement the Lax Wendroff method and use it to solve (11.7). For $N = 30, 60, 120, 240$, plot the analytic solution, the upwind solution, and the Lax-Wendroff solution. (You should have 4 separate plots, each with 3 graphs.) You should be able to tell that the Lax Wendroff method approximates the smooth portion of the signal much better, as it does not struggle with diffusion. Unfortunately, it has some difficulty with the discontinuous portion, where unphysical oscillations are seen. Recall that we saw something similar in the waves lab when there were discontinuous initial conditions.

Hint: Use equations 11.9 and 11.3.

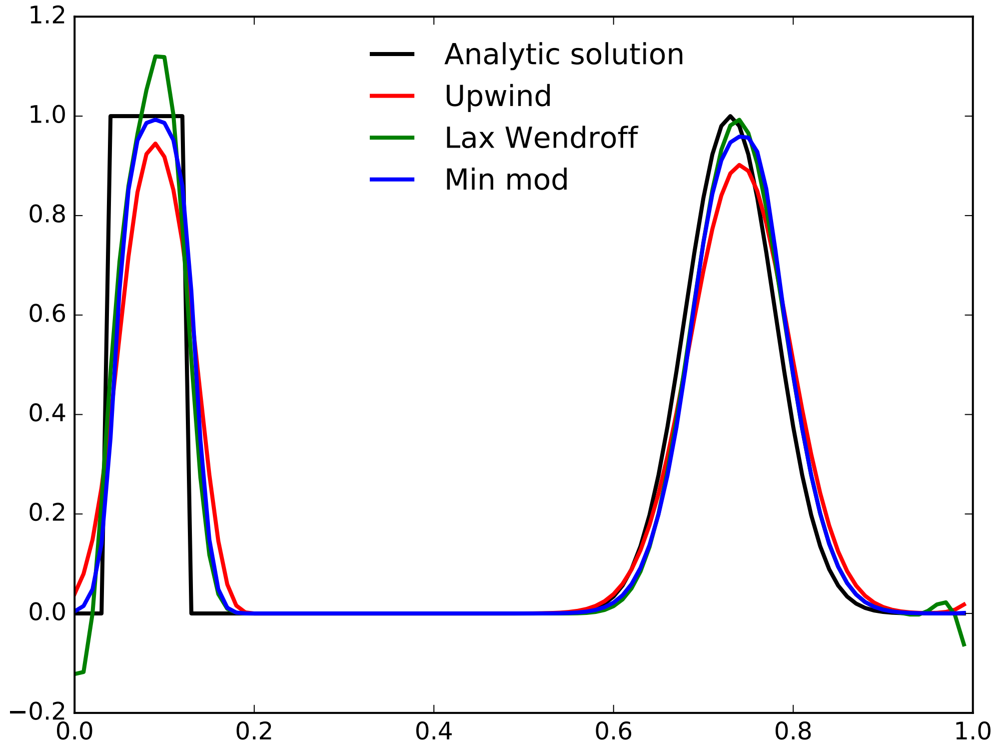


Figure 11.3: Solutions of (11.7) at time $t = 1.2$ using various methods. Here the advection coefficient is $a = 1.2$, and there are $N = 100$ subintervals in space, 150 subintervals in time.

Problem 2. Implement the Minmod method and use it to solve (11.7). For $N = 30, 60, 120, 240$, plot the anaytic solution, the upwind solution, the Lax-Wendroff solution, and the Minmod solution. (You should have 4 separate plots, each with 4 graphs.) Be sure to vectorize the minmod operation.

Hint: Use equations 11.9 and 11.3.

Beyond piecewise linear reconstructions

As you can imagine, using a linear approximation is not the only option. There are a host of high order finite volume methods that consider polynomial reconstructions of $\tilde{u}^n$ inside each cell. The key is then to use some nonlinear limiting technique that will ensure that when $\tilde{u}^n(x)$ is advocated that no new extrema are introduced. Choosing the correct limiter for the given application then becomes an art unto itself.

12 The Finite Element method

Lab Objective: *The finite element method is commonly used for numerically solving partial differential equations. We introduce the finite element method via a simple BVP describing the steady state distribution of heat in a pipe as fluid flows through.*

Advection-Diffusion of Heat in a Fluid

We begin with the heat equation

$$y_t = \varepsilon y_{xx} + f(x)$$

where $f(x)$ represents any heat sources in the system, and εy_{xx} models the diffusion of heat. We wish to study the distribution of heat in a fluid that is moving at some constant speed a. This can be modelled by adding an advection or transport term to the heat equation, giving us

$$y_t + a y_x = \varepsilon y_{xx} + f(x).$$

We consider a fluid flowing through a pipe from $x = 0$ to $x = 1$ with speed $a = 1$, and as it travels it is warmed at a constant rate $f = 1$. We will impose the condition that $y = 2$ at $x = 0$, so that the fluid is already at a constant temperature as it enters the pipe.

These conditions yield

$$\begin{aligned} &y_t + y_x = \varepsilon y_{xx} + 1, \quad 0 < x < 1, \\ &y(0) = 2 \end{aligned}$$

As time increases we expect the temperature of the fluid in the pipe to reach a steady state distribution, with $y_t = 0$. The heat distribution then satisfies

$$\begin{aligned} &\varepsilon y'' - y' = -1, \quad 0 < x < 1, \\ &y(0) = 2. \end{aligned}$$

This problem is not fully defined, since it has only one boundary condition. Suppose a device is installed on the end of the pipe that nearly instantaneously brings the heat of the water up to $y = 4$. Physically we expect this extra heat that is introduced at $x = 1$ to diffuse backward through the water in the pipe. This leads to a well defined BVP,

$$\begin{aligned} &\varepsilon y'' - y' = -1, \quad 0 < x < 1, \\ &y(0) = 2, \quad y(1) = 4. \end{aligned} \tag{12.1}$$

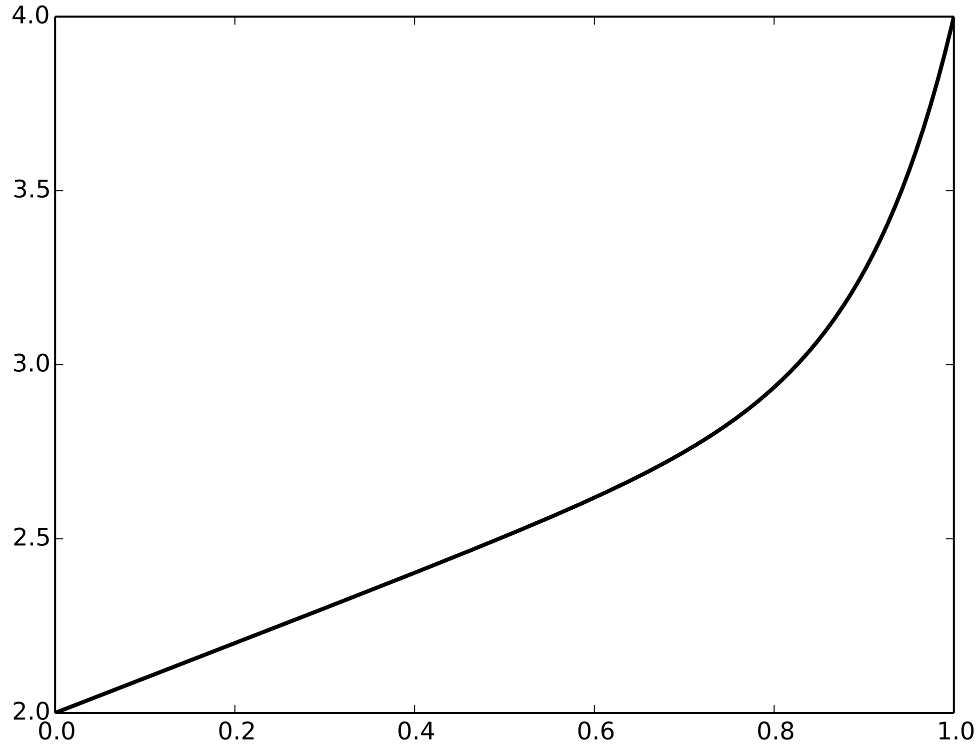


Figure 12.1: The solution of (12.1) for $\varepsilon = .1$.

The Weak Formulation

Consider the equation

$$\begin{aligned} &\varepsilon y'' - y' = f, \quad 0 < x < 1, \\ &y(0) = \alpha, \quad y(1) = \beta. \end{aligned} \tag{12.2}$$

To find the solution y using the finite element method, we reframe the problem and look at what is known as its weak formulation.

Let w be a smooth function on $[0, 1]$ satisfying $w(0) = w(1) = 0$. Multiplying (12.2) by w and integrating over $[0, 1]$ yields

$$\begin{aligned} \int_0^1 fw &= \int_0^1 \varepsilon y'' w - y'w, \\ &= \int_0^1 -\varepsilon y' w' - y'w. \end{aligned}$$

Define a bilinear function a and a linear function l by

$$a(y,w) = \int_0^1 -\varepsilon y'w' - y'w,$$
$$l(w) = \int_0^1 fw.$$

Rather than trying to solve (12.2), we instead consider the problem of finding a function y such that

$$a(y,w) = l(w), \quad \forall\, w \in V_0, \tag{12.3}$$

where V is some appropriate vector space that is expected to allow us to approximate the solution y, and $V_0 = \{w \in V | w(0) = w(1) = 0\}$. (For example, we could consider the space of functions that are piecewise linear with vertices at a fixed set of points. This example is discussed further below.) This equation is called the weak formulation of (12.2).

Let P_n be some partition of $[0,1]$, $0 = x_0 < x_1 < \ldots < x_n = 1$, and let V_n be the finite-dimensional vector space of continuous functions v on $[0,1]$ where v is linear on each subinterval $[x_j, x_{j+1}]$. These subintervals are the finite elements for which this method is named. V_n has dimension $n+1$, since there are $n+1$ degrees of freedom for continuous piecewise linear functions in V. Let V_{n0} be the subspace of V_n of dimension $n-1$ whose elements are zero at the endpoints of $[0,1]$, and let $\triangle x_n = \max_{0 \le j \le n-1} |x_{j+1} - x_j|$.

Let $\{\mathrm{P}_n\}$ be a sequence of partitions that are refinements of each other, such that $\triangle x_n \to 0$ as $n \to \infty$. Then in particular $V_1 \subset V_2 \subset \ldots \subset V_n \ldots \subset V$. For each partition P_n we can look for an approximation $y_n \in V_n$ for the true solution y; if this is done correctly then $y_n \to y$ as $n \to \infty$.

The Numerical Method

Consider a partition $\mathrm{P}_5 = \{x_0, x_1, \ldots, x_5\}$. We will define some basis functions ϕ_i, $i = 0, \ldots, 5$ for the corresponding vector space V_5. Let the ϕ_i be the hat functions

$$\phi_i(x) = \begin{cases} (x - x_{i-1})/h_i & \text{if } x \in [x_{i-1}, x_i] \\ (x_{i+1} - x)/h_{i+1} & \text{if } x \in [x_i, x_{i+1}] \\ 0 & \text{otherwise} \end{cases}$$

where $h_i = x_i - x_{i-1}$; see Figures 12.2 and 12.3.

We look for an approximation $\hat{y} = \sum_{i=0}^5 k_i \phi_i \in V_5$ of the true solution y; to do this we must determine appropriate values for the constants k_i. We impose the condition on $\hat{y}$ that

$$a(\hat{y}, w) = l(w) \quad \forall\, w \in V_5.$$

Equivalently, we require that

$$a\left(\sum_{i=0}^5 k_i \phi_i, \phi_j\right) = l(\phi_j) \quad \text{for } j = 1, 2, 3, 4,$$

since $\phi_1, \phi_2, \phi_3, \phi_4$ form a basis for V_5.

Since a is bilinear, we obtain

$$\sum_{i=0}^5 k_i a(\phi_i, \phi_j) = l(\phi_j) \quad \text{for } j = 1, 2, 3, 4.$$

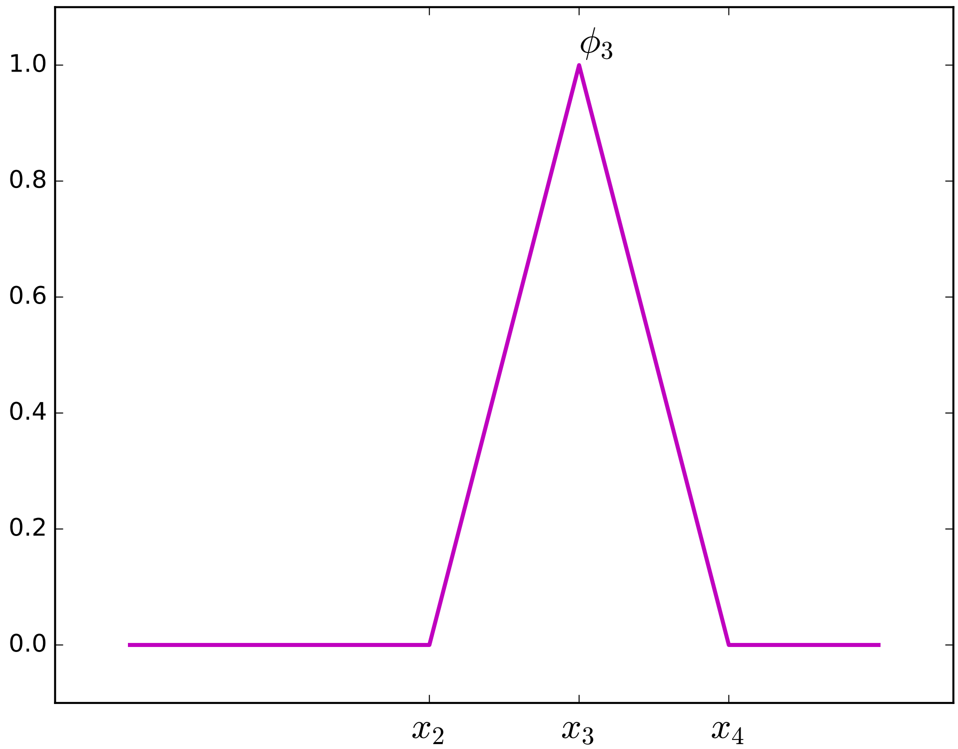


Figure 12.2: The basis function ϕ_3.

To satisfy the boundary conditions, we also require that $k_0 = \alpha$, $k_5 = \beta$. These equations can be written in matrix form as

$$AK = \Phi, \tag{12.4}$$

where

$$A = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ a(\phi_0,\phi_1) & a(\phi_1,\phi_1) & a(\phi_2,\phi_1) & 0 & 0 & 0 \\ 0 & a(\phi_1,\phi_2) & a(\phi_2,\phi_2) & a(\phi_3,\phi_2) & 0 & 0 \\ 0 & 0 & a(\phi_2,\phi_3) & a(\phi_3,\phi_3) & a(\phi_4,\phi_3) & 0 \\ 0 & 0 & 0 & a(\phi_3,\phi_4) & a(\phi_4,\phi_4) & a(\phi_5,\phi_4) \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

and

$$K = \begin{bmatrix} k_0 \\ k_1 \\ k_2 \\ k_3 \\ k_4 \\ k_5 \end{bmatrix}, \quad \Phi = \begin{bmatrix} \alpha \\ l(\phi_1) \\ l(\phi_2) \\ l(\phi_3) \\ l(\phi_4) \\ \beta \end{bmatrix}.$$

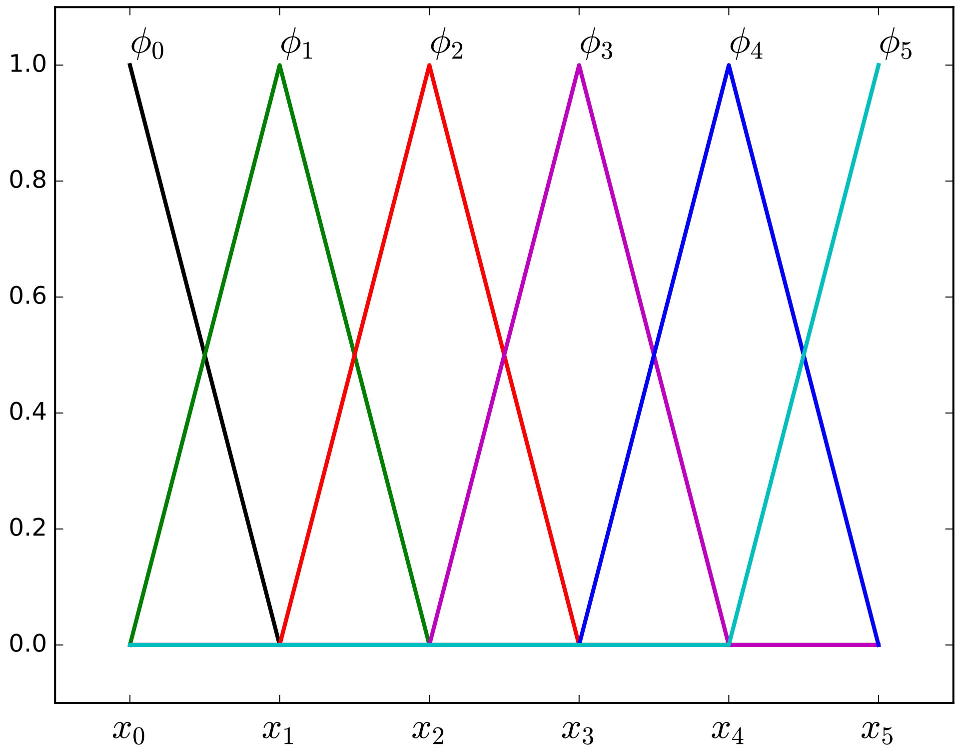


Figure 12.3: Basis functions for V_5.

Note that $a(\phi_i, \phi_j) = 0$ for most values of i, j (that is, when the hat functions do not have overlapping domains). Thus the finite element method results in a sparse linear system. To compute the coefficients of (12.4) we begin by evaluating some integrals. Since

$$\phi_i'(x) = \begin{cases} 1/h_i & \text{for } x_{i-1} < x < x_i, \\ -1/h_{i+1} & \text{for } x_i < x < x_{i+1}, \\ 0 & \text{otherwise,} \end{cases}$$

we obtain

$$\int_0^1 \phi_i'\phi_j' = \begin{cases} -1/h_{i+1} & \text{if } j = i+1, \\ 1/h_i + 1/h_{i+1} & \text{if } j = i, \\ 0 & \text{otherwise,} \end{cases}$$

$$\int_0^1 \phi_i'\phi_j = \begin{cases} -1/2 & \text{if } j = i+1, \\ 1/2 & \text{if } j = i-1, \\ 0 & \text{otherwise,} \end{cases}$$

$$a(\phi_i, \phi_j) = \begin{cases} \varepsilon/h_{i+1} + 1/2 & \text{if } j = i+1, \\ -\varepsilon/h_i - \varepsilon/h_{i+1} & \text{if } j = i, \\ \varepsilon/h_i - 1/2 & \text{if } j = i-1, \\ 0 & \text{otherwise,} \end{cases}$$

$$l(\phi_j) = -(1/2)(h_j + h_{j+1}).$$

Equation (12.4) may now be solved using any standard linear solver. To handle the large number of elements required for Problem 3, you will want to use the tridiagonal algorithm provided in several of the earlier labs or the banded matrix solver included in `scipy.linalg`.

Problem 1. Use the finite element method to solve

$$\begin{aligned} \varepsilon y'' - y' &= -1, \\ y(0) = \alpha, \quad y(1) &= \beta, \end{aligned} \tag{12.5}$$

where $\alpha = 2, \beta = 4$, and $\varepsilon = 0.02$. Use $N = 100$ finite elements (101 grid points). Compare your solution with the analytic solution

$$y(x) = \alpha + x + (\beta - \alpha - 1)\frac{e^{x/\varepsilon} - 1}{e^{1/\varepsilon} - 1}.$$

Problem 2. One of the strengths of the finite element method is the ability to generate grids that better suit the problem. The solution of (12.5) changes most rapidly near $x = 1$. Compare the numerical solution when the grid points are unevenly spaced versus when the grid points are clustered in the area of greatest change; see Figure 12.4. Specifically, use the grid points defined by

```
even_grid = np.linspace(0,1,15)
clustered_grid = np.linspace(0,1,15)**(1./8)
```

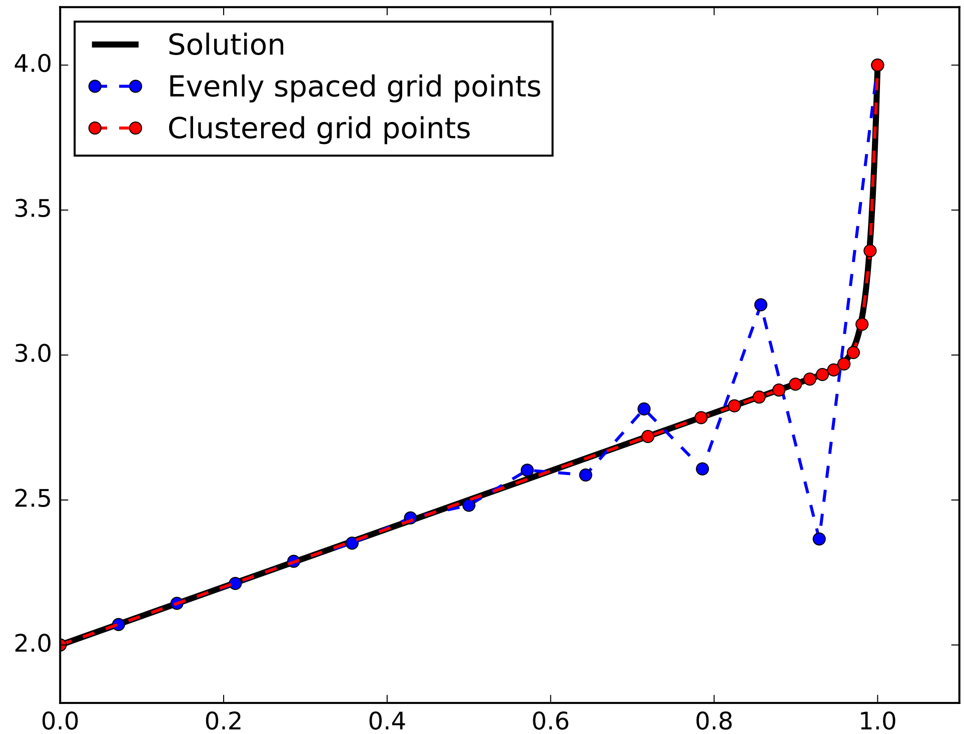


Figure 12.4: We plot two finite element approximations using 15 grid points.

Problem 3. Higher order methods promise faster convergence, but typically require more work to code. So why do we use them when a low order method will converge just as well, albeit with more grid points? The answer concerns the roundoff error associated with floating point arithmetic. Low order methods generally require more floating point operations, so roundoff error has a much greater effect.

The finite element method introduced here is a second order method, even though the approximate solution is piecewise linear. (To see this, note that if the grid points are evenly spaced, the matrix A in (12.4) is exactly the same as the matrix for the second order centered finite difference method.)

Solve (12.5) with the finite element method using $N = 2^i$ finite elements, $i = 4, 5, \ldots, 21$. Use a log-log plot to graph the error; see Figure 12.5.

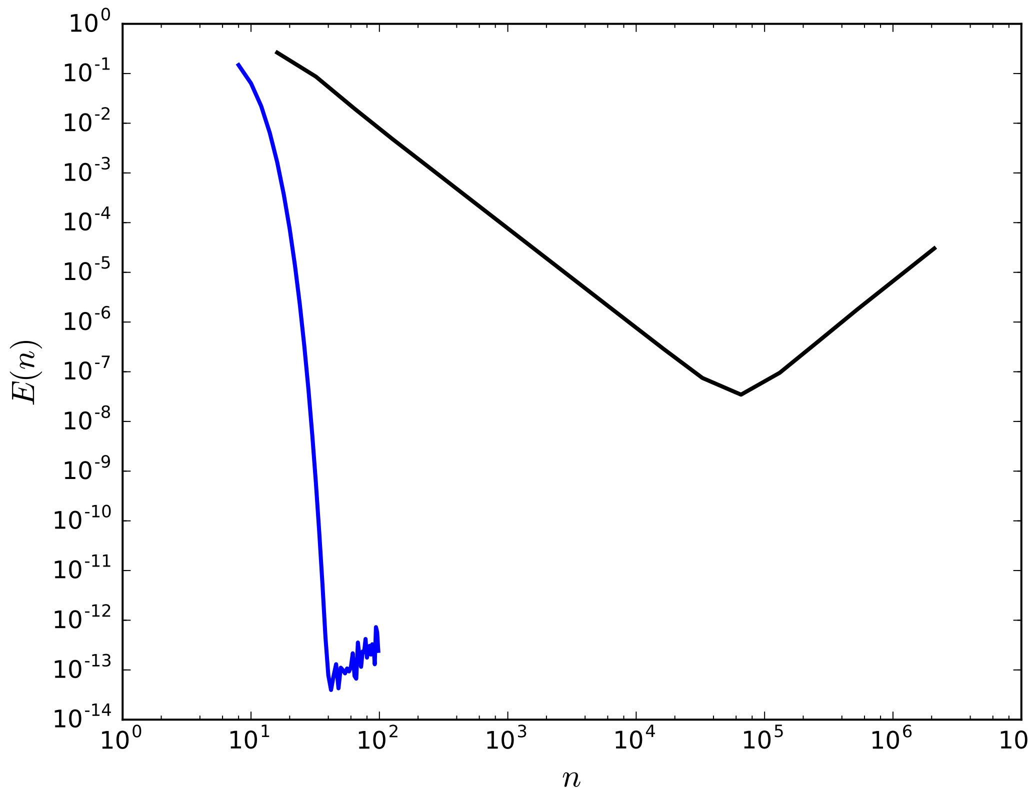


Figure 12.5: Error for the second order finite element method, as the number of subintervals n grows. Round-off error eventually overwhelms the approximation.

13 Stochastic Differential Equations

Lab Objective: *Stochastic differential equations are used to model stochastic processes. In this lab we will explore Brownian motion and then derive the Euler-Maruyama numerical method for SDEs. We will build an Euler-Maruyama numerical solver and use this solver to predict future stock prices.*

Stochastic differential equations combine the concepts of Brownian motion and differential equations in order to model stochastic processes. A stochastic process is a mathematical object made from a family of random variables. These processes model events that occur with random changes over time, such as bacterial population growth, movement of gas molecules, and fluctuating stock prices. To understand stochastic processes, it is imperative to understand Brownian motion.

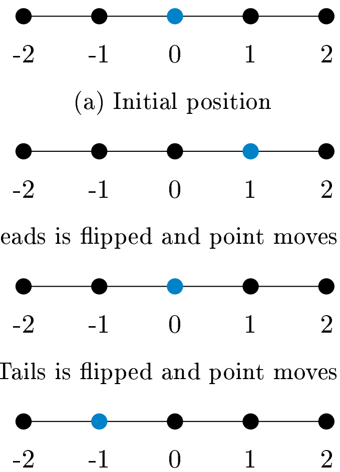
Brownian Motion

Brownian motion is random movement described by the Wiener process. The Wiener process is a stochastic process $W(t) \sim \mathcal{N}(0, t)$ which satisfies the following conditions:

1. $W(0) = 0$,

2. $W(t - s) = W(t) - W(s)$,

3. $W(t)$ is independent for all t.



(a) Initial position

(b) Heads is flipped and point moves right.

(c) Tails is flipped and point moves left.

(d) Tails is flipped and point moves left.

Figure 13.1: Example of Brownian motion. The blue dot travels left or right with equal probability. It is modeled by a coin flip. When heads, the dot moves right. When tails, the dot moves left.

For example, imagine a point at zero on a number line. The point can only move one number away and must move left or right. The probability of moving left and right is equal and can be modeled by a coin flip. Let's say that landing on heads moves the point right and tails moves the point left. On our first flip, we get heads and the point moves from 0 to 1. Now we flip the coin again. This coin flip does not depend on the previous coin flip and determines whether the point moves back to 0 or moves to 2. On the second flip, we get tails and the point moves back to 0. Continuing this process shows the random movement of the point on the number line.

As we flip the coin t times, the distribution of the point's position is approximately normally distributed with mean 0 and variance t. Note that $dW \sim \mathscr{N}(0, \Delta t)$ is also approximately normally distributed because $W(t-s) = W(t) - W(s)$ and $W(t-s) \sim \mathscr{N}(0, t-s)$. Using dW, we can show the movement of a point with the differential equation

$$\frac{dS_t}{S_t} = g(t, S_t)dW. \tag{13.1}$$

where $g(t, S_t)$ is a scalar function and S_t is the position of the point at time t. We can manipulate Equation 13.1 to model the position of the point numerically:

$$\begin{aligned} dS_t &\approx g(t, S_t)S_t dW \\ S_{t+1} - S_t &\approx g(t, S_t)S_t dW \\ S_{t+1} &\approx S_t + g(t, S_t)S_t dW \end{aligned}$$

where $dW \sim \mathscr{N}(0, 1)$. This model is itself a stochastic differential equation that is based completely on brownian motion.

Problem 1. Write a function `brownian_motion()` that accepts a scalar function `g`, initial condition `y0`, and an array of time points `t`. The function should return an array of the solution to Equation 13.1 evaluated at t.

Animate this function for $g(t, S_t) = 1$, $y_0 = (1, 1)$ and $t \in [0, 100)$. The animation should show a particle moving with a tail indicating it's previous position.

(Hint: Because $y_0 \in \mathbb{R}^2$, $dW \in \mathbb{R}^2 \times \mathbb{R}^2$ so that each dimension of y_0 moves independently. Thus, $dW = \begin{pmatrix} d_{w_1} & 0 \\ 0 & d_{w_2} \end{pmatrix}$ where $d_{w_i} \sim \mathcal{N}(0, 1)$).

Euler-Maruyama Method

A stochastic differential equation (SDE) is a differential equation that involves at least one stochastic component. Equation 13.1 is an example of a SDE, as its only component is stochastic. However, most SDEs are not made of just one stochastic component. A commonly used stochastic differential equation which contains a non-stochastic component is

$$\frac{dS_t}{S_t} = f(t, S_t)dt + g(t, S_t)dW \tag{13.2}$$

where $f(t, S_t)$ and $g(t, S_t)$ are scalar functions and $dW \sim \mathcal{N}(0, \Delta t)$. In this equation, the first term is a standard differential equation while the second term represents brownian motion. The combination allows for more accurate models of stochastic processes. To solve Equation 13.2, we apply the Euler-Maruyama method. This method combines the Euler method for ODEs with an additional stochastic component. Note that Problem 1 is the Euler-Maruyama method where $f(t, S_t) = 0$. We solve for S_{t+1} as follows:

$$\begin{aligned} dS_t &\approx f(t, S_t)S_t dt + g(t, S_t)S_t dW \\ S_{t+1} - S_t &\approx f(t, S_t)S_t dt + g(t, S_t)S_t dW \\ S_{t+1} &\approx S_t + f(t, S_t)S_t dt + g(t, S_t)S_t dW. \end{aligned}$$

Problem 2. Write a function `euler_maruyama()` which accepts a scalar function `f`, a scalar function `g`, initial condition `y0s`, and an array of time points `t`. The function should return an array of the solution to 13.2.

To test your function, set $f(t, S_t) = 1 - (S_t)^2$, $g(t, S_t) = 0.1$, $y_0 = 1$ and $t \in [0, 10)$. Your function should result in a plot which randomly oscillates with y generally in the interval $[0, 2]$. An example is shown in Figure 13.2.

Drift and Volatility

SDEs are often used in mathematical finance models. Particularly, the Geometric Brownian Motion (GBM) model is useful in predicting future stock prices. The GBM is defined as follows:

$$dS_t = \mu S_t dt + \sigma S_t dW, \tag{13.3}$$

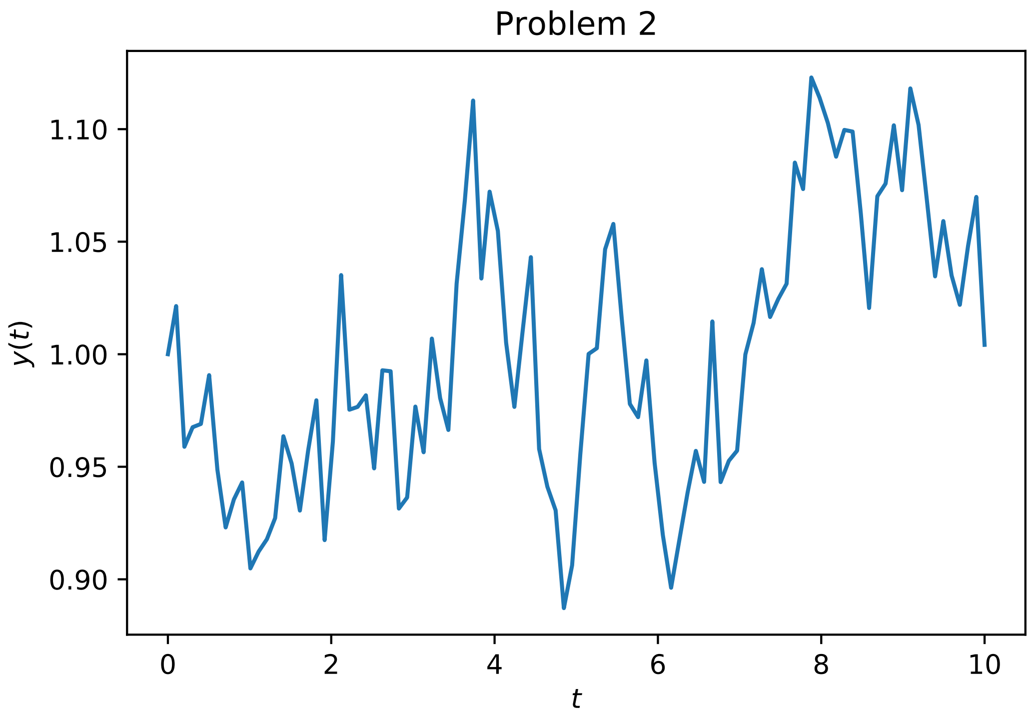


Figure 13.2: Possible solution for $f(t, S_t) = 1 - (S_t)^2$, $g(t, S_t) = 0.1$, $y_0 = 1$ and $t \in [0, 10)$.

where μ is the drift of the stock and σ is the volatility. The drift μ of a stock is the average change in return of historic stock data. The volatility of a stock is the standard deviation of the change in return of historic stock data. It is expected that μ and σ will remain the same for future stock data.

To find μ and σ, let $\theta = (\mu, \sigma)$. We want to find θ_{MAP} (maximum a posteriori) which maximizes the probability that μ and σ fit the historical data. We can calculate θ_{MAP} using Bayes Theorem:

$$\theta_{MAP}\left(\frac{dS}{S}\right) = \text{argmax}_\theta P\left(\theta|\frac{dS}{S}\right) = \text{argmax}_\theta \frac{P\left(\frac{dS}{S}|\theta\right)P(\theta)}{\int_\Theta P\left(\frac{dS}{S}|\vartheta\right)P(\vartheta)d\vartheta} = \text{argmax}_\theta P\left(\frac{dS}{S}|\theta\right)P(\theta), \tag{13.4}$$

where Θ is the collection of all possible θ. Since no information is known about $P(\theta)$, we choose $P(\theta)$ to be equal over all θ. This avoids giving bias to one value of θ over another. To ease calculations, we choose our improper prior to be uniformly 1, $P(\theta) = 1$. This implies $\theta_{MAP} = \text{argmax}_\theta P(\frac{dS}{S}|\theta) = \theta_{MLE}$.

Now it is necessary to determine the probability distribution of $P(\frac{dS}{S}|\theta)$. Plotting the change in stock price results in the following histogram: The change in stock price is approximately normally distributed and thus we consider $P(\frac{dS}{S}) \sim \mathcal{N}(\mu, \sigma^2)$. Now we can calculate θ_{MAP} as follows:

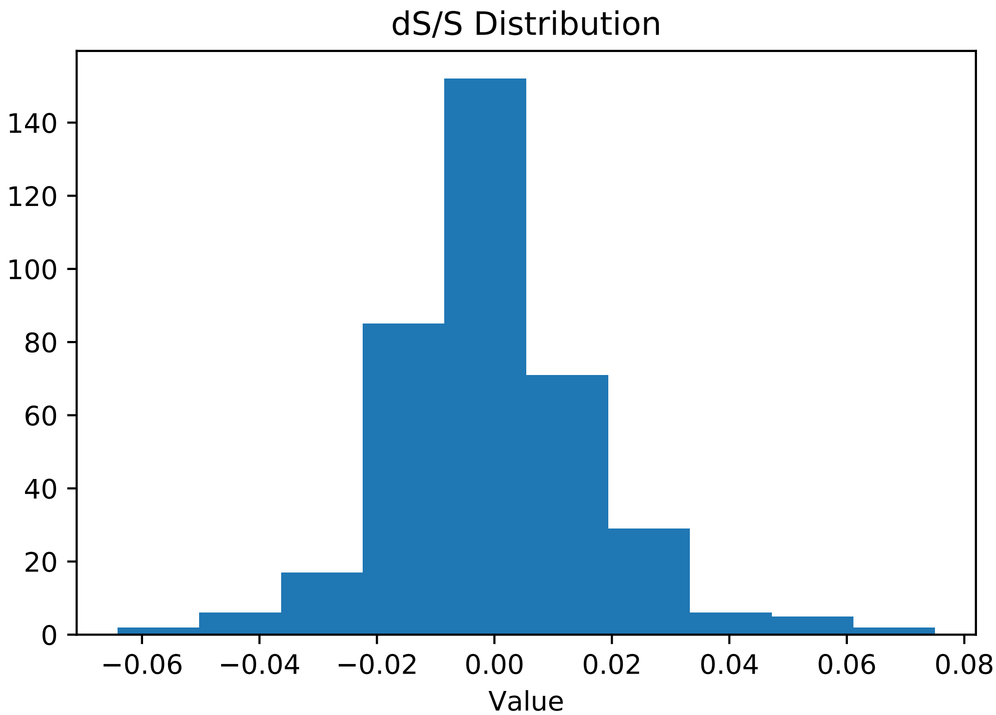


Figure 13.3: Distribution of change in stock price.

$$
\begin{aligned}
\theta_{MAP} &= \text{argmax}_\theta P(\frac{dS}{S}|\theta) \\
&= \text{argmax}_\theta \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi\sigma^2}} \exp(-\frac{((\frac{dS}{S})_i - \mu)^2}{2\sigma^2}) \\
&= \text{argmax}_\theta \log(\prod_{i=1}^{N} \frac{1}{\sqrt{2\pi\sigma^2}} \exp(-\frac{((\frac{dS}{S})_i - \mu)^2}{2\sigma^2})) \\
&= \text{argmax}_\theta \sum_{i=1}^{N} \log(\frac{1}{\sqrt{2\pi\sigma^2}} \exp(-\frac{((\frac{dS}{S})_i - \mu)^2}{2\sigma^2})) \\
&= \text{argmax}_\theta \sum_{i=1}^{N} \log(\frac{1}{\sqrt{2\pi\sigma^2}}) - \frac{((\frac{dS}{S})_i - \mu)^2}{2\sigma^2} \\
&= \text{argmax}_\theta N \log(\frac{1}{\sqrt{2\pi\sigma^2}}) - \sum_{i=1}^{N} \frac{((\frac{dS}{S})_i - \mu)^2}{2\sigma^2} \\
&= \text{argmin}_\theta N \log(\sqrt{2\pi\sigma^2}) + \sum_{i=1}^{N} \frac{((\frac{dS}{S})_i - \mu)^2}{2\sigma^2} \\
&= \text{argmin}_\theta N \log(\sqrt{2\pi\sigma^2}) + \frac{1}{2\sigma^2} \sum_{i=1}^{N} ((\frac{dS}{S})_i - \mu)^2
\end{aligned}
\tag{13.5}
$$

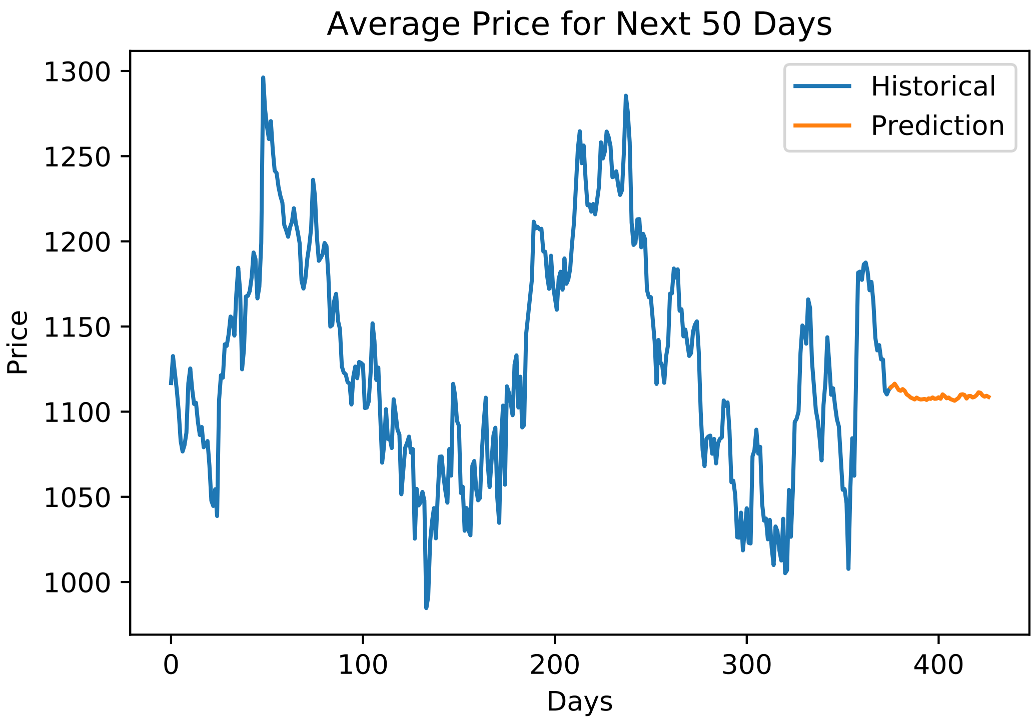


Figure 13.4: Possible plot of future Google stock prices.

The end result of Equation 13.5 gives an equation that can be optimized using `scipy.optimize.minimize` to find θ.

Problem 3. Write a function `theta()` which takes in an array of historical data. Use `scipy.optimize.minimize` and Equation 13.5 to calculate the optimal μ and σ. Return μ and σ. For the closing stock prices of `google_stock.csv`, $\mu \approx 1129.4321$ and $\sigma \approx 1.8548$.

(Hint: Use the sample mean and sample variance as an initial guess for `scipy.optimize.minimize`. Also use `method='Nelder-Mead'`.)

Problem 4. Use `euler_maruyama()` to predict the future closing stock prices of Google stock for $t \in [377, 427)$. Plot the original data and the average predicted stock prices. Return an array of the average future stock prices. Your plot should look similar to Figure 13.4.

(Hint: Let $f(t, S_t) = \mu$ and $g(t, S_t) = \sigma$. Each t represents one day, so there should be 50 predicted values.)

Convergence of Euler-Maruyama

The Euler-Maruyama method has strong convergence as $\Delta t \to \infty$. This can be seen heuristically by looking at the expected value of the error of the numerical method. Note equation 13.3 can be solved analytically to get the solution

$$S(t) = s_0 e^{\left(\mu - \frac{\sigma^2}{2}\right)t + \sigma W(t)} \tag{13.6}$$

where $s_0 = S(0)$. Let $A_{\Delta t}(t)$ be the approximation of $S(t)$ with step size Δt. Because we are working with SDEs, we take the expected value of the max error over all t and define the error as

$$E(A_{\Delta t}) = \sup_t \mathbb{E}\Big(|S(t) - A_{\Delta t}(t)|\Big) \approx C(\Delta t)^{\gamma}. \tag{13.7}$$

where γ is the order of convergence and C is some constant. Taking the log of both sides, we get

$$\log(E(A_{\Delta t})) = \log(C) + \gamma \log(\Delta t). \tag{13.8}$$

To find the order of convergence γ, we can plot $\Delta t \times E(A_{\Delta t}(t))$ as $\Delta t \to \infty$ with log axes. This should result is a straight line with slope γ, giving us the convergence rate. For Euler-Maruyama, $\gamma = \frac{1}{2}$.

Problem 5. Write a function `convergence()` that calculates the convergence of Euler-Maruyama. Calculate the drift and volatility of the closing prices in `google_stock.csv` and use Euler-Maruyama to predict stock values for $t \in [0, 50)$. Calculate the difference between the analytical solution 13.6 and predicted data from Euler-Maruyama. Plot the difference for $dt = 2^i$ for $i \in [0, 1, 2, 3, 4, 5]$ on a log-log plot. Your plot should be a straight line with slope $\frac{1}{2}$.

(Hint: Try using `np.arange`).

14 Obstacle Avoidance

Lab Objective: *Solve boundary value problems that arise when using Pontryagin's Maximum principle.*

General Boundary Value Problems

A boundary value problem is a differential equation with a set of constraints. It is similar to initial value problems, which give only initial constraints. An initial value problem may look something like this

$$\begin{aligned} y'' + y' + y &= f(t) \\ y(a) &= \alpha \\ y'(a) &= \beta \\ t &\in [a, b]. \end{aligned}$$

This problem gives a differential equation with initial conditions for y and y'. A boundary value problem may look something like this

$$\begin{aligned} y'' + y' + y &= f(t) \\ y(a) &= \alpha \\ y(b) &= \beta \\ t &\in [a, b], \end{aligned}$$

where we have both right and left hand boundary conditions on y.

Formulating and solving boundary value problems is an important tool when solving many types of problems. This is especially true in the world of variational calculus and optimal control. Many optimal control problems can be formulated as a boundary value problem by using Pontryagin's Maximum Principle, which may greatly simplify the problem.

SciPy has great tools that help us solve boundary value problems. We will be using `solve_bvp` from `scipy.integrate`. Consider the following example

$$y'' + 9y = cos(t), \quad y'(0) = 5, \quad y(\pi) = -\frac{5}{3}. \tag{14.1}$$

We begin by changing this second order ODE into a first order ODE system.

$$\text{Let } y_1 = y \text{ and } y_2 = y' \text{ so that,}$$
$$\begin{bmatrix} y_1 \\ y_2 \end{bmatrix}' = \begin{bmatrix} y_2 \\ \cos t - 9y_1 \end{bmatrix}.$$

This formulation allows us to use `solve_bvp()`.

```python
from scipy.integrate import solve_bvp
import numpy as np

def ode(t,y):
    ''' define the ode system '''
    return np.array([y[1], np.cos(t) - 9*y[0]])

def bc(ya,yb):
    ''' define the boundary conditions '''
    # ya are the initial values
    # yb are the final values
    # each entry of the return array will be set to zero
    return np.array([ya[1] - 5, yb[0] + 5/3])

# give the time domain
t_steps = 100
t = np.linspace(0,np.pi,t_steps)

# give an initial guess
y0 = np.ones((2,t_steps))


# solve the system
sol = solve_bvp(ode, bc, t, y0)
```

Then we can plot the solution with the following code

```python
import matplotlib.pyplot as plt

plt.plot(t, sol.y[0])
plt.xlabel('t')
plt.ylabel('y(t)')
plt.show()
```

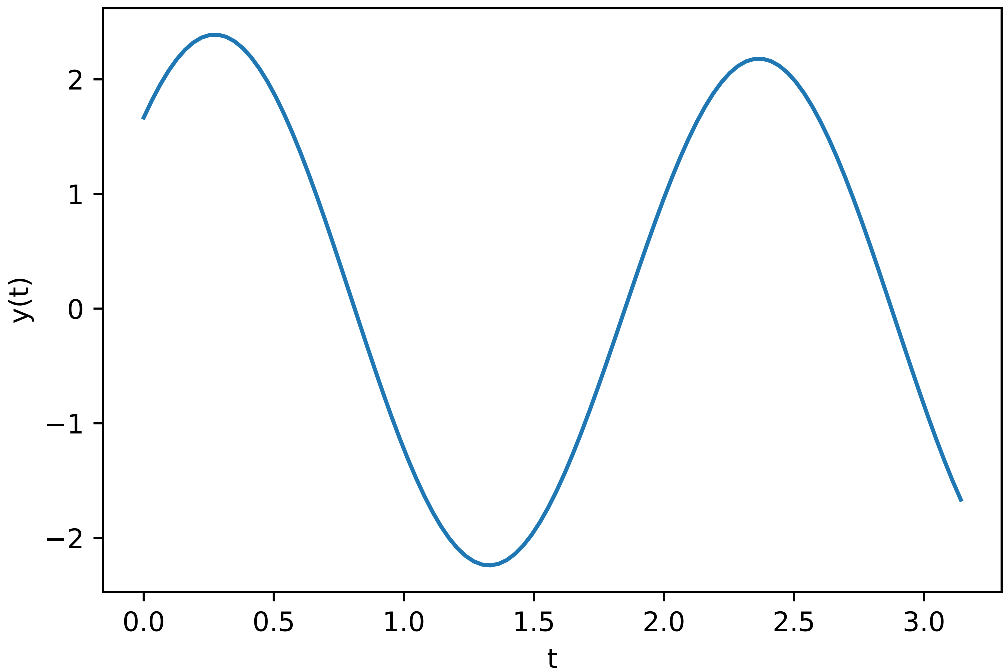


Figure 14.1: The solution to 14.1

Problem 1. Solve the following boundary value problem:

$$y'' + 3y = \sin(t)$$
$$y(0) = 0, \quad y(5\pi) = \frac{\pi}{2}.$$

Plot your solution.

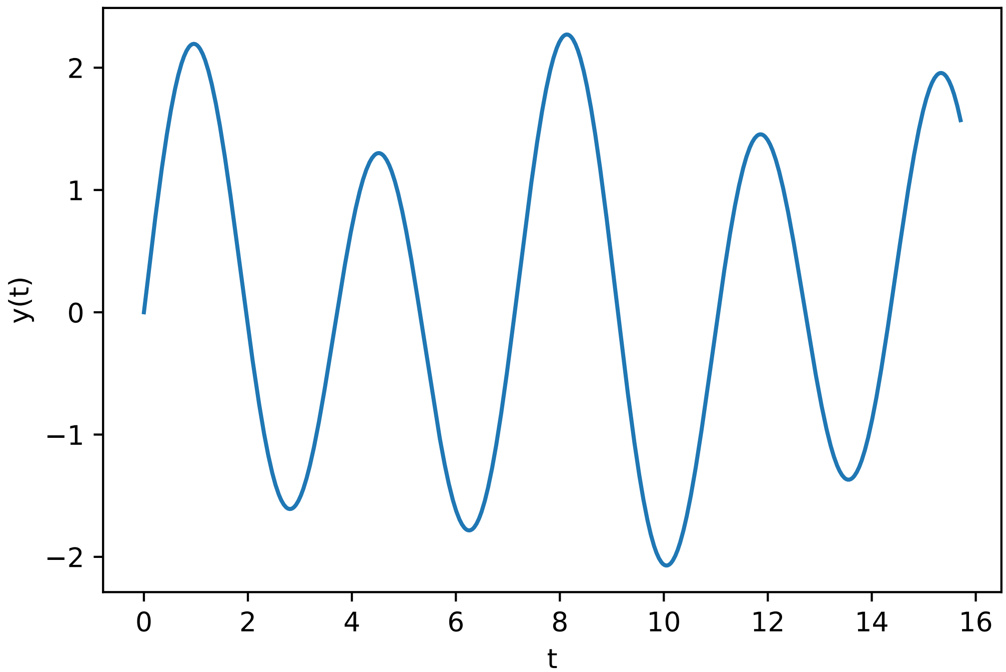


Figure 14.2: The solution to problem 1.

Pontryagin's Maximum Principle

Now that we understand how to solve boundary value problems, we can apply this to solve optimal control problems. Pontryagin's Maximum Principle is a very common way to formulate control problems as BVPs.

Fixed Time, Fixed Endpoint

We will begin with the more simple fixed time horizon problems. Fixed time horizon problems are commonly reformulated as boundary value problems, and we can apply what we have already learned about solving BVPs to make these problems easier to solve. We introduce fixed time horizon problems with a cost functional of the following form

$$J(u) = \int_{t_0}^{t_f} L(t, s(t), u(t))dt + K(t_f, s_f), \tag{14.2}$$

where t_0 and t_f are fixed. In this functional, $L(t, s(t), u(t))$ represents the cost of a certain path determined by the control u, and $K(t_f, s_f)$ is the terminal cost. We also have that

$$\dot{s} = f(t, s, u),\ s_0 = s(t_0),\ s_f = s(t_f). \tag{14.3}$$

In these equations t is time, s is the state variable, and u is the control variable. The maximum principle also uses the Hamiltonian equation

$$H(t, s, u, p) = \langle p, f(t, s, u)\rangle - L(t, s, u), \tag{14.4}$$

where p is a newly introduced variable called the costate. This Hamiltonian is then used to define an ODE system. This first equation defines a costate ODE system

$$\dot{p}^* = -H_s(t, s^*, u^*, p^*), \tag{14.5}$$

where a variable marked with an asterisk is the optimal choice of that variable, meaning that equation 14.5 is only true for the optimal state s^*, costate p^*, and control u^* functions. This next equation will allow us to solve for the control in terms of the state and costate

$$0 = H_u(t, s^*, u^*, p^*), \quad \forall t \in [t_0, t_f]. \tag{14.6}$$

The combination of these equations will allow us to create a BVP that will solve for the optimal control u^* and the associated states s^*. Our ODE comes from 14.3, 14.5, and 14.6, and the boundary values will come from our initial and final conditions on s.

Avoiding Collision

One area of application that relies heavily on optimal control is autonomous driving. A common problem in autonomous driving is the avoidance of obstacles. In this section we will outline a naïve solution to obstacle avoidance with a fixed time horizon.

First we can begin by defining our state variable s. We will want to understand the position and velocity at a given time so we will define the following state variable

$$s(t) = \begin{bmatrix} x(t) \\ y(t) \\ \dot{x}(t) \\ \dot{y}(t) \end{bmatrix} = \begin{bmatrix} s_1(t) \\ s_2(t) \\ s_3(t) \\ s_4(t) \end{bmatrix}, \tag{14.7}$$

which allows us to track those states in $\mathbb{R}^2$.

We can then establish the ODE defined in equation 14.3 by examining $\dot{s}(t)$

$$\dot{s}(t) = \begin{bmatrix} \dot{s_1}(t) \\ \dot{s_2}(t) \\ \dot{s_3}(t) \\ \dot{s_4}(t) \end{bmatrix} = \begin{bmatrix} \dot{x}(t) \\ \dot{y}(t) \\ \ddot{x}(t) \\ \ddot{y}(t) \end{bmatrix},$$

and if we define our control u_1 and u_2 to be acceleration in the x and y directions respectively, then we have

$$\dot{s}(t) = f(t, s, u) = \begin{bmatrix} s_3(t) \\ s_4(t) \\ u_1(t) \\ u_2(t) \end{bmatrix}. \tag{14.8}$$

Next we will define an obstacle. Since we are using integration to define cost, a reasonable way to model an obstacle in this problem would be to use a function. It would be helpful if this function is malleable, allowing us to reposition and resize it, based on the needs of the specific situation. This function also needs to have a large, preferably positive, value in a concentrated location, and it needs to vanish relatively quickly. A decent selection could be a function based on an ellipse, such as this function

$$C(x, y) = \frac{W_1}{((x - c_x)^2/r_x + (y - c_y)^2/r_y)^\lambda + 1}. \tag{14.9}$$

With the function 14.9 we can manipulate the center by changing c_x and c_y, and we can control the size by changing r_x and r_y. Changing the constant W_1 allows us to change the relative penalty of occupying the same location as the obstacle, and a reasonable value for λ will control the vanishing rate. We will also include a term in the cost functional that weights against high acceleration. This will allow us to model the real world more accurately, though the term we will be using is not a perfect representation of real world acceleration limitations. Our cost functional is the following

$$J(u) = \int_{t_0}^{t_f} 1 + C(x(t), y(t)) + W_2 |u(t)|^2 \, dt, \tag{14.10}$$

where $W_2 > 0$ defines the relative penalty of high acceleration. This functional will penalize passing near the obstacle and high levels of acceleration.

With the cost functional defined, we can now create the Hamiltonian and the rest of our BVP. We get the following Hamiltonian

$$H(t, p, s, u) = p_1 s_3 + p_2 s_4 + p_3 u_1 + p_4 u_2 - \left(1 + C(x, y) + W_2 |u(t)|^2\right), \tag{14.11}$$

which gives the following costate ODE by equation 14.5

$$\dot{p} = \begin{bmatrix} \dot{p}_1 \\ \dot{p}_2 \\ \dot{p}_3 \\ \dot{p}_4 \end{bmatrix} = \begin{bmatrix} C_x(x, y) \\ C_y(x, y) \\ -p_1 \\ -p_2 \end{bmatrix}. \tag{14.12}$$

Since we're given $H_u = 0$ in equation 14.6, then we also have the following relations

$$\begin{aligned} u_1(t) &= \frac{1}{2W_2} p_3(t) \\ u_2(t) &= \frac{1}{2W_2} p_4(t). \end{aligned} \tag{14.13}$$

Problem 2. Using the ODEs found in 14.8 and 14.12, the obstacle function 14.9, and the following boundary conditions and parameters solve for and plot the optimal path.

$$\begin{gathered} t_0 = 0, \quad t_f = 20 \\ (c_x, c_y) = (4, 1) \\ (r_x, r_y) = (5, .5) \\ \lambda = 20 \\ s_0 = \begin{bmatrix} 6 \\ 1.5 \\ 0 \\ 0 \end{bmatrix}, \quad s_f = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \end{gathered}$$

You will need to choose a W_1 and W_2 which allow the solver to find a valid path. If these parameters are not chosen correctly, the solver may find a path which goes through the obstacle, not around it. Plot the obstacle using `plt.contour()` to see be certain path doesn't pass through the obstacle.

Hint: The default for a parameter of `solve_bvp` called `max_nodes` is not large enough. Try at least `max_nodes = 30000`. You may also find it helpful to use the function `partial` from the module `functools` to preset the parameters for the functions you will be using.

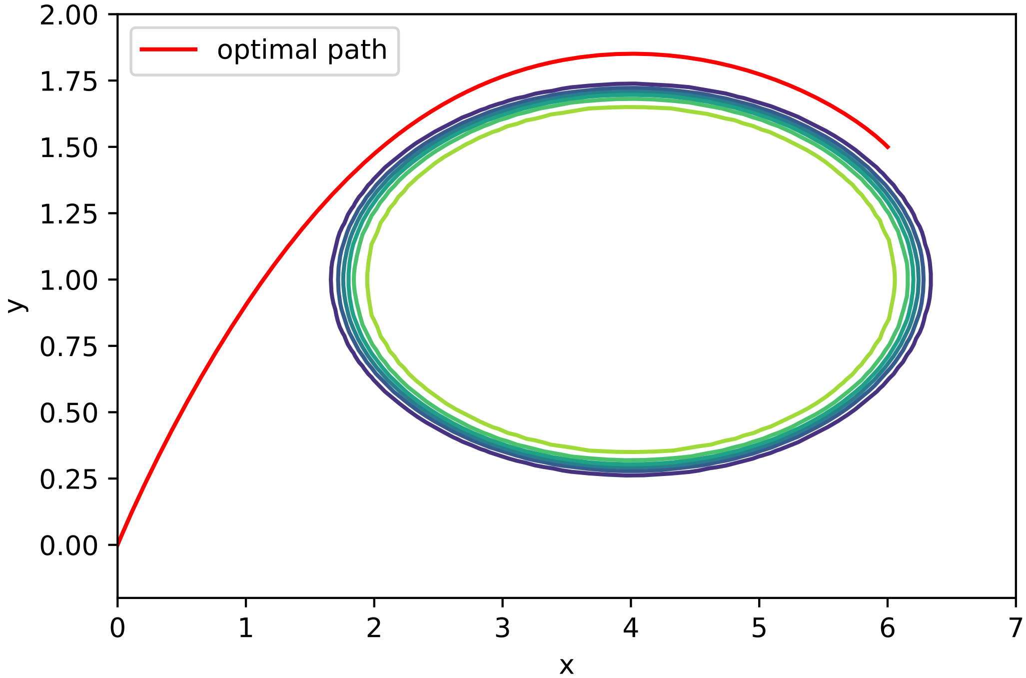


Figure 14.3: Solution to problem 2 for certain choice of parameters

Free Time Horizon Problems

In the previous sections and problems, we were working with BVPs that had a fixed start time t_0, and a fixed end time t_f. However, we may also encounter systems that have a free end time. In order to solve these problems we will need to make some alterations to the problem. First we will perform a change of basis so that we can work with a fixed end time. Consider the following system

$$\dot{x}(t) = f(x(t), t) \quad t \in [0, t_f],$$

we can do the following change of basis for the time variable

$$\begin{aligned} t &= t_f \hat{t} \\ \implies \frac{d}{dt} &= \frac{d}{d\hat{t}} \frac{d\hat{t}}{dt} \\ \implies \frac{d}{dt} &= \frac{d}{d\hat{t}} \frac{1}{t_f}. \end{aligned}$$

We can now define $z(\hat{t}) := x(t_f \hat{t})$ which gives us the following new system

$$\dot{z}\left(\hat{t}\right) = t_f f\left(z\left(\hat{t}\right), \hat{t}\right) \quad \hat{t} \in [0,1].$$

This system can be solved in the same way we solve the fixed time horizon problems. But you may notice that we now have an extra unknown parameter, the final time. Because of this, a free time horizon problem will need one more boundary value to make the system solvable.

So lets examine the earlier example as a free time horizon problem. We start with the ODE system we derived from the second order equation, replacing the fixed final time with a free final time and including the needed third boundary condition

$$\begin{bmatrix} y_1 \\ y_2 \end{bmatrix}' = \begin{bmatrix} y_2 \\ cos(t) - 9y_1 \end{bmatrix}, \quad y_1(0) = 5/3, \quad y_2(0) = 5, \quad y_1(t_f) = -\frac{5}{3}.$$

Now we make the coordinate change giving the following system

$$\begin{bmatrix} z_1 \\ z_2 \end{bmatrix}' = t_f \begin{bmatrix} z_2 \\ cos(\hat{t}) - 9z_1 \end{bmatrix}, \quad z_1(0) = 5/3, \quad z_2(0) = 5, \quad z_1(1) = -\frac{5}{3}. \tag{14.14}$$

Now we can solve this system using `solve_bvp` in python. The new argument `p` that we have included in `ode()` and `bc()` is an `ndarray` that contains our parameter t_f.

```
def ode(t,y,p):
    ''' define the ode system '''
    return p[0]*np.array([y[1], np.cos(t) - 9*y[0]])

def bc(ya,yb,p):
    ''' define the boundary conditions '''
    return np.array([ya[0] - (5/3), ya[1] - 5, yb[0] + 5/3])

# give the time domain
t_steps = 100
t = np.linspace(0,1,t_steps)

# give an initial guess
y0 = np.ones((2,t_steps))
p0 = np.array([6])

# solve the system
sol = solve_bvp(ode, bc, t, y0, p0)
```

The attribute `sol.p[0]` will give the final time the solver found.

When plotting we need to make sure that we remember that $x(t_f \hat{t}) = z(\hat{t})$, so we plot in the following way

```
plt.plot(sol.p[0]*t,sol.sol(t)[0])
plt.xlabel('t')
plt.ylabel('y(t)')
plt.show()
```

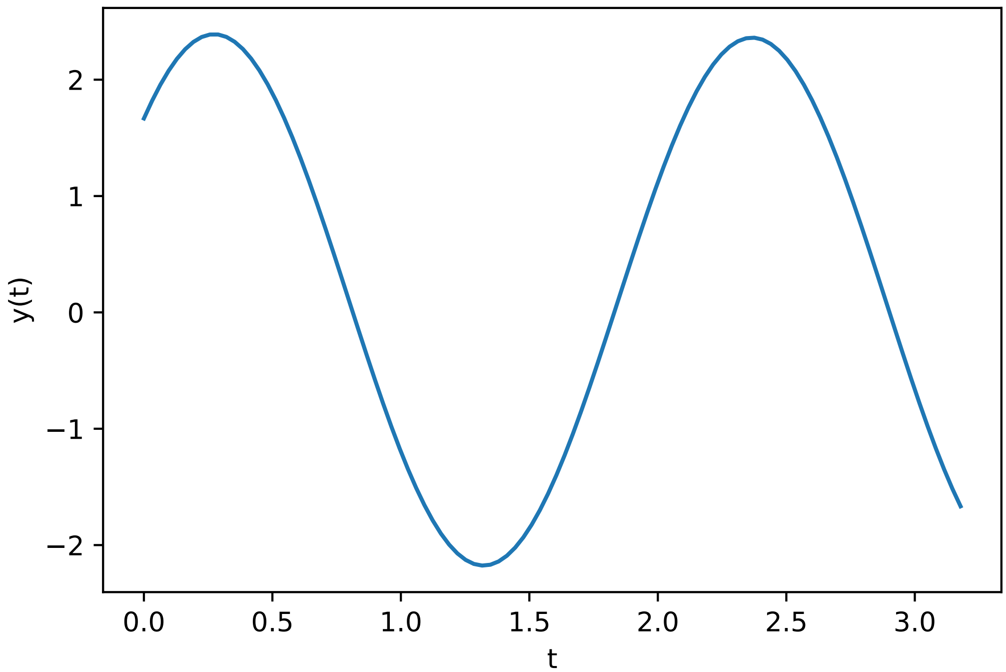


Figure 14.4: The solution to 14.14

Problem 3. Solve the following boundary value problem:

$$y'' + 3y = \sin(t)$$
$$y(0) = 0, \quad y(t_f) = \frac{\pi}{2}, \quad y'(t_f) = \frac{1}{2}\left(\sqrt{3}\pi\cot(\pi\sqrt{75}) - 1\right).$$

Plot your solution. What t_f did the solver find?

Free Time, Fixed Endpoint Control Problems

Now that we understand how to formulate free time horizon problems, we can modify our optimal control BVP to become a free time horizon problem. This is actually the best way to formulate many optimal control problems, as we usually don't know exactly how long it takes to traverse the optimal path. The methodology is exactly the same as we used in the last problem, we only need to find the extra boundary value which will allow us to make the end time a free variable.

To find this extra boundary value we will use the fact that the Hamiltonian is 0 for all t along the optimal path. It is standard to use the final time as the representative so we will assert that

$$H(t_f, p(t_f), s(t_f), u(t_f)) = 0. \tag{14.15}$$

You may notice that when you solve an optimal control problem as a free end time BVP, the optimal path you get is different than what you found when it was a fixed end time BVP. This is because the free end time solution actually arrives faster. The solution found in the fixed end time formulation is the optimal path for a certain fixed end time, but it may not be the overall fastest path that avoids the obstacle.

Problem 4. Refactor your code from problem 2 to create a free end time BVP and use a new boundary value derived from 14.15. Plot the solution you found. What is the optimal time?

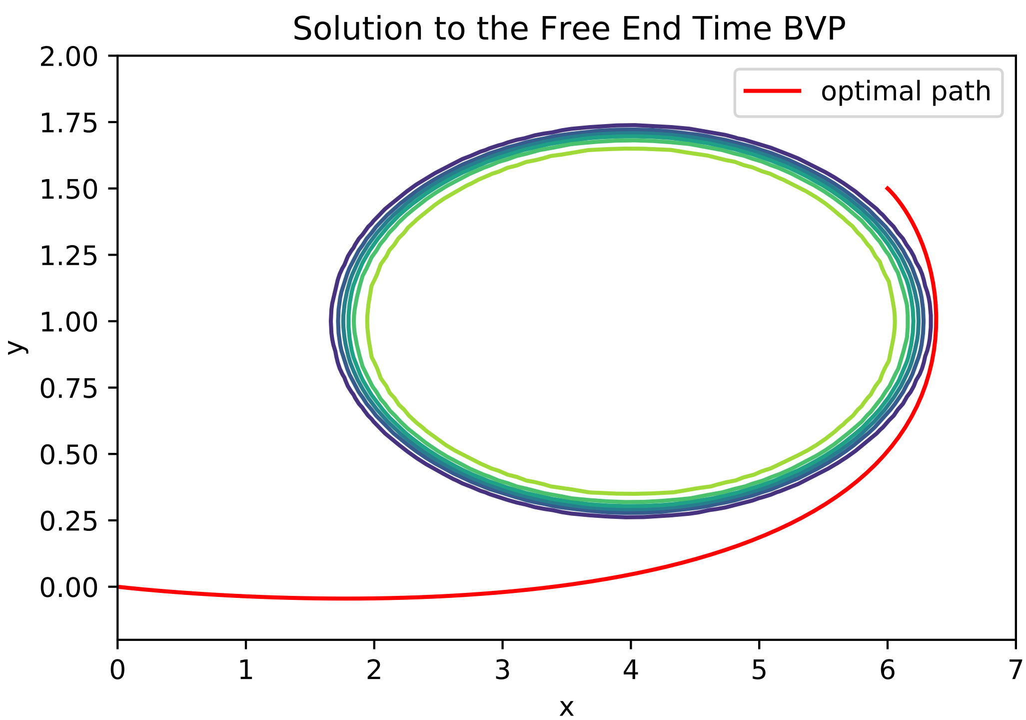


Figure 14.5: The solution to 4

A Getting Started

The labs in this curriculum aim to introduce computational and mathematical concepts, walk through implementations of those concepts in Python, and use industrial-grade code to solve interesting, relevant problems. Lab assignments are usually about 5–10 pages long and include code examples (yellow boxes), important notes (green boxes), warnings about common errors (red boxes), and about 3–7 exercises (blue boxes). Get started by downloading the lab manual(s) for your course from `http://foundations-of-applied-mathematics.github.io/`.

Submitting Assignments

Labs

Every lab has a corresponding specifications file with some code to get you started and to make your submission compatible with automated test drivers. Like the lab manuals, these materials are hosted at `http://foundations-of-applied-mathematics.github.io/`.

Download the `.zip` file for your course, unzip the folder, and move it somewhere where it won't get lost. This folder has some setup scripts and a collection of folders, one per lab, each of which contains the specifications file(s) for that lab. See `Student-Materials/wiki/Lab-Index` for the complete list of labs, their specifications and data files, and the manual that each lab belongs to.

> **Achtung!**
>
> Do **not** move or rename the lab folders or the enclosed specifications files; if you do, the test drivers will not be able to find your assignment. Make sure your folder and file names match `Student-Materials/wiki/Lab-Index`.

To submit a lab, modify the provided specifications file and use the file-sharing program specified by your instructor (discussed in the next section). The instructor will drop feedback files in the lab folder after grading the assignment. For example, the Introduction to Python lab has the specifications file `PythonIntro/python_intro.py`. To complete that assignment, modify `PythonIntro/python_intro.py` and submit it via your instructor's file-sharing system. After grading, the instructor will create a file called `PythonIntro/PythonIntro_feedback.txt` with your score and some feedback.

Homework

Non-lab coding homework should be placed in the `_Homework/` folder and submitted like a lab assignment. Be careful to name your assignment correctly so the instructor (and test driver) can find it. The instructor may drop specifications files and/or feedback files in this folder as well.

Setup

Achtung!

We strongly recommend using a Unix-based operating system (Mac or Linux) for the labs. Unix has a true bash terminal, works well with git and python, and is the preferred platform for computational and data scientists. It is possible to do this curriculum with Windows, but expect some road bumps along the way.

There are two ways to submit code to the instructor: with git (`http://git-scm.com/`), or with a file-syncing service like Google Drive. Your instructor will indicate which system to use.

Setup With Git

Git is a program that manages updates between an online code repository and the copies of the repository, called *clones*, stored locally on computers. If git is not already installed on your computer, download it at `http://git-scm.com/downloads`. If you have never used git, you might want to read a few of the following resources.

- Official git tutorial: `https://git-scm.com/docs/gittutorial`
- Bitbucket git tutorials: `https://www.atlassian.com/git/tutorials`
- GitHub git cheat sheet: `services.github.com/.../github-git-cheat-sheet.pdf`
- GitLab git tutorial: `https://docs.gitlab.com/ce/gitlab-basics/start-using-git.html`
- Codecademy git lesson: `https://www.codecademy.com/learn/learn-git`
- Training video series by GitHub: `https://www.youtube.com/playlist?list=PLg7.../`

There are many websites for hosting online git repositories. Your instructor will indicate which web service to use, but we only include instructions here for setup with Bitbucket.

1. *Sign up.* Create a Bitbucket account at `https://bitbucket.org`. If you use an academic email address (ending in `.edu`, etc.), you will get free unlimited public and private repositories.
2. *Make a new repository.* On the Bitbucket page, click the + button from the menu on the left and, under **CREATE**, select **Repository**. Provide a name for the repository, mark the repository as **private**, and make sure the repository type is **Git**. For **Include a README?**, select **No** (if you accidentally include a `README`, delete the repository and start over). Under **Advanced settings**, enter a short description for your repository, select **No forks** under forking, and select **Python** as the language. Finally, click the blue **Create repository** button. Take note of the URL of the webpage that is created; it should be something like `https://bitbucket.org/<name>/<repo>`.

3. *Give the instructor access to your repository.* On your newly created Bitbucket repository page (`https://bitbucket.org/<name>/<repo>` or similar), go to **Settings** in the menu to the left and select **User and group access**, the second option from the top. Enter your instructor's Bitbucket username under **Users** and click **Add**. Select the blue **Write** button so your instructor can read from and write feedback to your repository.

4. *Connect your folder to the new repository.* In a shell application (Terminal on Linux or Mac, or Git Bash (`https://gitforwindows.org/`) on Windows), enter the following commands.

```
# Navigate to your folder.
$ cd /path/to/folder  # cd means 'change directory'.

# Make sure you are in the right place.
$ pwd                 # pwd means 'print working directory'.
/path/to/folder
$ ls *.md             # ls means 'list files'.
README.md             # This means README.md is in the working directory.

# Connect this folder to the online repository.
$ git init
$ git remote add origin https://<name>@bitbucket.org/<name>/<repo>.git

# Record your credentials.
$ git config --local user.name "your name"
$ git config --local user.email "your email"

# Add the contents of this folder to git and update the repository.
$ git add --all
$ git commit -m "initial commit"
$ git push origin master
```

For example, if your Bitbucket username is `greek314`, the repository is called `acmev1`, and the folder is called `Student-Materials/` and is on the desktop, enter the following commands.

```
# Navigate to the folder.
$ cd ~/Desktop/Student-Materials

# Make sure this is the right place.
$ pwd
/Users/Archimedes/Desktop/Student-Materials
$ ls *.md
README.md

# Connect this folder to the online repository.
$ git init
$ git remote add origin https://greek314@bitbucket.org/greek314/acmev1.git

# Record credentials.
$ git config --local user.name "archimedes"
```

```
$ git config --local user.email "greek314@example.com"

# Add the contents of this folder to git and update the repository.
$ git add --all
$ git commit -m "initial commit"
$ git push origin master
```

At this point you should be able to see the files on your repository page from a web browser. If you enter the repository URL incorrectly in the `git remote add origin` step, you can reset it with the following line.

```
$ git remote set-url origin https://<name>@bitbucket.org/<name>/<repo>.git
```

5. *Download data files.* Many labs have accompanying data files. To download these files, navigate to your clone and run the `download_data.sh` bash script, which downloads the files and places them in the correct lab folder for you. You can also find individual data files through `Student-Materials/wiki/Lab-Index`.

```
# Navigate to your folder and run the script.
$ cd /path/to/folder
$ bash download_data.sh
```

6. *Install Python package dependencies.* The labs require several third-party Python packages that don't come bundled with Anaconda. Run the following command to install the necessary packages.

```
# Navigate to your folder and run the script.
$ cd /path/to/folder
$ bash install_dependencies.sh
```

7. (Optional) *Clone your repository.* If you want your repository on another computer after completing steps 1–4, use the following commands.

```
# Navigate to where you want to put the folder.
$ cd ~/Desktop/or/something/

# Clone the folder from the online repository.
$ git clone https://<name>@bitbucket.org/<name>/<repo>.git <foldername>

# Record your credentials in the new folder.
$ cd <foldername>
$ git config --local user.name "your name"
$ git config --local user.email "your email"

# Download data files to the new folder.
$ bash download_data.sh
```

Setup Without Git

Even if you aren't using git to submit files, you must install it (http://git-scm.com/downloads) in order to get the data files for each lab. Share your folder with your instructor according to their directions, and follow steps 5 and 6 of the previous section to download the data files and install package dependencies.

Using Git

Git manages the history of a file system through *commits*, or checkpoints. Use git status to see the files that have been changed since the last commit. These changes are then moved to the *staging area*, a list of files to save during the next commit, with git add <filename(s)>. Save the changes in the staging area with git commit -m "<A brief message describing the changes>".

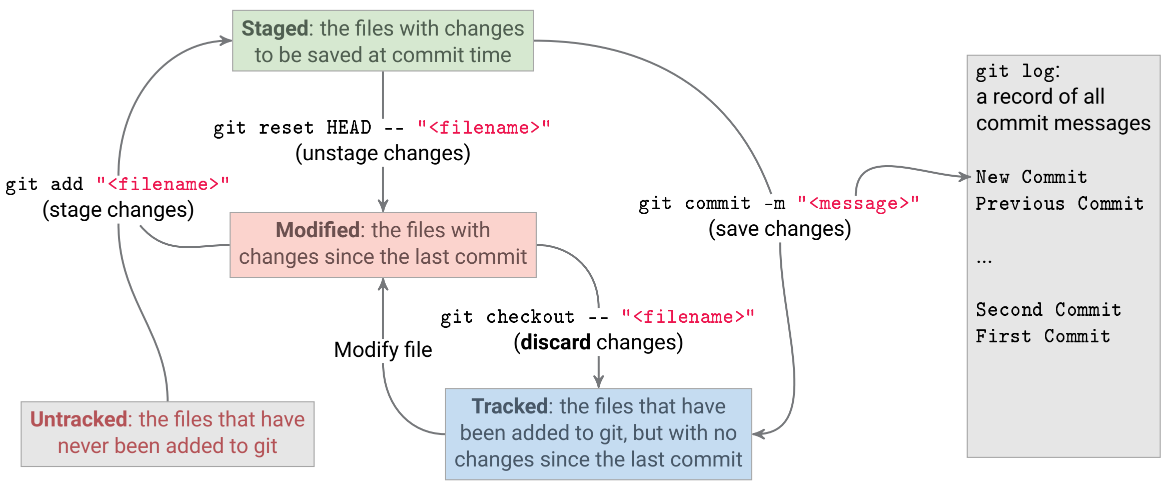


Figure A.1: Git commands to stage, unstage, save, or discard changes. Commit messages are recorded in the log.

All of these commands are done within a clone of the repository, stored somewhere on a computer. This repository must be manually synchronized with the online repository via two other git commands: git pull origin master, to pull updates from the web to the computer; and git push origin master, to push updates from the computer to the web.

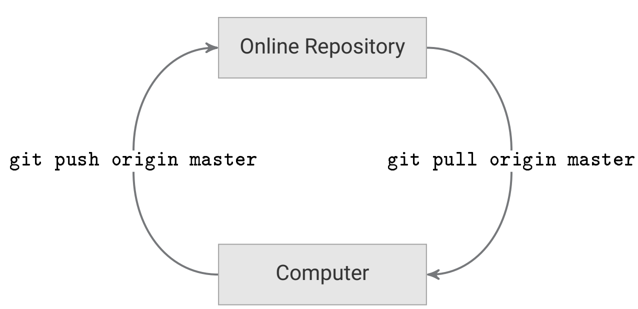


Figure A.2: Exchanging git commits between the repository and a local clone.

Command	Explanation
git status	Display the staging area and untracked changes.
git pull origin master	Pull changes from the online repository.
git push origin master	Push changes to the online repository.
git add <filename(s)>	Add a file or files to the staging area.
git add -u	Add all modified, tracked files to the staging area.
git commit -m "<message>"	Save the changes in the staging area with a given message.
git checkout -- <filename>	Revert changes to an unstaged file since the last commit.
git reset HEAD -- <filename>	Remove a file from the staging area.
git diff <filename>	See the changes to an unstaged file since the last commit.
git diff --cached <filename>	See the changes to a staged file since the last commit.
git config --local <option>	Record your credentials (user.name, user.email, etc.).

Table A.1: Common git commands.

Note

When pulling updates with git pull origin master, your terminal may sometimes display the following message.

```
Merge branch 'master' of https://bitbucket.org/<name>/<repo> into master

# Please enter a commit message to explain why this merge is necessary,
# especially if it merges an updated upstream into a topic branch.
#
# Lines starting with '#' will be ignored, and an empty message aborts
# the commit.
~
~
```

This means that someone else (the instructor) has pushed a commit that you do not yet have, while you have also made one or more commits locally that they do not have. This screen, displayed in *vim* (https://en.wikipedia.org/wiki/Vim_(text_editor)), is asking you to enter a message (or use the default message) to create a *merge commit* that will reconcile both changes. To close this screen and create the merge commit, type :wq and press enter.

Example Work Sessions

```
$ cd ~/Desktop/Student-Materials/
$ git pull origin master                           # Pull updates.
### Make changes to a file.
$ git add -u                                       # Track changes.
$ git commit -m "Made some changes."               # Commit changes.
$ git push origin master                           # Push updates.
```

```
# Pull any updates from the online repository (such as TA feedback).
$ cd ~/Desktop/Student-Materials/
$ git pull origin master
From https://bitbucket.org/username/repo
 * branch            master     -> FETCH_HEAD
Already up-to-date.

### Work on the labs. For example, modify PythonIntro/python_intro.py.

$ git status
On branch master
Your branch is up-to-date with 'origin/master'.
Changes not staged for commit:
  (use "git add <file>..." to update what will be committed)
  (use "git checkout -- <file>..." to discard changes in working directory)

    PythonIntro/python_intro.py

# Track the changes with git.
$ git add PythonIntro/python_intro.py
$ git status
On branch master
Your branch is up-to-date with 'origin/master'.
Changes to be committed:
  (use "git reset HEAD <file>..." to unstage)

    modified:   PythonIntro/python_intro.py

# Commit the changes to the repository with an informative message.
$ git commit -m "Made some changes"
[master fed9b34] Made some changes
 1 file changed, 10 insertion(+) 1 deletion(-)

# Push the changes to the online repository.
$ git push origin master
Counting objects: 3, done.
Delta compression using up to 2 threads.
Compressing objects: 100% (2/2), done.
Writing objects: 100% (3/3), 327 bytes | 0 bytes/s, done.
Total 3 (delta 0), reused 0 (delta 0)
To https://username@bitbucket.org/username/repo.git
   5742a1b..fed9b34  master -> master

$ git status
On branch master
Your branch is up-to-date with 'origin/master'.
nothing to commit, working directory clean
```

B Installing and Managing Python

Lab Objective: *One of the great advantages of Python is its lack of overhead: it is relatively easy to download, install, start up, and execute. This appendix introduces tools for installing and updating specific packages and gives an overview of possible environments for working efficiently in Python.*

Installing Python via Anaconda

A *Python distribution* is a single download containing everything needed to install and run Python, together with some common packages. For this curriculum, we **strongly** recommend using the *Anaconda* distribution to install Python. Anaconda includes IPython, a few other tools for developing in Python, and a large selection of packages that are common in applied mathematics, numerical computing, and data science. Anaconda is free and available for Windows, Mac, and Linux.

Follow these steps to install Anaconda.

1. Go to `https://www.anaconda.com/download/`.
2. Download the **Python 3.6** graphical installer specific to your machine.
3. Open the downloaded file and proceed with the default configurations.

For help with installation, see `https://docs.anaconda.com/anaconda/install/`. This page contains links to detailed step-by-step installation instructions for each operating system, as well as information for updating and uninstalling Anaconda.

> ACHTUNG!
>
> This curriculum uses Python 3.6, **not** Python 2.7. With the wrong version of Python, some example code within the labs may not execute as intended or result in an error.

Managing Packages

A *Python package manager* is a tool for installing or updating Python packages, which involves downloading the right source code files, placing those files in the correct location on the machine, and linking the files to the Python interpreter. **Never** try to install a Python package without using a package manager (see `https://xkcd.com/349/`).

Conda

Many packages are not included in the default Anaconda download but can be installed via Anaconda's package manager, `conda`. See `https://docs.anaconda.com/anaconda/packages/pkg-docs` for the complete list of available packages. When you need to update or install a package, **always** try using `conda` first.

Command	Description
`conda install <package-name>`	Install the specified package.
`conda update <package-name>`	Update the specified package.
`conda update conda`	Update `conda` itself.
`conda update anaconda`	Update **all** packages included in Anaconda.
`conda --help`	Display the documentation for `conda`.

For example, the following terminal commands attempt to install and update `matplotlib`.

```
$ conda update conda                # Make sure that conda is up to date.
$ conda install matplotlib          # Attempt to install matplotlib.
$ conda update matplotlib           # Attempt to update matplotlib.
```

See `https://conda.io/docs/user-guide/tasks/manage-pkgs.html` for more examples.

Note

The best way to ensure a package has been installed correctly is to try importing it in IPython.

```
# Start IPython from the command line.
$ ipython
IPython 6.5.0 -- An enhanced Interactive Python. Type '?' for help.

# Try to import matplotlib.
In [1]: from matplotlib import pyplot as plt      # Success!
```

Achtung!

Be careful not to attempt to update a Python package while it is in use. It is safest to update packages while the Python interpreter is not running.

Pip

The most generic Python package manager is called `pip`. While it has a larger package list, `conda` is the cleaner and safer option. Only use `pip` to manage packages that are not available through `conda`.

Command	Description
`pip install package-name`	Install the specified package.
`pip install --upgrade package-name`	Update the specified package.
`pip freeze`	Display the version number on all installed packages.
`pip --help`	Display the documentation for `pip`.

See `https://pip.pypa.io/en/stable/user_guide/` for more complete documentation.

Workflows

There are several different ways to write and execute programs in Python. Try a variety of workflows to find what works best for you.

Text Editor + Terminal

The most basic way of developing in Python is to write code in a text editor, then run it using either the Python or IPython interpreter in the terminal.

There are many different text editors available for code development. Many text editors are designed specifically for computer programming which contain features such as syntax highlighting and error detection, and are highly customizable. Try installing and using some of the popular text editors listed below.

- Atom: `https://atom.io/`
- Sublime Text: `https://www.sublimetext.com/`
- Notepad++ (Windows): `https://notepad-plus-plus.org/`
- Geany: `https://www.geany.org/`
- Vim: `https://www.vim.org/`
- Emacs: `https://www.gnu.org/software/emacs/`

Once Python code has been written in a text editor and saved to a file, that file can be executed in the terminal or command line.

```
$ ls                        # List the files in the current directory.
hello_world.py
$ cat hello_world.py        # Print the contents of the file to the terminal.
print("hello, world!")
$ python hello_world.py     # Execute the file.
hello, world!

# Alternatively, start IPython and run the file.
$ ipython
IPython 6.5.0 -- An enhanced Interactive Python. Type '?' for help.

In [1]: %run hello_world.py
hello, world!
```

IPython is an enhanced version of Python that is more user-friendly and interactive. It has many features that cater to productivity such as tab completion and object introspection.

> **Note**
>
> While Mac and Linux computers come with a built-in bash terminal, Windows computers do not. Windows does come with *Powershell*, a terminal-like application, but some commands in Powershell are different than their bash analogs, and some bash commands are missing from Powershell altogether. There are two good alternatives to the bash terminal for Windows:
>
> - Windows subsystem for linux: `docs.microsoft.com/en-us/windows/wsl/`.
> - Git bash: `https://gitforwindows.org/`.

Jupyter Notebook

The Jupyter Notebook (previously known as IPython Notebook) is a browser-based interface for Python that comes included as part of the Anaconda Python Distribution. It has an interface similar to the IPython interpreter, except that input is stored in cells and can be modified and re-evaluated as desired. See `https://github.com/jupyter/jupyter/wiki/` for some examples.

To begin using Jupyter Notebook, run the command `jupyter notebook` in the terminal. This will open your file system in a web browser in the Jupyter framework. To create a Jupyter Notebook, click the **New** drop down menu and choose **Python 3** under the **Notebooks** heading. A new tab will open with a new Jupyter Notebook.

Jupyter Notebooks differ from other forms of Python development in that notebook files contain not only the raw Python code, but also formatting information. As such, Juptyer Notebook files cannot be run in any other development environment. They also have the file extension `.ipynb` rather than the standard Python extension `.py`.

Jupyter Notebooks also support Markdown—a simple text formatting language—and $\LaTeX$, and can embedded images, sound clips, videos, and more. This makes Jupyter Notebook the ideal platform for presenting code.

Integrated Development Environments

An *integrated development environment* (IDEs) is a program that provides a comprehensive environment with the tools necessary for development, all combined into a single application. Most IDEs have many tightly integrated tools that are easily accessible, but come with more overhead than a plain text editor. Consider trying out each of the following IDEs.

- JupyterLab: `http://jupyterlab.readthedocs.io/en/stable/`
- PyCharm: `https://www.jetbrains.com/pycharm/`
- Spyder: `http://code.google.com/p/spyderlib/`
- Eclipse with PyDev: `http://www.eclipse.org/`, `https://www.pydev.org/`

See `https://realpython.com/python-ides-code-editors-guide/` for a good overview of these (and other) workflow tools.

C NumPy Visual Guide

Lab Objective: *NumPy operations can be difficult to visualize, but the concepts are straightforward. This appendix provides visual demonstrations of how NumPy arrays are used with slicing syntax, stacking, broadcasting, and axis-specific operations. Though these visualizations are for 1- or 2-dimensional arrays, the concepts can be extended to n-dimensional arrays.*

Data Access

The entries of a 2-D array are the rows of the matrix (as 1-D arrays). To access a single entry, enter the row index, a comma, and the column index. Remember that indexing begins with 0.

$$\texttt{A[0]} = \begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \end{bmatrix} \qquad \texttt{A[2,1]} = \begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \boxed{\times} & \times & \times & \times \\ \times & \times & \times & \times & \times \end{bmatrix}$$

Slicing

A lone colon extracts an entire row or column from a 2-D array. The syntax `[a:b]` can be read as "the ath entry up to (but not including) the bth entry." Similarly, `[a:]` means "the ath entry to the end" and `[:b]` means "everything up to (but not including) the bth entry."

$$\texttt{A[1]} = \texttt{A[1,:]} = \begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \end{bmatrix} \qquad \texttt{A[:,2]} = \begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \end{bmatrix}$$

$$\texttt{A[1:,:2]} = \begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \end{bmatrix} \qquad \texttt{A[1:-1,1:-1]} = \begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \end{bmatrix}$$

Stacking

`np.hstack()` stacks sequence of arrays horizontally and `np.vstack()` stacks a sequence of arrays vertically.

$$\texttt{A} = \begin{bmatrix} \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \end{bmatrix} \qquad \texttt{B} = \begin{bmatrix} * & * & * \\ * & * & * \\ * & * & * \end{bmatrix}$$

$$\texttt{np.hstack((A,B,A))} = \begin{bmatrix} \times & \times & \times & * & * & * & \times & \times & \times \\ \times & \times & \times & * & * & * & \times & \times & \times \\ \times & \times & \times & * & * & * & \times & \times & \times \end{bmatrix}$$

$$\texttt{np.vstack((A,B,A))} = \begin{bmatrix} \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \\ * & * & * \\ * & * & * \\ * & * & * \\ \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \end{bmatrix}$$

Because 1-D arrays are flat, `np.hstack()` concatenates 1-D arrays and `np.vstack()` stacks them vertically. To make several 1-D arrays into the columns of a 2-D array, use `np.column_stack()`.

$$\texttt{x} = \begin{bmatrix} \times & \times & \times & \times \end{bmatrix} \qquad \texttt{y} = \begin{bmatrix} * & * & * & * \end{bmatrix}$$

$$\texttt{np.hstack((x,y,x))} = \begin{bmatrix} \times & \times & \times & \times & * & * & * & * & \times & \times & \times & \times \end{bmatrix}$$

$$\texttt{np.vstack((x,y,x))} = \begin{bmatrix} \times & \times & \times & \times \\ * & * & * & * \\ \times & \times & \times & \times \end{bmatrix} \qquad \texttt{np.column\_stack((x,y,x))} = \begin{bmatrix} \times & * & \times \\ \times & * & \times \\ \times & * & \times \\ \times & * & \times \end{bmatrix}$$

The functions `np.concatenate()` and `np.stack()` are more general versions of `np.hstack()` and `np.vstack()`, and `np.row_stack()` is an alias for `np.vstack()`.

Broadcasting

NumPy automatically aligns arrays for component-wise operations whenever possible. See `http://docs.scipy.org/doc/numpy/user/basics.broadcasting.html` for more in-depth examples and broadcasting rules.

$$\texttt{A} = \begin{bmatrix} 1 & 2 & 3 \\ 1 & 2 & 3 \\ 1 & 2 & 3 \end{bmatrix} \qquad \texttt{x} = \begin{bmatrix} 10 & 20 & 30 \end{bmatrix}$$

$$\texttt{A + x} = \begin{matrix} \begin{bmatrix} 1 & 2 & 3 \\ 1 & 2 & 3 \\ 1 & 2 & 3 \end{bmatrix} \\ + \\ \begin{bmatrix} 10 & 20 & 30 \end{bmatrix} \end{matrix} = \begin{bmatrix} 11 & 22 & 33 \\ 11 & 22 & 33 \\ 11 & 22 & 33 \end{bmatrix}$$

$$\texttt{A + x.reshape((1,-1))} = \begin{bmatrix} 1 & 2 & 3 \\ 1 & 2 & 3 \\ 1 & 2 & 3 \end{bmatrix} + \begin{bmatrix} 10 \\ 20 \\ 30 \end{bmatrix} = \begin{bmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{bmatrix}$$

Operations along an Axis

Most array methods have an `axis` argument that allows an operation to be done along a given axis. To compute the sum of each column, use `axis=0`; to compute the sum of each row, use `axis=1`.

$$A = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \end{bmatrix}$$

$$\texttt{A.sum(axis=0)} = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \end{bmatrix} = \begin{bmatrix} 4 & 8 & 12 & 16 \end{bmatrix}$$

$$\texttt{A.sum(axis=1)} = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \end{bmatrix} = \begin{bmatrix} 10 & 10 & 10 & 10 \end{bmatrix}$$

D Plot Customization and Matplotlib Syntax Guide

Lab Objective: *The documentation for Matplotlib can be a little difficult to maneuver and basic information is sometimes difficult to find. This appendix condenses and demonstrates some of the more applicable and useful information on plot customizations. For an introduction to Matplotlib, see lab* **??**.

Colors

By default, every plot is assigned a different color specified by the "color cycle". It can be overwritten by specifying what color is desired in a few different ways.

•

Matplotlib recognizes some basic built-in colors.

Code	Color
'b'	blue
'g'	green
'r'	red
'c'	cyan
'm'	magenta
'y'	yellow
'k'	black
'w'	white

The following displays how these colors can be implemented. The result is displayed in Figure D.1.

```
import numpy as np
from matplotlib import pyplot as plt

colors = np.array(["k", "g", "b", "r", "c", "m", "y", "w"])
x = np.linspace(0, 5, 1000)
y = np.ones(1000)
```

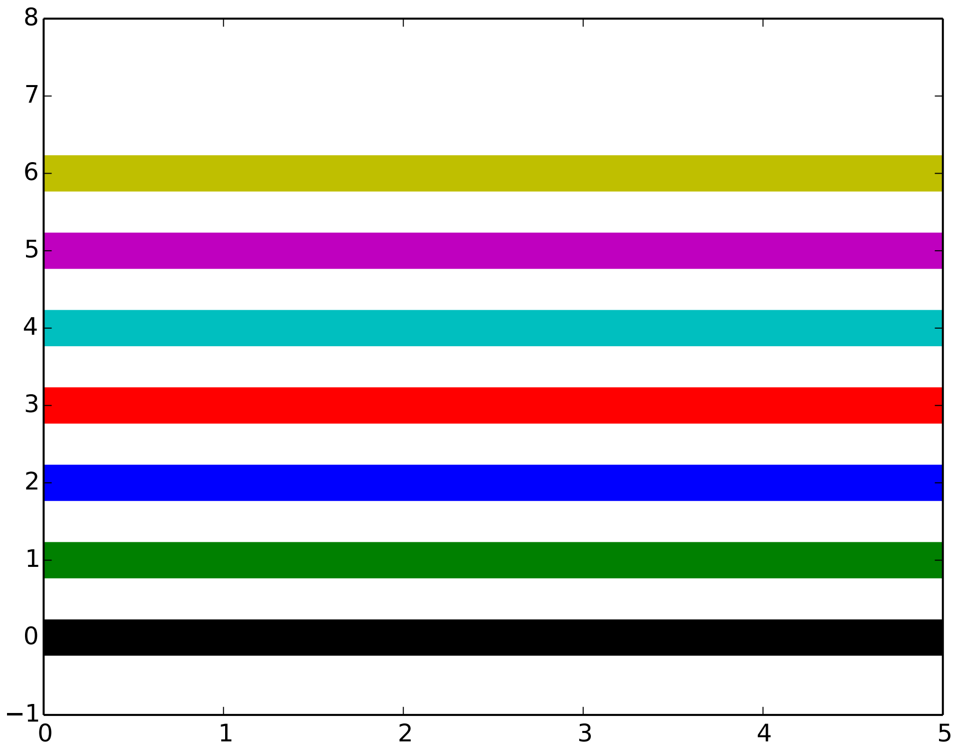


Figure D.1: A display of all the built-in colors.

```
for i in xrange(8):
    plt.plot(x, i*y, colors[i], linewidth=18)

plt.ylim([-1, 8])
plt.savefig("colors.pdf", format='pdf')
plt.clf()
```

colors.py

There are many other ways to specific colors. A popular method to access colors that are not built-in is to use a `RGB` tuple. Colors can also be specified using an html hex string or its associated html color name like `"DarkOliveGreen"`, `"FireBrick"`, `"LemonChiffon"`, `"MidnightBlue"`, `"PapayaWhip"`, or `"SeaGreen"`.

Window Limits

You may have noticed the use of `plt.ylim([ymin, ymax])` in the previous code. This explicitly sets the boundary of the y-axis. Similarily, `plt.xlim([xmin, xmax])` can be used to set the boundary of the x-axis. Doing both commands simultaneously is possible with the `plt.axis([xmin, xmax, ymin, ymax])`. Remember that these commands must be executed after the plot.

Lines

Thickness

You may have noticed that the width of the lines above seemed thin considering we wanted to inspect the line color. `linewidth` is a keyword argument that is defaulted to be `None` but can be given any real number to adjust the line width.

The following displays how `linewidth` is implemented. It is displayed in Figure D.2.

```
lw = np.linspace(.5, 15, 8)

for i in xrange(8):
    plt.plot(x, i*y, colors[i], linewidth=lw[i])

plt.ylim([-1, 8])
plt.show()
```

linewidth.py

Style

By default, plots are drawn with a solid line. The following are accepted format string characters to indicate line style.

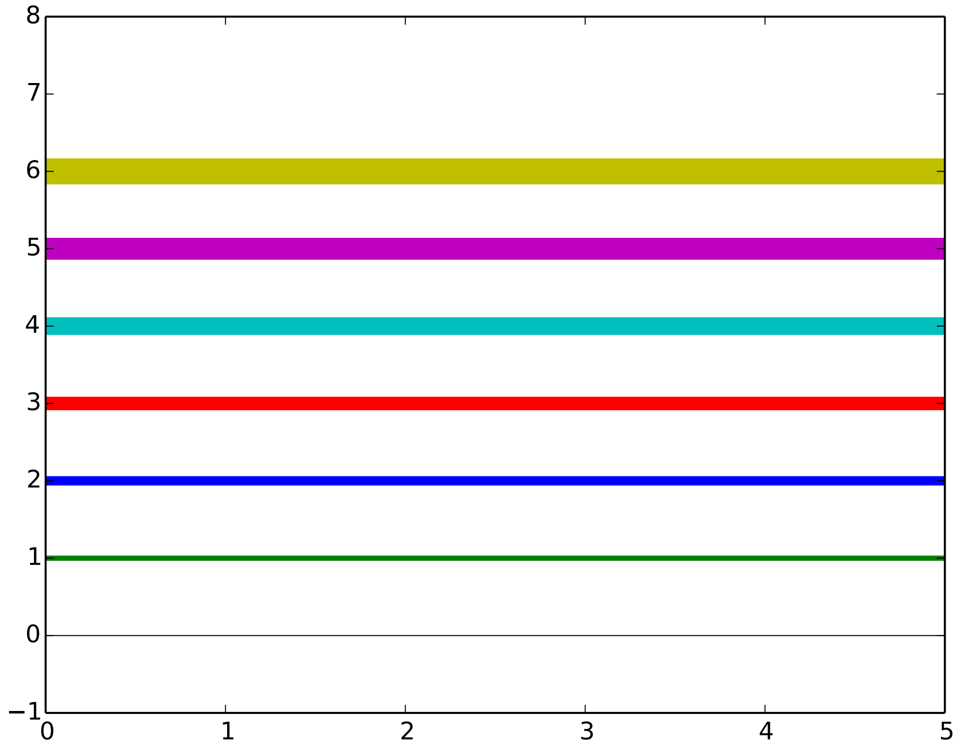


Figure D.2: plot of varying linewidths.

character	description
-	solid line style
--	dashed line style
-.	dash-dot line style
:	dotted line style
.	point marker
,	pixel marker
o	circle marker
v	triangle_down marker
^	triangle_up marker
<	triangle_left marker
>	triangle_right marker
1	tri_down marker
2	tri_up marker
3	tri_left marker
4	tri_right marker
s	square marker
p	pentagon marker
*	star marker
h	hexagon1 marker
H	hexagon2 marker
+	plus marker
x	x marker
D	diamond marker
d	thin_diamond marker
|	vline marker
_	hline marker

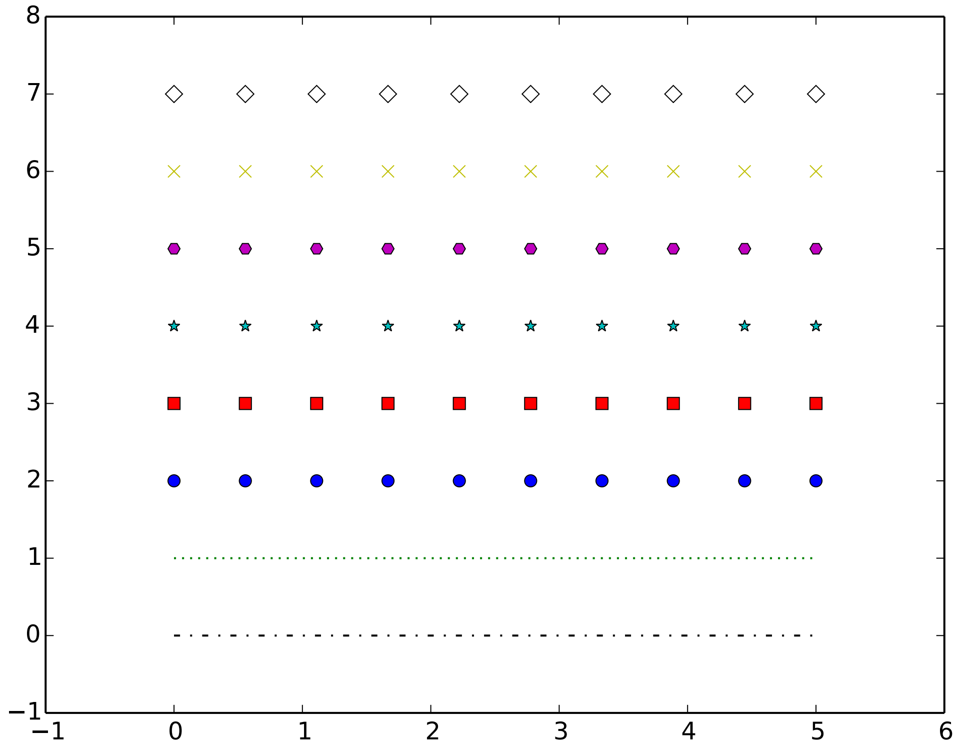


Figure D.3: plot of varying linestyles.

The following displays how `linestyle` can be implemented. It is displayed in Figure D.3.

```
x = np.linspace(0, 5, 10)
y = np.ones(10)
ls = np.array(['-.', ':', 'o', 's', '*', 'H', 'x', 'D'])

for i in xrange(8):
    plt.plot(x, i*y, colors[i]+ls[i])

plt.axis([-1, 6, -1, 8])
plt.show()
```

linestyle.py

Text

It is also possible to add text to your plots. To label your axes, the `plt.xlabel()` and the `plt.ylabel()` can both be used. The function `plt.title()` will add a title to a plot. If you are working with subplots, this command will add a title to the subplot you are currently modifying. To add a title above the entire figure, use `plt.suptitle()`.

All of the `text()` commands can be customized with `fontsize` and `color` keyword arguments.

We can add these elements to our previous example. It is displayed in Figure D.4.

```
for i in xrange(8):
    plt.plot(x, i*y, colors[i]+ls[i])

plt.title("My Plot of Varying Linestyles", fontsize = 20, color = "gold")
plt.xlabel("x-axis", fontsize = 10, color = "darkcyan")
plt.ylabel("y-axis", fontsize = 10, color = "darkcyan")

plt.axis([-1, 6, -1, 8])
plt.show()
```

text.py

See `http://matplotlib.org` for Matplotlib documentation.

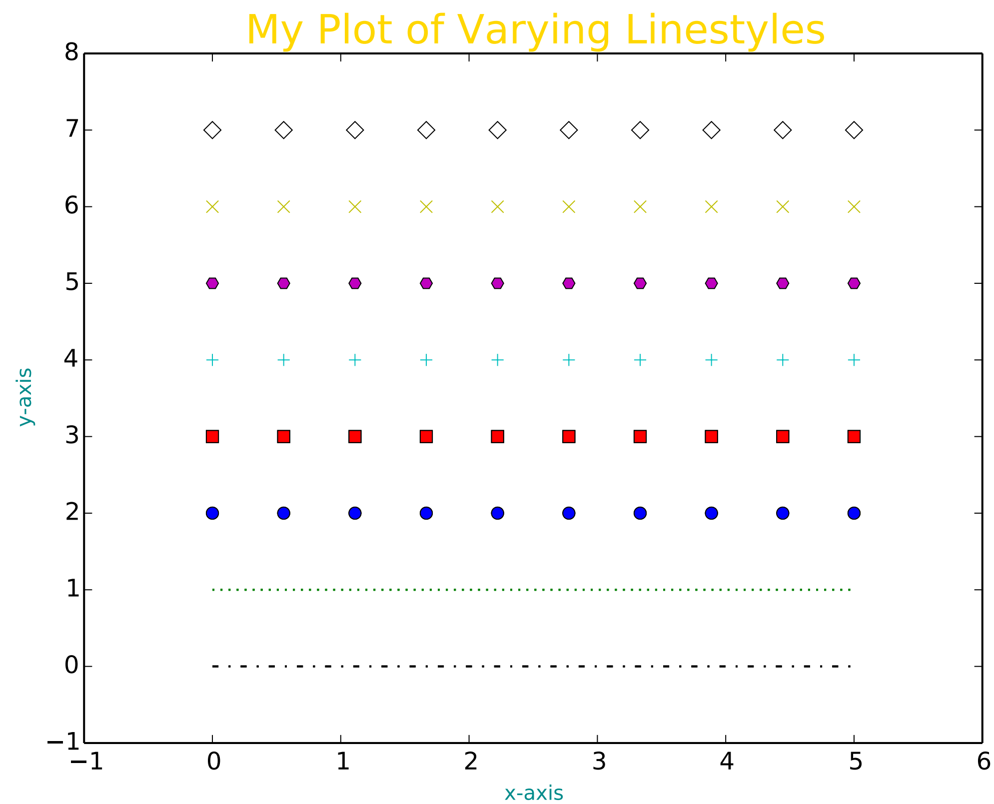


Figure D.4: plot of varying linestyles using text labels.

Bibliography

[ADH+01] David Ascher, Paul F Dubois, Konrad Hinsen, Jim Hugunin, Travis Oliphant, et al. Numerical python, 2001.

[Hun07] J. D. Hunter. Matplotlib: A 2d graphics environment. *Computing In Science & Engineering*, 9(3):90–95, 2007.

[Kim09] Seongjai Kim. Edge-preserving noise removal, part i: Second order anisotropic diffusion. Technical report, University of Kentucky Department of Mathematics, 2009.

[LeV02] Randall J. LeVeque. *Finite volume methods for hyperbolic problems*. Cambridge Texts in Applied Mathematics. Cambridge University Press, Cambridge, 2002.

[Oli06] Travis E Oliphant. *A guide to NumPy*, volume 1. Trelgol Publishing USA, 2006.

[Oli07] Travis E Oliphant. Python for scientific computing. *Computing in Science & Engineering*, 9(3), 2007.

[PM88] Pietro Perona and Jitendra Malik. Scale-space and edge detection using anisotropic diffusion. Technical Report UCB/CSD-88-483, EECS Department, University of California, Berkeley, Dec 1988.

[VD10] Guido VanRossum and Fred L Drake. *The python language reference*. Python software foundation Amsterdam, Netherlands, 2010.