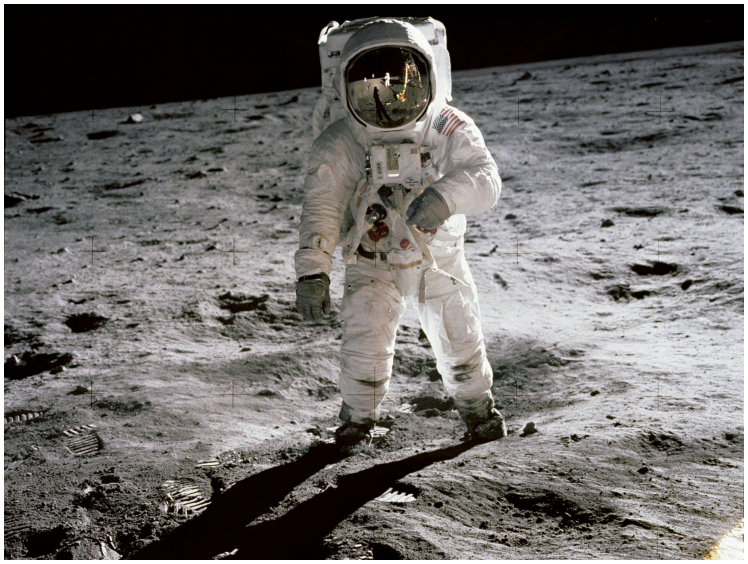
Labs for Foundations of Applied Mathematics

Volume I
Mathematical Analysis



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Preface

This lab manual is designed to accompany the textbook *Foundations of Applied Mathematics* by Humpherys, Jarvis and Evans.

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Part I

Labs

1 Linear Transformations

Lab Objective: *Linear transformations are the most basic and essential operators in vector space theory. In this lab we visually explore how linear transformations alter points in the Cartesian plane. We also empirically explore the computational cost of applying linear transformations via matrix multiplication.*

Linear Transformations

A *linear transformation* is a mapping between vector spaces that preserves addition and scalar multiplication. More precisely, let V and W be vector spaces over a common field $\mathbb{F}$. A map $L : V \to W$ is a linear transformation from V into W if

$$L(a\mathbf{x}_1 + b\mathbf{x}_2) = aL\mathbf{x}_1 + bL\mathbf{x}_2$$

for all vectors $\mathbf{x}_1,\ \mathbf{x}_2 \in V$ and scalars $a,\ b \in \mathbb{F}$.

Every linear transformation L from an m-dimensional vector space into an n-dimensional vector space can be represented by an $m \times n$ matrix A, called the *matrix representation* of L. To apply L to a vector $\mathbf{x}$, left multiply by its matrix representation. This results in a new vector $\mathbf{x}'$, where each component is some linear combination of the elements of $\mathbf{x}$. For linear transformations from $\mathbb{R}^2$ to $\mathbb{R}^2$, this process has the following form.

$$A\mathbf{x} = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} ax + by \\ cx + dy \end{bmatrix} = \begin{bmatrix} x' \\ y' \end{bmatrix} = \mathbf{x}'$$

Linear transformations can be interpreted geometrically. To demonstrate this, consider the array of points H that collectively form a picture of a horse, stored in the file `horse.npy`. The coordinate pairs $\mathbf{x}_i$ are organized by column, so the array has two rows: one for x-coordinates, and one for y-coordinates. Matrix multiplication on the left transforms each coordinate pair, resulting in another matrix H' whose columns are the transformed coordinate pairs.

$$AH = A\begin{bmatrix} x_1 & x_2 & x_3 & \dots \\ y_1 & y_2 & y_3 & \dots \end{bmatrix} = A\left[\begin{array}{c|c|c|c} \mathbf{x}_1 & \mathbf{x}_2 & \mathbf{x}_3 & \dots \end{array}\right] = \left[\begin{array}{c|c|c|c} A\mathbf{x}_1 & A\mathbf{x}_2 & A\mathbf{x}_3 & \dots \end{array}\right]$$
$$= \left[\begin{array}{c|c|c|c} \mathbf{x}_1' & \mathbf{x}_2' & \mathbf{x}_3' & \dots \end{array}\right] = \begin{bmatrix} x_1' & x_2' & x_3' & \dots \\ y_1' & y_2' & y_3' & \dots \end{bmatrix} = H'$$

To begin, use `np.load()` to extract the array from the `.npy` file, then plot the unaltered points as individual pixels. See Figure 1.1 for the result.

```
>>> import numpy as np
>>> from matplotlib import pyplot as plt

# Load the array from the .npy file.
>>> data = np.load("horse.npy")

# Plot the x row against the y row with black pixels.
>>> plt.plot(data[0], data[1], 'k,')

# Set the window limits to [-1, 1] by [-1, 1] and make the window square.
>>> plt.axis([-1,1,-1,1])
>>> plt.gca().set_aspect("equal")
>>> plt.show()
```

Types of Linear Transformations

Linear transformations from $\mathbb{R}^2$ into $\mathbb{R}^2$ can be classified in a few ways.

- **Stretch**: Stretches or compresses the vector along each axis. The matrix representation is diagonal:

$$\begin{bmatrix} a & 0 \\ 0 & b \end{bmatrix}$$

  If $a = b$, the transformation is called a *dilation*. The stretch in Figure 1.1 uses $a = \frac{1}{2}$ and $b = \frac{6}{5}$ to compress the x-axis and stretch the y-axis.

- **Shear**: Slants the vector by a scalar factor horizontally or vertically. There are two matrix representations:

$$\text{horizontal shear: } \begin{bmatrix} 1 & a \\ 0 & 1 \end{bmatrix} \qquad \text{vertical shear: } \begin{bmatrix} 1 & 0 \\ b & 1 \end{bmatrix}$$

  Horizontal shears skew the x-coordinate of the vector while vertical shears skew the y-coordinate. Figure 1.1 has a horizontal shear with $a = \frac{1}{2}$.

- **Reflection**: Reflects the vector about a line that passes through the origin. The reflection about the line spanned by the vector $[a, b]^\mathsf{T}$ has the matrix representation

$$\frac{1}{a^2 + b^2} \begin{bmatrix} a^2 - b^2 & 2ab \\ 2ab & b^2 - a^2 \end{bmatrix}.$$

  The reflection in Figure 1.1 reflects the image about the y-axis ($a = 0$, $b = 1$).

- **Rotation**: Rotates the vector around the origin. A counterclockwise rotation of θ radians has the following matrix representation:

$$\begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}$$

  A negative value of θ performs a clockwise rotation. Choosing $\theta = \frac{\pi}{2}$ produces the rotation in Figure 1.1.

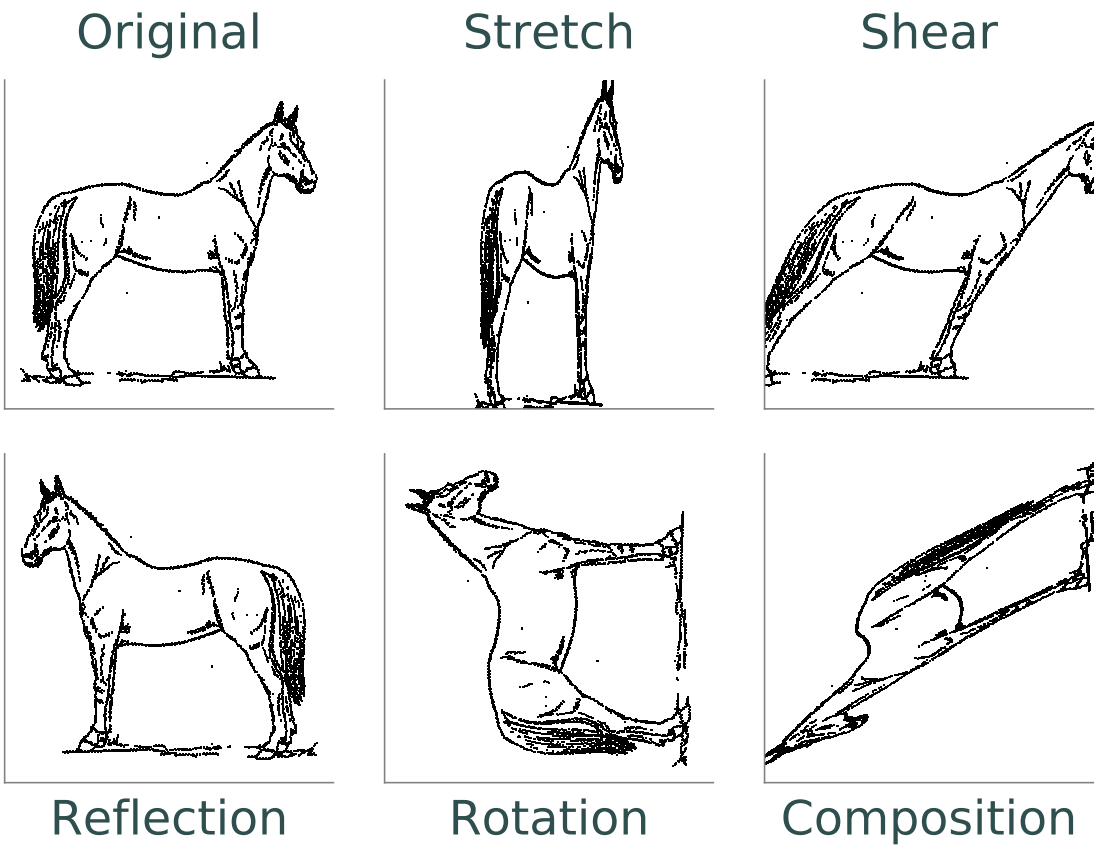


Figure 1.1: The points stored in `horse.npy` under various linear transformations.

Problem 1. Write a function for each type of linear transformation. Each function should accept an array to transform and the scalars that define the transformation (a and b for stretch, shear, and reflection, and θ for rotation). Construct the matrix representation, left multiply it with the input array, and return the transformed array.

To test these functions, write a function to plot the original points in `horse.npy` together with the transformed points in subplots for a side-by-side comparison. Compare your results to Figure 1.1.

Compositions of Linear Transformations

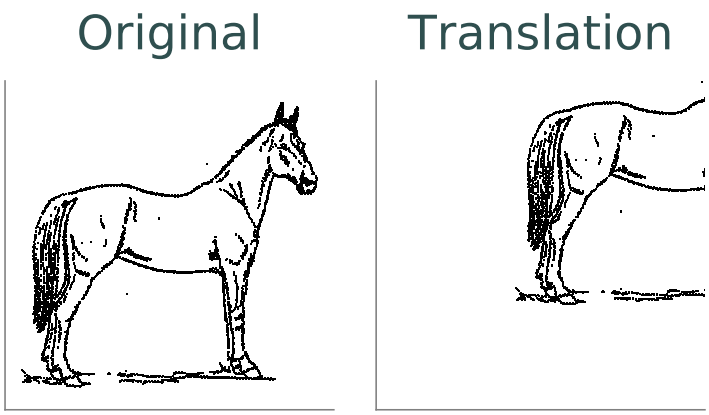
Let V, W, and Z be finite-dimensional vector spaces. If $L : V \to W$ and $K : W \to Z$ are linear transformations with matrix representations A and B, respectively, then the *composition* function $KL : V \to Z$ is also a linear transformation, and its matrix representation is the matrix product BA.

For example, if S is a matrix representing a shear and R is a matrix representing a rotation, then RS represents a shear followed by a rotation. In fact, any linear transformation $L : \mathbb{R}^2 \to \mathbb{R}^2$ is a composition of the four transformations discussed above. Figure 1.1 displays the composition of all four previous transformations, applied in order (stretch, shear, reflection, then rotation).

Affine Transformations

All linear transformations map the origin to itself. An *affine transformation* is a mapping between vector spaces that preserves the relationships between points and lines, but that may not preserve the origin. Every affine transformation T can be represented by a matrix A and a vector $\mathbf{b}$. To apply T to a vector x, calculate $A\mathbf{x}+\mathbf{b}$. If $\mathbf{b}=\mathbf{0}$ then the transformation is linear, and if $A=I$ but $\mathbf{b}\neq\mathbf{0}$ then it is called a *translation*.

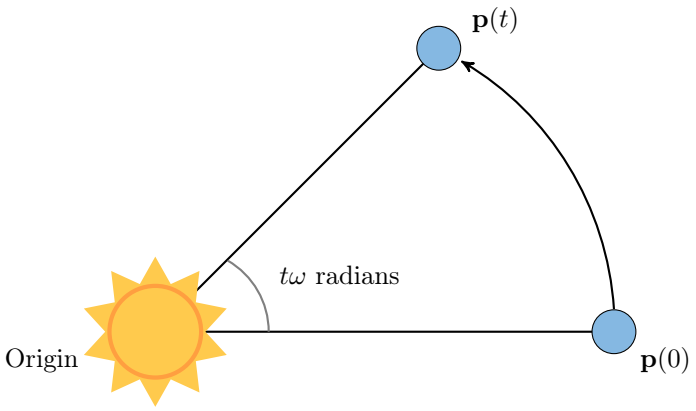
For example, if T is the translation with $\mathbf{b}=\left[\frac{3}{4},\frac{1}{2}\right]^{\mathsf{T}}$, then applying T to an image will shift it right by $\frac{3}{4}$ and up by $\frac{1}{2}$. This translation is illustrated below.



Affine transformations include all compositions of stretches, shears, rotations, reflections, and translations. For example, if S represents a shear and R a rotation, and if $\mathbf{b}$ is a vector, then $RS\mathbf{x}+\mathbf{b}$ shears, then rotates, then translates $\mathbf{x}$.

Modeling Motion with Affine Transformations

Affine transformations can be used to model particle motion, such as a planet rotating around the sun. Let the sun be the origin, the planet's location at time t be given by the vector $\mathbf{p}(t)$, and suppose the planet has angular momentum ω (a measure of how fast the planet goes around the sun). To find the planet's position at time t given the planet's initial position $\mathbf{p}(0)$, rotate the vector $\mathbf{p}(0)$ around the origin by $t\omega$ radians. Thus if $R(\theta)$ is the matrix representation of the linear transformation that rotates a vector around the origin by θ radians, then $\mathbf{p}(t)=R(t\omega)\mathbf{p}(0)$.



Composing the rotation with a translation shifts the center of rotation away from the origin, yielding more complicated motion.

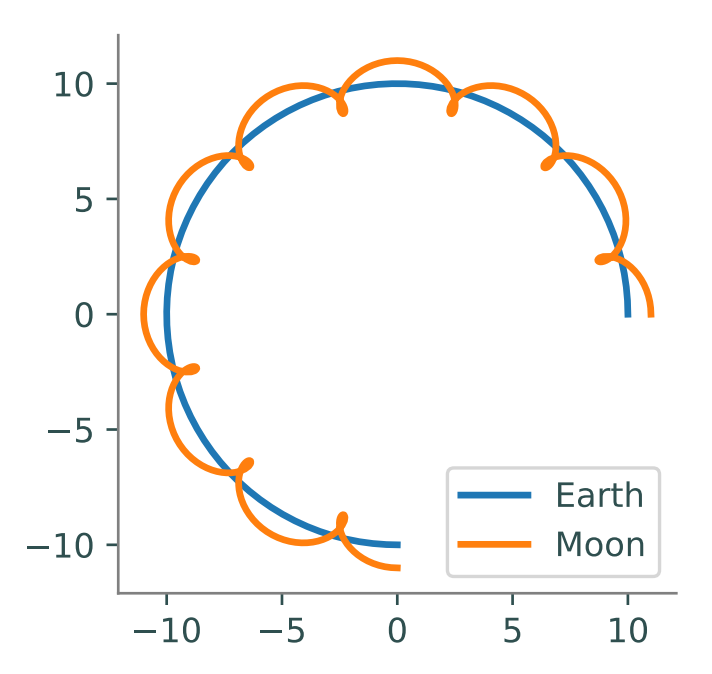
Problem 2. The moon orbits the earth while the earth orbits the sun. Assuming circular orbits, we can compute the trajectories of both the earth and the moon using only linear and affine transformations.

Assume an orientation where both the earth and moon travel counterclockwise, with the sun at the origin. Let $\mathbf{p}_e(t)$ and $\mathbf{p}_m(t)$ be the positions of the earth and the moon at time t, respectively, and let ω_e and ω_m be each celestial body's angular momentum. For a particular time t, we calculate $\mathbf{p}_e(t)$ and $\mathbf{p}_m(t)$ with the following steps:

1. Compute $\mathbf{p}_e(t)$ by rotating the initial vector $\mathbf{p}_e(0)$ counterclockwise about the origin by $t\omega_e$ radians.
2. Calculate the position of the moon relative to the earth at time t by rotating the vector $\mathbf{p}_m(0) - \mathbf{p}_e(0)$ counterclockwise about the origin by $t\omega_m$ radians.
3. To compute $\mathbf{p}_m(t)$, translate the vector resulting from the previous step by $\mathbf{p}_e(t)$.

Write a function that accepts a final time T and the angular momenta ω_e and ω_m. Assuming initial positions $\mathbf{p}_e(0) = (10, 0)$ and $\mathbf{p}_m(0) = (11, 0)$, plot $\mathbf{p}_e(t)$ and $\mathbf{p}_m(t)$ over the time interval $t \in [0, T]$.

The moon travels around the earth approximately 13 times every year. With $T = \frac{3\pi}{2}$, $\omega_e = 1$, and $\omega_m = 13$, your plot should resemble the following figure (fix the aspect ratio with `ax.set_aspect("equal")`).



Timing Matrix Operations

Linear transformations are easy to perform via matrix multiplication. However, performing matrix multiplication with very large matrices can strain a machine's time and memory constraints. For the remainder of this lab we take an empirical approach in exploring how much time and memory different matrix operations require.

Timing Code

Recall that the `time` module's `time()` function measures the number of seconds since the Epoch. To measure how long it takes for code to run, record the time just before and just after the code in question, then subtract the first measurement from the second to get the number of seconds that have passed. Additionally, in IPython, the quick command `%timeit` uses the `timeit` module to quickly time a single line of code.

```
In [1]: import time

In [2]: def for_loop():
   ...:     """Go through ten million iterations of nothing."""
   ...:     for _ in range(int(1e7)):
   ...:         pass

In [3]: def time_for_loop():
   ...:     """Time for_loop() with time.time()."""
   ...:     start = time.time()             # Clock the starting time.
   ...:     for_loop()
   ...:     return time.time() - start      # Return the elapsed time.

In [4]: time_for_loop()
0.24458789825439453

In [5]: %timeit for_loop()
248 ms +- 5.35 ms per loop (mean +- std. dev. of 7 runs, 1 loop each)
```

Timing an Algorithm

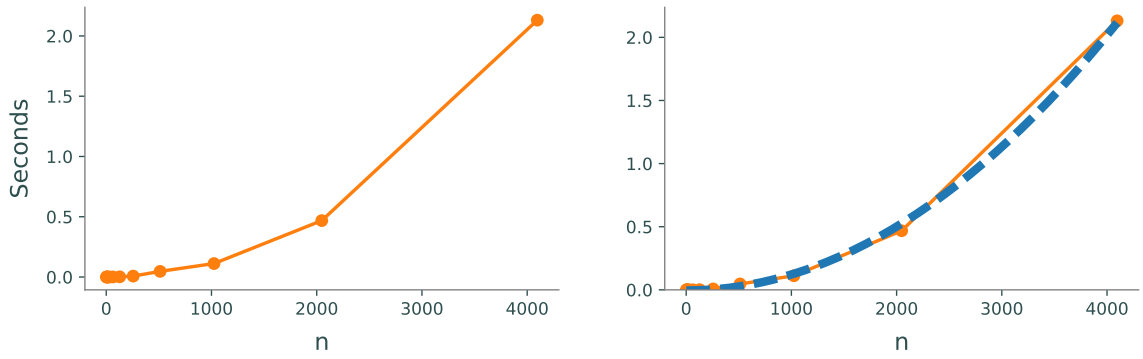
Most algorithms have at least one input that dictates the size of the problem to be solved. For example, the following functions take in a single integer n and produce a random vector of length n as a list or a random $n \times n$ matrix as a list of lists.

```
from random import random
def random_vector(n):       # Equivalent to np.random.random(n).tolist()
    """Generate a random vector of length n as a list."""
    return [random() for i in range(n)]

def random_matrix(n):       # Equivalent to np.random.random((n,n)).tolist()
    """Generate a random nxn matrix as a list of lists."""
    return [[random() for j in range(n)] for i in range(n)]
```

Executing `random_vector(n)` calls `random()` n times, so doubling n should about double the amount of time `random_vector(n)` takes to execute. By contrast, executing `random_matrix(n)` calls `random()` n^2 times (n times per row with n rows). Therefore doubling n will likely more than double the amount of time `random_matrix(n)` takes to execute, especially if n is large.

To visualize this phenomenon, we time `random_matrix()` for $n = 2^1,\ 2^2,\ \ldots,\ 2^{12}$ and plot n against the execution time. The result is displayed below on the left.

```
>>> domain = 2**np.arange(1,13)
>>> times = []
>>> for n in domain:
...     start = time.time()
...     random_matrix(n)
...     times.append(time.time() - start)
...
>>> plt.plot(domain, times, 'g.-', linewidth=2, markersize=15)
>>> plt.xlabel("n", fontsize=14)
>>> plt.ylabel("Seconds", fontsize=14)
>>> plt.show()
```



The figure on the left shows that the execution time for `random_matrix(n)` increases quadratically in n. In fact, the blue dotted line in the figure on the right is the parabola $y = an^2$, which fits nicely over the timed observations. Here a is a small constant, but it is much less significant than the exponent on the n. To represent this algorithm's growth, we ignore a altogether and write `random_matrix(n)` $\sim n^2$.

Note

An algorithm like `random_matrix(n)` whose execution time increases quadratically with n is called $O(n^2)$, notated by `random_matrix(n)` $\in O(n^2)$. Big-oh notation is common for indicating both the *temporal complexity* of an algorithm (how the execution time grows with n) and the *spatial complexity* (how the memory usage grows with n).

Problem 3. Let A be an $m \times n$ matrix with entries a_{ij}, $\mathbf{x}$ be an $n \times 1$ vector with entries x_k, and B be an $n \times p$ matrix with entries b_{ij}. The matrix-vector product $A\mathbf{x} = \mathbf{y}$ is a new $m \times 1$ vector and the matrix-matrix product $AB = C$ is a new $m \times p$ matrix. The entries y_i of $\mathbf{y}$ and c_{ij} of C are determined by the following formulas:

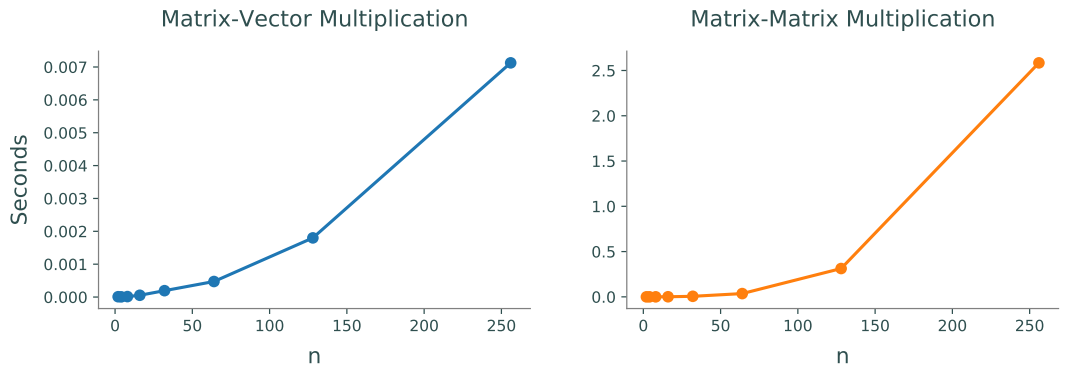
$$y_i = \sum_{k=1}^{n} a_{ik}x_k \qquad\qquad c_{ij} = \sum_{k=1}^{n} a_{ik}b_{kj}$$

These formulas are implemented below **without** using NumPy arrays or operations.

```
def matrix_vector_product(A, x):    # Equivalent to np.dot(A,x).tolist()
    """Compute the matrix-vector product Ax as a list."""
    m, n = len(A), len(x)
    return [sum([A[i][k] * x[k] for k in range(n)]) for i in range(m)]

def matrix_matrix_product(A, B):    # Equivalent to np.dot(A,B).tolist()
    """Compute the matrix-matrix product AB as a list of lists."""
    m, n, p = len(A), len(B), len(B[0])
    return [[sum([A[i][k] * B[k][j] for k in range(n)])
                                    for j in range(p) ]
                                    for i in range(m) ]
```

Time each of these functions with increasingly large inputs. Generate the inputs A, $\mathbf{x}$, and B with `random_matrix()` and `random_vector()` (so each input will be $n \times n$ or $n \times 1$). Only time the multiplication functions, not the generating functions.

Report your findings in a single figure with two subplots: one with matrix-vector times, and one with matrix-matrix times. Choose a domain for n so that your figure accurately describes the growth, but avoid values of n that lead to execution times of more than 1 minute. Your figure should resemble the following plots.



Logarithmic Plots

Though the two plots from Problem 3 look similar, the scales on the y-axes show that the actual execution times differ greatly. To be compared correctly, the results need to be viewed differently.

A *logarithmic plot* uses a logarithmic scale—with values that increase exponentially, such as 10^1, 10^2, 10^3, ...—on one or both of its axes. The three kinds of log plots are listed below.

- **log-lin**: the x-axis uses a logarithmic scale but the y-axis uses a linear scale.
  Use `plt.semilogx()` instead of `plt.plot()`.
- **lin-log**: the x-axis is uses a linear scale but the y-axis uses a log scale.
  Use `plt.semilogy()` instead of `plt.plot()`.
- **log-log**: both the x and y-axis use a logarithmic scale.
  Use `plt.loglog()` instead of `plt.plot()`.

Since the domain $n = 2^1, 2^2, \ldots$ is a logarithmic scale and the execution times increase quadratically, we visualize the results of the previous problem with a log-log plot. The default base for the logarithmic scales on logarithmic plots in Matplotlib is 10. To change the base to 2 on each axis, specify the keyword arguments `basex=2` and `basey=2`.

Suppose the domain of n values are stored in `domain` and the corresponding execution times for `matrix_vector_product()` and `matrix_matrix_product()` are stored in `vector_times` and `matrix_times`, respectively. Then the following code produces Figure 1.5.

```
>>> ax1 = plt.subplot(121)  # Plot both curves on a regular lin-lin plot.
>>> ax1.plot(domain, vector_times, 'b.-', lw=2, ms=15, label="Matrix-Vector")
>>> ax1.plot(domain, matrix_times, 'g.-', lw=2, ms=15, label="Matrix-Matrix")
>>> ax1.legend(loc="upper left")

>>> ax2 = plot.subplot(122) # Plot both curves on a base 2 log-log plot.
>>> ax2.loglog(domain, vector_times, 'b.-', basex=2, basey=2, lw=2)
>>> ax2.loglog(domain, matrix_times, 'g.-', basex=2, basey=2, lw=2)

>>> plt.show()
```

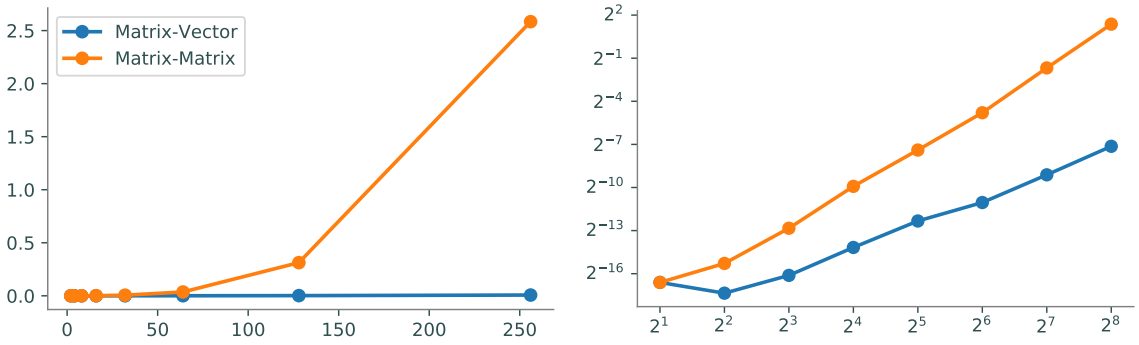


Figure 1.5

In the log-log plot, the slope of the `matrix_matrix_product()` line is about 3 and the slope of the `matrix_vector_product()` line is about 2. This reflects the fact that matrix-matrix multiplication (which uses 3 loops) is $O(n^3)$, while matrix-vector multiplication (which only has 2 loops) is only $O(n^2)$.

Problem 4. NumPy is built specifically for fast numerical computations. Repeat the experiment of Problem 3, timing the following operations:

- matrix-vector multiplication with `matrix_vector_product()`.
- matrix-matrix multiplication with `matrix_matrix_product()`.
- matrix-vector multiplication with `np.dot()` or `@`.
- matrix-matrix multiplication with `np.dot()` or `@`.

Create a single figure with two subplots: one with all four sets of execution times on a regular linear scale, and one with all four sets of execution times on a log-log scale. Compare your results to Figure 1.5.

Note

Problem 4 shows that **matrix operations are significantly faster in NumPy than in plain Python**. Matrix-matrix multiplication grows cubically regardless of the implementation; however, with lists the times grows at a rate of an^3 while with NumPy the times grow at a rate of bn^3, where a is much larger than b. NumPy is more efficient for several reasons:

1. Iterating through loops is very expensive. Many of NumPy's operations are implemented in C, which are much faster than Python loops.
2. Arrays are designed specifically for matrix operations, while Python lists are general purpose.
3. NumPy takes careful advantage of computer hardware, efficiently using different levels of computer memory.

However, in Problem 4, the execution times for matrix multiplication with NumPy seem to increase somewhat inconsistently. This is because the fastest layer of computer memory can only handle so much information before the computer has to begin using a larger, slower layer of memory.

Additional Material

Image Transformation as a Class

Consider organizing the functions from Problem 1 into a class. The constructor might accept an array or the name of a file containing an array. This structure would makes it easy to do several linear or affine transformations in sequence.

```
>>> horse = ImageTransformer("horse.npy")
>>> horse.stretch(.5, 1.2)
>>> horse.shear(.5, 0)
>>> horse.relect(0, 1)
>>> horse.rotate(np.pi/2.)
>>> horse.translate(.75, .5)
>>> horse.display()
```

Animating Parametrizations

The plot in Problem 2 fails to fully convey the system's evolution over time because time itself is not part of the plot. The following function creates an animation for the earth and moon trajectories.

```
from matplotlib.animation import FuncAnimation

def solar_system_animation(earth, moon):
    """Animate the moon orbiting the earth and the earth orbiting the sun.
    Parameters:
        earth ((2,N) ndarray): The earth's postion with x-coordinates on the
            first row and y coordinates on the second row.
        moon ((2,N) ndarray): The moon's postion with x-coordinates on the
            first row and y coordinates on the second row.
    """
    fig, ax = plt.subplots(1,1)                     # Make a figure explicitly.
    plt.axis([-15,15,-15,15])                       # Set the window limits.
    ax.set_aspect("equal")                          # Make the window square.
    earth_dot,  = ax.plot([],[], 'bo', ms=10)       # Blue dot for the earth.
    earth_path, = ax.plot([],[], 'b-')              # Blue line for the earth.
    moon_dot,   = ax.plot([],[], 'go', ms=5)        # Green dot for the moon.
    moon_path,  = ax.plot([],[], 'g-')              # Green line for the moon.
    ax.plot([0],[0],'y*', ms=30)                    # Yellow star for the sun.

    def animate(index):
        earth_dot.set_data(earth[0,index], earth[1,index])
        earth_path.set_data(earth[0,:index], earth[1,:index])
        moon_dot.set_data(moon[0,index], moon[1,index])
        moon_path.set_data(moon[0,:index], moon[1,:index])
        return earth_dot, earth_path, moon_dot, moon_path,
    a = FuncAnimation(fig, animate, frames=earth.shape[1], interval=25)
    plt.show()
```

2 Linear Systems

Lab Objective: *The fundamental problem of linear algebra is solving the linear system $A\mathbf{x} = \mathbf{b}$, given that a solution exists. There are many approaches to solving this problem, each with different pros and cons. In this lab we implement the LU decomposition and use it to solve square linear systems. We also introduce SciPy, together with its libraries for linear algebra and working with sparse matrices.*

Gaussian Elimination

The standard approach for solving the linear system $A\mathbf{x} = \mathbf{b}$ on paper is reducing the augmented matrix $[A \mid \mathbf{b}]$ to row-echelon form (REF) via *Gaussian elimination*, then using back substitution. The matrix is in REF when the leading non-zero term in each row is the diagonal term, so the matrix is upper triangular.

At each step of Gaussian elimination, there are three possible operations: swapping two rows, multiplying one row by a scalar value, or adding a scalar multiple of one row to another. Many systems, like the one displayed below, can be reduced to REF using only the third type of operation. First, use multiples of the first row to get zeros below the diagonal in the first column, then use a multiple of the second row to get zeros below the diagonal in the second column.

$$\left[\begin{array}{ccc|c} 1 & 1 & 1 & 1 \\ 1 & 4 & 2 & 3 \\ 4 & 7 & 8 & 9 \end{array}\right] \longrightarrow \left[\begin{array}{ccc|c} 1 & 1 & 1 & 1 \\ 0 & 3 & 1 & 2 \\ 4 & 7 & 8 & 9 \end{array}\right] \longrightarrow \left[\begin{array}{ccc|c} 1 & 1 & 1 & 1 \\ 0 & 3 & 1 & 2 \\ 0 & 3 & 4 & 5 \end{array}\right] \longrightarrow \left[\begin{array}{ccc|c} 1 & 1 & 1 & 1 \\ 0 & 3 & 1 & 2 \\ 0 & 0 & 3 & 3 \end{array}\right]$$

Each of these operations is equivalent to left-multiplying by a *type III elementary matrix*, the identity with one non-diagonal non-zero term. If row operation k corresponds to matrix E_k, the following equation is $E_3E_2E_1A = U$.

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -4 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \left[\begin{array}{ccc|c} 1 & 1 & 1 & 1 \\ 1 & 4 & 2 & 3 \\ 4 & 7 & 8 & 9 \end{array}\right] = \left[\begin{array}{ccc|c} 1 & 1 & 1 & 1 \\ 0 & 3 & 1 & 2 \\ 0 & 0 & 3 & 3 \end{array}\right]$$

However, matrix multiplication is an inefficient way to implement row reduction. Instead, modify the matrix in place (without making a copy), changing only those entries that are affected by each row operation.

```
>>> import numpy as np

>>> A = np.array([[1, 1, 1, 1],
...               [1, 4, 2, 3],
...               [4, 7, 8, 9]], dtype=np.float)

# Reduce the 0th column to zeros below the diagonal.
>>> A[1,0:] -= (A[1,0] / A[0,0]) * A[0]
>>> A[2,0:] -= (A[2,0] / A[0,0]) * A[0]

# Reduce the 1st column to zeros below the diagonal.
>>> A[2,1:] -= (A[2,1] / A[1,1]) * A[1,1:]
>>> print(A)
[[ 1.  1.  1.  1.]
 [ 0.  3.  1.  2.]
 [ 0.  0.  3.  3.]]
```

Note that the final row operation modifies only part of the third row to avoid spending the computation time of adding 0 to 0.

If a 0 appears on the main diagonal during any part of row reduction, the approach given above tries to divide by 0. Swapping the current row with one below it that does not have a 0 in the same column solves this problem. This is equivalent to left-multiplying by a type II elementary matrix, also called a *permutation matrix*.

Achtung!

Gaussian elimination is not always numerically stable. In other words, it is susceptible to rounding error that may result in an incorrect final matrix. Suppose that, due to roundoff error, the matrix A has a very small entry on the diagonal.

$$A = \begin{bmatrix} 10^{-15} & 1 \\ -1 & 0 \end{bmatrix}$$

Though 10^{-15} is essentially zero, instead of swapping the first and second rows to put A in REF, a computer might multiply the first row by 10^{15} and add it to the second row to eliminate the -1. The resulting matrix is far from what it would be if the 10^{-15} were actually 0.

$$\begin{bmatrix} 10^{-15} & 1 \\ -1 & 0 \end{bmatrix} \longrightarrow \begin{bmatrix} 10^{-15} & 1 \\ 0 & 10^{15} \end{bmatrix}$$

Round-off error can propagate through many steps in a calculation. The NumPy routines that employ row reduction use several tricks to minimize the impact of round-off error, but these tricks cannot fix every matrix.

Problem 1. Write a function that reduces an arbitrary square matrix A to REF. You may assume that A is invertible and that a 0 will never appear on the main diagonal (so only use type III row reductions, not type II). Avoid operating on entries that you know will be 0 before and after a row operation. Use at most two nested loops.

Test your function with small test cases that you can check by hand. Consider using `np.random.randint()` to generate a few manageable tests cases.

The LU Decomposition

The *LU decomposition* of a square matrix A is a factorization $A = LU$ where U is the **upper** triangular REF of A and L is the **lower** triangular product of the type III elementary matrices whose inverses reduce A to U. The LU decomposition of A exists when A can be reduced to REF using only type III elementary matrices (without any row swaps). However, the rows of A can always be permuted in a way such that the decomposition exists. If P is a permutation matrix encoding the appropriate row swaps, then the decomposition $PA = LU$ always exists.

Suppose A has an LU decomposition (not requiring row swaps). Then A can be reduced to REF with k row operations, corresponding to left-multiplying the type III elementary matrices $E_1, \dots, E_k$. Because there were no row swaps, each E_i is lower triangular, so each inverse E_i^{-1} is also lower triangular. Furthermore, since the product of lower triangular matrices is lower triangular, L is lower triangular.

$$\begin{aligned} E_k \dots E_2 E_1 A = U \quad \longrightarrow \quad A &= (E_k \dots E_2 E_1)^{-1} U \\ &= E_1^{-1} E_2^{-1} \dots E_k^{-1} U \\ &= LU \end{aligned}$$

Thus L can be computed by right-multiplying the identity by the matrices used to reduce U. However, in this special situation, each right-multiplication only changes one entry of L, matrix multiplication can be avoided altogether. The entire process, only slightly different than row reduction, is summarized below.

Algorithm 2.1

procedure LU DECOMPOSITION(A)
  $m, n \leftarrow \text{shape}(A)$ ▷ Store the dimensions of A.
  $U \leftarrow \text{copy}(A)$ ▷ Make a copy of A with `np.copy()`.
  $L \leftarrow I_m$ ▷ The $m \times m$ identity matrix.
  for $j = 0 \dots n-1$ **do**
    for $i = j+1 \dots m-1$ **do**
      $L_{i,j} \leftarrow U_{i,j} / U_{j,j}$
      $U_{i,j:} \leftarrow U_{i,j:} - L_{i,j} U_{j,j:}$
  return L, U

Problem 2. Write a function that finds the LU decomposition of a square matrix. You may assume that the decomposition exists and requires no row swaps.

Forward and Backward Substitution

If $PA = LU$ and $A\mathbf{x} = \mathbf{b}$, then $LU\mathbf{x} = PA\mathbf{x} = P\mathbf{b}$. This system can be solved by first solving $L\mathbf{y} = P\mathbf{b}$, then $U\mathbf{x} = \mathbf{y}$. Since L and U are both triangular, these systems can be solved with backward and forward substitution. We can thus compute the LU factorization of A once, then use substitution to efficiently solve $A\mathbf{x} = \mathbf{b}$ for various values of $\mathbf{b}$.

Since the diagonal entries of L are all 1, the triangular system $L\mathbf{y} = \mathbf{b}$ has the following form.

$$\begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ l_{21} & 1 & 0 & \cdots & 0 \\ l_{31} & l_{32} & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ l_{n1} & l_{n2} & l_{n3} & \cdots & 1 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_n \end{bmatrix}.$$

Matrix multiplication yields the following equations.

$$\begin{aligned} y_1 &= b_1 & y_1 &= b_1 \\ l_{21}y_1 + y_2 &= b_2 & y_2 &= b_2 - l_{21}y_1 \\ &\vdots & &\vdots \\ \sum_{j=1}^{k-1} l_{kj}y_j + y_k &= b_k & y_k &= b_k - \sum_{j=1}^{k-1} l_{kj}y_j \end{aligned} \tag{2.1}$$

The triangular system $U\mathbf{x} = \mathbf{y}$ yields similar equations, but in reverse order.

$$\begin{bmatrix} u_{11} & u_{12} & u_{13} & \cdots & u_{1n} \\ 0 & u_{22} & u_{23} & \cdots & u_{2n} \\ 0 & 0 & u_{33} & \cdots & u_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & u_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_n \end{bmatrix}$$

$$\begin{aligned} u_{nn}x_n &= y_n & x_n &= \frac{1}{u_{nn}}y_n \\ u_{n-1,n-1}x_{n-1} + u_{n-1,n}x_n &= y_{n-1} & x_{n-1} &= \frac{1}{u_{n-1,n-1}}\left(y_{n-1} - u_{n-1,n}x_n\right) \\ &\vdots & &\vdots \\ \sum_{j=k}^{n} u_{kj}x_j &= y_k & x_k &= \frac{1}{u_{kk}}\left(y_k - \sum_{j=k+1}^{n} u_{kj}x_j\right) \end{aligned} \tag{2.2}$$

Problem 3. Write a function that, given A and $\mathbf{b}$, solves the square linear system $A\mathbf{x} = \mathbf{b}$. Use the function from Problem 2 to compute L and U, then use (2.1) and (2.2) to solve for $\mathbf{y}$, then $\mathbf{x}$. You may again assume that no row swaps are required ($P = I$ in this case).

SciPy

SciPy is a powerful scientific computing library built upon NumPy. It includes high-level tools for linear algebra, statistics, signal processing, integration, optimization, machine learning, and more.

SciPy is typically imported with the convention `import scipy as sp`. However, SciPy is set up in a way that requires its submodules to be imported individually.[1]

```
>>> import scipy as sp
>>> hasattr(sp, "stats")            # The stats module isn't loaded yet.
False

>>> from scipy import stats         # Import stats explicitly. Access it
>>> hasattr(sp, "stats")            # with 'stats' or 'sp.stats'.
True
```

Linear Algebra

NumPy and SciPy both have a linear algebra module, each called `linalg`, but SciPy's module is the larger of the two. Some of SciPy's common `linalg` functions are listed below.

Function	Returns
`det()`	The determinant of a square matrix.
`eig()`	The eigenvalues and eigenvectors of a square matrix.
`inv()`	The inverse of an invertible matrix.
`norm()`	The norm of a vector or matrix norm of a matrix.
`solve()`	The solution to $A\mathbf{x} = \mathbf{b}$ (the system need not be square).

This library also includes routines for computing matrix decompositions.

```
>>> from scipy import linalg as la

# Make a random matrix and a random vector.
>>> A = np.random.random((1000,1000))
>>> b = np.random.random(1000)

# Compute the LU decomposition of A, including pivots.
>>> L, P = la.lu_factor(A)

# Use the LU decomposition to solve Ax = b.
>>> x = la.lu_solve((L,P), b)

# Check that the solution is legitimate.
>>> np.allclose(A @ x, b)
True
```

[1] SciPy modules like `linalg` are really *packages*, which need to be initialized separately. For example, to import SciPy's `linalg` package use `from scipy import linalg as la`.

As with NumPy, SciPy's routines are all highly optimized. However, some algorithms are, by nature, faster than others.

Problem 4. Write a function that times different `scipy.linalg` functions for solving square linear systems.

For various values of n, generate a random $n \times n$ matrix A and a random n-vector $\mathbf{b}$ using `np.random.random()`. Time how long it takes to solve the system $A\mathbf{x} = \mathbf{b}$ with each of the following approaches:

1. Invert A with `la.inv()` and left-multiply the inverse to $\mathbf{b}$.
2. Use `la.solve()`.
3. Use `la.lu_factor()` and `la.lu_solve()` to solve the system with the LU decomposition.
4. Use `la.lu_factor()` and `la.lu_solve()`, but only time `la.lu_solve()` (not the time it takes to do the factorization with `la.lu_factor()`).

Plot the system size n versus the execution times. Use log scales if needed.

ACHTUNG!

Problem 4 demonstrates that computing a matrix inverse is computationally expensive. In fact, numerically inverting matrices is so costly that there is hardly ever a good reason to do it. Use a specific solver like `la.lu_solve()` whenever possible instead of using `la.inv()`.

Sparse Matrices

Large linear systems can have tens of thousands of entries. Storing the corresponding matrices in memory can be difficult: a $10^5 \times 10^5$ system requires around 40 GB to store in a NumPy array (4 bytes per entry $\times$ 10^{10} entries). This is well beyond the amount of RAM in a normal laptop.

In applications where systems of this size arise, it is often the case that the system is *sparse*, meaning that most of the entries of the matrix are 0. SciPy's `sparse` module provides tools for efficiently constructing and manipulating 1- and 2-D sparse matrices. A `sparse` matrix only stores the nonzero values and the positions of these values. For sufficiently sparse matrices, storing the matrix as a `sparse` matrix may only take megabytes, rather than gigabytes.

For example, diagonal matrices are sparse. Storing an $n \times n$ diagonal matrix in the naïve way means storing n^2 values in memory. It is more efficient to instead store the diagonal entries in a 1-D array of n values. In addition to using less storage space, this allows for much faster matrix operations: the standard algorithm to multiply a matrix by a diagonal matrix involves n^3 steps, but most of these are multiplying by or adding 0. A smarter algorithm can accomplish the same task much faster.

SciPy has seven sparse matrix types. Each type is optimized either for storing sparse matrices whose nonzero entries follow certain patterns, or for performing certain computations.

Name	Description	Advantages
`bsr_matrix`	Block Sparse Row	Specialized structure.
`coo_matrix`	Coordinate Format	Conversion among sparse formats.
`csc_matrix`	Compressed Sparse Column	Column-based operations and slicing.
`csr_matrix`	Compressed Sparse Row	Row-based operations and slicing.
`dia_matrix`	Diagonal Storage	Specialized structure.
`dok_matrix`	Dictionary of Keys	Element access, incremental construction.
`lil_matrix`	Row-based Linked List	Incremental construction.

Creating Sparse Matrices

A regular, non-sparse matrix is called *full* or *dense*. Full matrices can be converted to each of the sparse matrix formats listed above. However, it is more memory efficient to never create the full matrix in the first place. There are three main approaches for creating sparse matrices from scratch.

- **Coordinate Format**: When all of the nonzero values and their positions are known, create the entire sparse matrix at once as a `coo_matrix`. All nonzero values are stored as a coordinate and a value. This format also converts quickly to other sparse matrix types.

```
>>> from scipy import sparse

# Define the rows, columns, and values separately.
>>> rows = np.array([0, 1, 0])
>>> cols = np.array([0, 1, 1])
>>> vals = np.array([3, 5, 2])
>>> A = sparse.coo_matrix((vals, (rows,cols)), shape=(3,3))
>>> print(A)
  (0, 0)    3
  (1, 1)    5
  (0, 1)    2

# The toarray() method casts the sparse matrix as a NumPy array.
>>> print(A.toarray())              # Note that this method forfeits
[[3 2 0]                            # all sparsity-related optimizations.
 [0 5 0]
 [0 0 0]]
```

- **DOK and LIL Formats**: If the matrix values and their locations are not known beforehand, construct the matrix incrementally with a `dok_matrix` or a `lil_matrix`. Indicate the size of the matrix, then change individual values with regular slicing syntax.

```
>>> B = sparse.lil_matrix((2,6))
>>> B[0,2] = 4
>>> B[1,3:] = 9

>>> print(B.toarray())
[[ 0.  0.  4.  0.  0.  0.]
 [ 0.  0.  0.  9.  9.  9.]]
```

- **DIA Format**: Use a `dia_matrix` to store matrices that have nonzero entries on only certain diagonals. The function `sparse.diags()` is one convenient way to create a `dia_matrix` from scratch. Additionally, every sparse matrix has a `setdiags()` method for modifying specified diagonals.

```
# Use sparse.diags() to create a matrix with diagonal entries.
>>> diagonals = [[1,2],[3,4,5],[6]]     # List the diagonal entries.
>>> offsets = [-1,0,3]                  # Specify the diagonal they go on.
>>> print(sparse.diags(diagonals, offsets, shape=(3,4)).toarray())
[[ 3.  0.  0.  6.]
 [ 1.  4.  0.  0.]
 [ 0.  2.  5.  0.]]

# If all of the diagonals have the same entry, specify the entry alone.
>>> A = sparse.diags([1,3,6], offsets, shape=(3,4))
>>> print(A.toarray())
[[ 3.  0.  0.  6.]
 [ 1.  3.  0.  0.]
 [ 0.  1.  3.  0.]]

# Modify a diagonal with the setdiag() method.
>>> A.setdiag([4,4,4], 0)
>>> print(A.toarray())
[[ 4.  0.  0.  6.]
 [ 1.  4.  0.  0.]
 [ 0.  1.  4.  0.]]
```

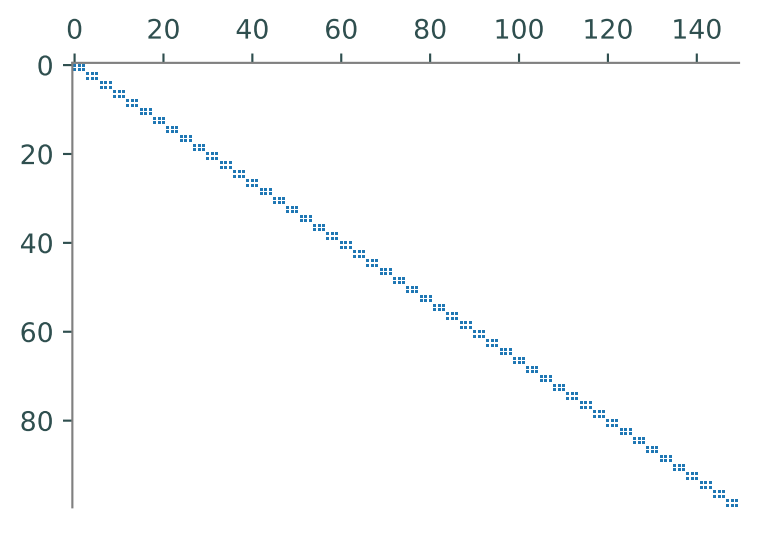
- **BSR Format**: Many sparse matrices can be formulated as block matrices, and a block matrix can be stored efficiently as a `bsr_matrix`. Use `sparse.bmat()` or `sparse.block_diag()` to create a block matrix quickly.

```
# Use sparse.bmat() to create a block matrix. Use 'None' for zero blocks.
>>> A = sparse.coo_matrix(np.ones((2,2)))
>>> B = sparse.coo_matrix(np.full((2,2), 2.))
>>> print(sparse.bmat([[  A , None,  A  ],
                       [None,  B  , None]], format='bsr').toarray())
[[ 1.  1.  0.  0.  1.  1.]
 [ 1.  1.  0.  0.  1.  1.]
 [ 0.  0.  2.  2.  0.  0.]
 [ 0.  0.  2.  2.  0.  0.]]

 # Use sparse.block_diag() to construct a block diagonal matrix.
 >>> print(sparse.block_diag((A,B)).toarray())
[[ 1.  1.  0.  0.]
 [ 1.  1.  0.  0.]
 [ 0.  0.  2.  2.]
 [ 0.  0.  2.  2.]]
```

Note

If a sparse matrix is too large to fit in memory as an array, it can still be visualized with Matplotlib's `plt.spy()`, which colors in the locations of the non-zero entries of the matrix.

```
>>> from matplotlib import pyplot as plt

# Construct and show a matrix with 50 2x3 diagonal blocks.
>>> B = sparse.coo_matrix([[1,3,5],[7,9,11]])
>>> A = sparse.block_diag([B]*50)
>>> plt.spy(A, markersize=1)
>>> plt.show()
```



Problem 5. Let I be the $n \times n$ identity matrix, and define

$$A = \begin{bmatrix} B & I & & & \\ I & B & I & & \\ & I & \ddots & \ddots & \\ & & \ddots & \ddots & I \\ & & & I & B \end{bmatrix}, \qquad B = \begin{bmatrix} -4 & 1 & & & \\ 1 & -4 & 1 & & \\ & 1 & \ddots & \ddots & \\ & & \ddots & \ddots & 1 \\ & & & 1 & -4 \end{bmatrix},$$

where A is $n^2 \times n^2$ and each block B is $n \times n$. The large matrix A is used in finite difference methods for solving Laplace's equation in two dimensions, $\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0$.

Write a function that accepts an integer n and constructs and returns A as a sparse matrix. Use `plt.spy()` to check that your matrix has nonzero values in the correct places.

Sparse Matrix Operations

Once a sparse matrix has been constructed, it should be converted to a `csr_matrix` or a `csc_matrix` with the matrix's `tocsr()` or `tocsc()` method. The CSR and CSC formats are optimized for row or column operations, respectively. To choose the correct format to use, determine what direction the matrix will be traversed.

For example, in the matrix-matrix multiplication AB, A is traversed row-wise, but B is traversed column-wise. Thus A should be converted to a `csr_matrix` and B should be converted to a `csc_matrix`.

```
# Initialize a sparse matrix incrementally as a lil_matrix.
>>> A = sparse.lil_matrix((10000,10000))
>>> for k in range(10000):
...     A[np.random.randint(0,9999), np.random.randint(0,9999)] = k
...
>>> A
<10000x10000 sparse matrix of type '<type 'numpy.float64'>'
    with 9999 stored elements in LInked List format>

# Convert A to CSR and CSC formats to compute the matrix product AA.
>>> Acsr = A.tocsr()
>>> Acsc = A.tocsc()
>>> Acsr.dot(Acsc)
<10000x10000 sparse matrix of type '<type 'numpy.float64'>'
    with 10142 stored elements in Compressed Sparse Row format>
```

Beware that row-based operations on a `csc_matrix` are very slow, and similarly, column-based operations on a `csr_matrix` are very slow.

Achtung!

Many familiar NumPy operations have analogous routines in the `sparse` module. These methods take advantage of the sparse structure of the matrices and are, therefore, usually significantly faster. However, SciPy's `sparse` matrices behave a little differently than NumPy arrays.

Operation	`numpy`	`scipy.sparse`
Component-wise Addition	`A + B`	`A + B`
Scalar Multiplication	`2 * A`	`2 * A`
Component-wise Multiplication	`A * B`	`A.multiply(B)`
Matrix Multiplication	`A.dot(B)`, `A @ B`	`A * B`, `A.dot(B)`, `A @ B`

Note in particular the difference between `A * B` for NumPy arrays and SciPy sparse matrices. Do **not** use `np.dot()` to try to multiply sparse matrices, as it may treat the inputs incorrectly. The syntax `A.dot(B)` is safest in most cases.

SciPy's sparse module has its own linear algebra library, `scipy.sparse.linalg`, designed for operating on sparse matrices. Like other SciPy modules, it must be imported explicitly.

```
>>> from scipy.sparse import linalg as spla
```

Problem 6. Write a function that times regular and sparse linear system solvers.

For various values of n, generate the $n^2 \times n^2$ matrix A described in Problem 5 and a random vector $\mathbf{b}$ with n^2 entries. Time how long it takes to solve the system $A\mathbf{x} = \mathbf{b}$ with each of the following approaches:

1. Convert A to CSR format and use `scipy.sparse.linalg.spsolve()` (`spla.spsolve()`).
2. Convert A to a NumPy array and use `scipy.linalg.solve()` (`la.solve()`).

In each experiment, only time how long it takes to solve the system (not how long it takes to convert A to the appropriate format).

Plot the system size n^2 versus the execution times. As always, use log scales where appropriate and use a legend to label each line.

Achtung!

Even though there are fast algorithms for solving certain sparse linear system, it is still very computationally difficult to invert sparse matrices. In fact, the inverse of a sparse matrix is usually not sparse. There is rarely a good reason to invert a matrix, sparse or dense.

See `http://docs.scipy.org/doc/scipy/reference/sparse.html` for additional details on SciPy's `sparse` module.

Additional Material

Improvements on the LU Decomposition

Vectorization

Algorithm 2.1 uses two loops to compute the LU decomposition. With a little vectorization, the process can be reduced to a single loop.

Algorithm 2.2

1: **procedure** FAST LU DECOMPOSITION(A)
2: $m, n \leftarrow \text{shape}(A)$
3: $U \leftarrow \text{copy}(A)$
4: $L \leftarrow I_m$
5: **for** $k = 0 \dots n-1$ **do**
6: $L_{k+1:,k} \leftarrow U_{k+1:,k} / U_{k,k}$
7: $U_{k+1:,k:} \leftarrow U_{k+1:,k:} - L_{k+1:,k} U_{k,k:}^\mathsf{T}$
8: **return** L, U

Note that step 7 is an *outer product*, not the regular dot product ($\mathbf{x}\mathbf{y}^\mathsf{T}$ instead of the usual $\mathbf{x}^\mathsf{T}\mathbf{y}$). Use `np.outer()` instead of `np.dot()` or `@` to get the desired result.

Pivoting

Gaussian elimination iterates through the rows of a matrix, using the diagonal entry $x_{k,k}$ of the matrix at the kth iteration to zero out all of the entries in the column below $x_{k,k}$ ($x_{i,k}$ for $i \geq k$). This diagonal entry is called the *pivot*. Unfortunately, Gaussian elimination, and hence the LU decomposition, can be very numerically unstable if at any step the pivot is a very small number. Most professional row reduction algorithms avoid this problem via *partial pivoting*.

The idea is to choose the largest number (in magnitude) possible to be the pivot by swapping the pivot row[2] with another row before operating on the matrix. For example, the second and fourth rows of the following matrix are exchanged so that the pivot is -6 instead of 2.

$$\begin{bmatrix} \times & \times & \times & \times \\ 0 & 2 & \times & \times \\ 0 & 4 & \times & \times \\ 0 & -6 & \times & \times \end{bmatrix} \longrightarrow \begin{bmatrix} \times & \times & \times & \times \\ 0 & -6 & \times & \times \\ 0 & 4 & \times & \times \\ 0 & 2 & \times & \times \end{bmatrix} \longrightarrow \begin{bmatrix} \times & \times & \times & \times \\ 0 & -6 & \times & \times \\ 0 & 0 & \times & \times \\ 0 & 0 & \times & \times \end{bmatrix}$$

A row swap is equivalent to left-multiplying by a type II elementary matrix, also called a *permutation matrix*.

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} \times & \times & \times & \times \\ 0 & 2 & \times & \times \\ 0 & 4 & \times & \times \\ 0 & -6 & \times & \times \end{bmatrix} = \begin{bmatrix} \times & \times & \times & \times \\ 0 & -6 & \times & \times \\ 0 & 4 & \times & \times \\ 0 & 2 & \times & \times \end{bmatrix}$$

For the LU decomposition, if the permutation matrix at step k is P_k, then $P = P_k \dots P_2 P_1$ yields $PA = LU$. The complete algorithm is given below.

[2] *Complete pivoting* involves row and column swaps, but doing both operations is usually considered overkill.

Algorithm 2.3

procedure LU Decomposition with Partial Pivoting(A)
  $m, n \leftarrow \text{shape}(A)$
  $U \leftarrow \text{copy}(A)$
  $L \leftarrow I_m$
  $P \leftarrow [0,\ 1,\ \ldots,\ n-1]$ ▷ See tip 2 below.
  for $k = 0 \ldots n-1$ **do**
    Select $i \geq k$ that maximizes $|U_{i,k}|$
    $U_{k,k:} \leftrightarrow U_{i,k:}$ ▷ Swap the two rows.
    $L_{k,:k} \leftrightarrow L_{i,:k}$ ▷ Swap the two rows.
    $P_k \leftrightarrow P_i$ ▷ Swap the two entries.
    $L_{k+1:,k} \leftarrow U_{k+1:,k}/U_{k,k}$
    $U_{k+1:,k:} \leftarrow U_{k+1:,k:} - L_{k+1:,k}U_{k,k:}^{\mathsf{T}}$
  return L, U, P

The following tips may be helpful for implementing this algorithm:

1. Since NumPy arrays are mutable, use `np.copy()` to reassign the rows of an array simultaneously.
2. Instead of storing P as an $n \times n$ array, fancy indexing allows us to encode row swaps in a 1-D array of length n. Initialize P as the array $[0, 1, \ldots, n]$. After performing a row swap on A, perform the same operations on P. Then the matrix product PA will be the same as `A[P]`.

```
>>> A = np.zeros(3) + np.vstack(np.arange(3))
>>> P = np.arange(3)
>>> print(A)
[[ 0.  0.  0.]
 [ 1.  1.  1.]
 [ 2.  2.  2.]]

# Swap rows 1 and 2.
>>> A[1], A[2] = np.copy(A[2]), np.copy(A[1])
>>> P[1], P[2] = P[2], P[1]
>>> print(A)                        # A with the new row arrangement.
[[ 0.  0.  0.]
 [ 2.  2.  2.]
 [ 1.  1.  1.]]
>>> print(P)                        # The permutation of the rows.
[0 2 1]
>>> print(A[P])                     # A with the original row arrangement.
[[ 0.  0.  0.]
 [ 1.  1.  1.]
 [ 2.  2.  2.]]
```

There are potential cases where even partial pivoting does not eliminate catastrophic numerical errors in Gaussian elimination, but the odds of having such an amazingly poor matrix are essentially zero. The numerical analyst J.H. Wilkinson captured the likelihood of encountering such a matrix in a natural application when he said, "Anyone that unlucky has already been run over by a bus!"

In Place

The LU decomposition can be performed in place (overwriting the original matrix A) by storing U on and above the main diagonal of the array and storing L below it. The main diagonal of L does not need to be stored since all of its entries are 1. This format saves an entire array of memory, and is how `scipy.linalg.lu_factor()` returns the factorization.

More Applications of the LU Decomposition

The LU decomposition can also be used to compute inverses and determinants.

- **Inverse**: $(PA)^{-1} = (LU)^{-1} \longrightarrow A^{-1}P^{-1} = U^{-1}L^{-1} \longrightarrow LUA^{-1} = P$. Solve $LU\mathbf{a}_i = \mathbf{p}_i$ with forward and backward substitution (as in Problem 3) for every column $\mathbf{p}_i$ of P. Then

$$A^{-1} = \left[\begin{array}{c|c|c|c} & & & \\ \mathbf{a}_1 & \mathbf{a}_2 & \cdots & \mathbf{a}_n \\ & & & \end{array}\right],$$

  the matrix where $\mathbf{a}_k$ is the kth column.

- **Determinant**: $\det(A) = \det(P^{-1}LU) = \frac{\det(L)\det(U)}{\det(P)}$. The determinant of a triangular matrix is the product of its diagonal entries. Since every diagonal entry of L is 1, $\det(L) = 1$. Also, P is just a row permutation of the identity matrix (which has determinant 1), and a single row swap negates the determinant. Then if S is the number of row swaps, the determinant is given by the following equation.

$$\det(A) = (-1)^S \prod_{i=1}^{n} u_{ii}$$

The Cholesky Decomposition

A square matrix A is called *positive definite* if $\mathbf{z}^\mathsf{T}A\mathbf{z} > 0$ for all nonzero vectors $\mathbf{z}$. In addition, A is called *Hermitian* if $A = A^\mathsf{H} = \overline{A^\mathsf{T}}$. If A is Hermitian positive definite, it has a *Cholesky Decomposition* $A = U^\mathsf{H}U$ where U is upper triangular with real, positive entries on the diagonal. This is the matrix equivalent to taking the square root of a positive real number.

The Cholesky decomposition takes advantage of the conjugate symmetry of A to simultaneously reduce the columns *and* rows of A to zeros (except for the diagonal). It thus requires only half of the calculations and memory of the LU decomposition. Furthermore, the algorithm is *numerically stable*, which means that round-off errors do not propagate throughout the computation. This decomposition is used when possible to solve least squares, optimization, and state estimation problems.

Algorithm 2.4

```
1: procedure CHOLESKY DECOMPOSITION(A)
2:     U ← A                                   ▷ Copy A if desired.
3:     for i = 0 ... n − 1 do
4:         for j = i + 1 ... n − 1 do
5:             U_{j,j:} ← U_{j,j:} − U_{i,j:} conj(U_{ij}) / U_{ii}
6:         U_{i,i:} ← U_{i,i:} / sqrt(U_{ii})
7:     return U
```

As with the LU decomposition, SciPy's `linalg` module has optimized routines, `la.cho_factor()` and `la.cho_solve()`, for using the Cholesky decomposition.

3 The QR Decomposition

Lab Objective: *The QR decomposition is a fundamentally important matrix factorization. It is straightforward to implement, is numerically stable, and provides the basis of several important algorithms. In this lab, we explore several ways to produce the QR decomposition and implement a few immediate applications.*

The QR decomposition of a matrix A is a factorization $A = QR$, where Q is has orthonormal columns and R is upper triangular. Every $m \times n$ matrix A of rank $n \leq m$ has a QR decomposition, with two main forms.

- **Reduced QR**: Q is $m \times n$, R is $n \times n$, and the columns $\{\mathbf{q}_j\}_{j=1}^{n}$ of Q form an orthonormal basis for the column space of A.
- **Full QR**: Q is $m \times m$ and R is $m \times n$. In this case, the columns $\{\mathbf{q}_j\}_{j=1}^{m}$ of Q form an orthonormal basis for all of $\mathbb{F}^m$, and the last $m - n$ rows of R only contain zeros. If $m = n$, this is the same as the reduced factorization.

We distinguish between these two forms by writing $\widehat{Q}$ and $\widehat{R}$ for the reduced decomposition and Q and R for the full decomposition.

$$\underset{\widehat{Q}\ (m\times n)}{\begin{bmatrix} \mathbf{q}_1 & \cdots & \mathbf{q}_n \end{bmatrix}} \underset{Q\ (m\times m)}{\begin{bmatrix} \mathbf{q}_{n+1} & \cdots & \mathbf{q}_m \end{bmatrix}} \underset{\widehat{R}\ (n\times n)}{\begin{bmatrix} r_{11} & \cdots & r_{1n} \\ & \ddots & \vdots \\ & & r_{nn} \end{bmatrix}} \underset{R\ (m\times n)}{\begin{bmatrix} 0 & \cdots & 0 \\ \vdots & & \vdots \\ 0 & \cdots & 0 \end{bmatrix}} = A\ (m \times n)$$

QR via Gram-Schmidt

The *classical Gram-Schmidt algorithm* takes a linearly independent set of vectors and constructs an orthonormal set of vectors with the same span. Applying Gram-Schmidt to the columns of A, which are linearly independent since A has rank n, results in the columns of Q.

Let $\{\mathbf{x}_j\}_{j=1}^n$ be the columns of A. Define

$$\mathbf{q}_1 = \frac{\mathbf{x}_1}{\|\mathbf{x}_1\|}, \qquad \mathbf{q}_k = \frac{\mathbf{x}_k - \mathbf{p}_{k-1}}{\|\mathbf{x}_k - \mathbf{p}_{k-1}\|}, \quad k = 2,\ \dots,\ n,$$

$$\mathbf{p}_0 = \mathbf{0}, \quad \text{and} \qquad \mathbf{p}_{k-1} = \sum_{j=1}^{k-1} \langle \mathbf{q}_j, \mathbf{x}_k \rangle \mathbf{q}_j, \quad k = 2,\ \dots,\ n.$$

Each $\mathbf{p}_{k-1}$ is the projection of $\mathbf{x}_k$ onto the span of $\{\mathbf{q}_j\}_{j=1}^{k-1}$, so $\mathbf{q}_k' = \mathbf{x}_k - \mathbf{p}_{k-1}$ is the residual vector of the projection. Thus $\mathbf{q}_k'$ is orthogonal to each of the vectors in $\{\mathbf{q}_j\}_{j=1}^{k-1}$. Therefore, normalizing each $\mathbf{q}_k'$ produces an orthonormal set $\{\mathbf{q}_j\}_{j=1}^n$.

To construct the reduced QR decomposition, let $\widehat{Q}$ be the matrix with columns $\{\mathbf{q}_j\}_{j=1}^n$, and let $\widehat{R}$ be the upper triangular matrix with the following entries:

$$r_{kk} = \|\mathbf{x}_k - \mathbf{p}_{k-1}\|, \qquad r_{jk} = \langle \mathbf{q}_j, \mathbf{x}_k \rangle = \mathbf{q}_j^\mathsf{T} \mathbf{x}_k,\ j < k.$$

This clever choice of entries for $\widehat{R}$ reverses the Gram-Schmidt process and ensures that $\widehat{Q}\widehat{R} = A$.

Modified Gram-Schmidt

If the columns of A are close to being linearly dependent, the classical Gram-Schmidt algorithm often produces a set of vectors $\{\mathbf{q}_j\}_{j=1}^n$ that are not even close to orthonormal due to rounding errors. The *modified Gram-Schmidt algorithm* is a slight variant of the classical algorithm which more consistently produces a set of vectors that are "very close" to orthonormal.

Let $\mathbf{q}_1$ be the normalization of $\mathbf{x}_1$ as before. Instead of making just $\mathbf{x}_2$ orthogonal to $\mathbf{q}_1$, make *each* of the vectors $\{\mathbf{x}_j\}_{j=2}^n$ orthogonal to $\mathbf{q}_1$:

$$\mathbf{x}_k = \mathbf{x}_k - \langle \mathbf{q}_1, \mathbf{x}_k \rangle \mathbf{q}_1, \quad k = 2,\ \dots,\ n.$$

Next, define $\mathbf{q}_2 = \frac{\mathbf{x}_2}{\|\mathbf{x}_2\|}$. Proceed by making each of $\{\mathbf{x}_j\}_{j=3}^n$ orthogonal to $\mathbf{q}_2$:

$$\mathbf{x}_k = \mathbf{x}_k - \langle \mathbf{q}_2, \mathbf{x}_k \rangle \mathbf{q}_2, \quad k = 3, \dots, n.$$

Since each of these new vectors is a linear combination of vectors orthogonal to $\mathbf{q}_1$, they are orthogonal to $\mathbf{q}_1$ as well. Continuing this process results in the desired orthonormal set $\{\mathbf{q}_j\}_{j=1}^n$. The entire modified Gram-Schmidt algorithm is described below.

Algorithm 3.1

```
procedure MODIFIED GRAM-SCHMIDT(A)
    m, n ← shape(A)                          ▷ Store the dimensions of A.
    Q ← copy(A)                              ▷ Make a copy of A with np.copy().
    R ← zeros(n, n)                          ▷ An n × n array of all zeros.
    for i = 0 ... n − 1 do
        R_{i,i} ← ‖Q_{:,i}‖
        Q_{:,i} ← Q_{:,i} / R_{i,i}          ▷ Normalize the ith column of Q.
        for j = i + 1 ... n − 1 do
            R_{i,j} ← Q_{:,j}^T Q_{:,i}
            Q_{:,j} ← Q_{:,j} − R_{i,j} Q_{:,i}   ▷ Orthogonalize the jth column of Q.
    return Q, R
```

Problem 1. Write a function that accepts an $m \times n$ matrix A of rank n. Use Algorithm 3.1 to compute the reduced QR decomposition of A.

Consider the following tips for implementing the algorithm.

- Use `scipy.linalg.norm()` to compute the norm of the vector in step 6.
- Note that steps 7 and 10 employ scalar multiplication or division, while step 9 uses vector multiplication.

To test your function, generate test cases with NumPy's `np.random` module. Verify that R is upper triangular, Q is orthonormal, and $QR = A$. You may also want to compare your results to SciPy's QR factorization routine, `scpiy.linalg.qr()`.

```
>>> import numpy as np
>>> from scipy import linalg as la

# Generate a random matrix and get its reduced QR decomposition via SciPy.
>>> A = np.random.random((6,4))
>>> Q,R = la.qr(A, mode="economic") # Use mode="economic" for reduced QR.
>>> print(A.shape, Q.shape, R.shape)
(6,4) (6,4) (4,4)

# Verify that R is upper triangular, Q is orthonormal, and QR = A.
>>> np.allclose(np.triu(R), R)
True
>>> np.allclose(Q.T @ Q, np.identity(4))
True
>>> np.allclose(Q @ R, A)
True
```

Consequences of the QR Decomposition

The special structures of Q and R immediately provide some simple applications.

Determinants

Let A be $n \times n$. Then Q and R are both $n \times n$ as well.[1] Since Q is orthonormal and R is upper-triangular,

$$\det(Q) = \pm 1 \qquad \text{and} \qquad \det(R) = \prod_{i=1}^{n} r_{i,i}.$$

Then since $\det(AB) = \det(A)\det(B)$,

$$|\det(A)| = |\det(QR)| = |\det(Q)\det(R)| = |\det(Q)|\,|\det(R)| = \left|\prod_{i=1}^{n} r_{i,i}\right|. \tag{3.1}$$

[1] An $n \times n$ orthonormal matrix is sometimes called *unitary* in other texts.

Problem 2. Write a function that accepts an invertible matrix A. Use the QR decomposition of A and (3.1) to calculate $|\det(A)|$. You may use your QR decomposition algorithm from Problem 1 or SciPy's QR routine. Can you implement this function in a single line?
(Hint: `np.diag()` and `np.prod()` may be useful.)

Check your answer against `la.det()`, which calculates the determinant.

Linear Systems

The LU decomposition is usually the matrix factorization of choice to solve the linear system $A\mathbf{x} = \mathbf{b}$ because the triangular structures of L and U facilitate forward and backward substitution. However, the QR decomposition avoids the potential numerical issues that come with Gaussian elimination.

Since Q is orthonormal, $Q^{-1} = Q^\mathsf{T}$. Therefore, solving $A\mathbf{x} = \mathbf{b}$ is equivalent to solving the system $R\mathbf{x} = Q^\mathsf{T}\mathbf{b}$. Since R is upper-triangular, $R\mathbf{x} = Q^\mathsf{T}\mathbf{b}$ can be solved quickly with back substitution.[2]

Problem 3. Write a function that accepts an invertible $n \times n$ matrix A and a vector $\mathbf{b}$ of length n. Use the QR decomposition to solve $A\mathbf{x} = \mathbf{b}$ in the following steps:

1. Compute Q and R.
2. Calculate $\mathbf{y} = Q^\mathsf{T}\mathbf{b}$.
3. Use back substitution to solve $R\mathbf{x} = \mathbf{y}$ for $\mathbf{x}$.

QR via Householder

The Gram-Schmidt algorithm orthonormalizes A using a series of transformations that are stored in an upper triangular matrix. Another way to compute the QR decomposition is to take the opposite approach: triangularize A through a series of orthonormal transformations. Orthonormal transformations are numerically stable, meaning that they are less susceptible to rounding errors. In fact, this approach is usually faster and more accurate than Gram-Schmidt methods.

The idea is for the kth orthonormal transformation Q_k to map the kth column of A to the span of $\{\mathbf{e}_j\}_{j=1}^k$, where the $\mathbf{e}_j$ are the standard basis vectors in $\mathbb{R}^m$. In addition, to preserve the work of the previous transformations, Q_k should not modify any entries of A that are above or to the left of the kth diagonal term of A. For a 4×3 matrix A, the process can be visualized as follows.

$$Q_3Q_2Q_1\begin{bmatrix}\boxed{\begin{matrix}*&*&*\\*&*&*\\*&*&*\\*&*&*\end{matrix}}\end{bmatrix} = Q_3Q_2\begin{bmatrix}*&*&*\\0&\boxed{\begin{matrix}*&*\\*&*\\*&*\end{matrix}}\end{bmatrix} = Q_3\begin{bmatrix}*&*&*\\0&*&*\\0&0&\boxed{\begin{matrix}*\\*\\*\end{matrix}}\end{bmatrix} = \begin{bmatrix}*&*&*\\0&*&*\\0&0&*\\0&0&0\end{bmatrix}$$

Thus $Q_3Q_2Q_1A = R$, so that $A = Q_1^\mathsf{T}Q_2^\mathsf{T}Q_3^\mathsf{T}R$ since each Q_k is orthonormal. Furthermore, the product of square orthonormal matrices is orthonormal, so setting $Q = Q_1^\mathsf{T}Q_2^\mathsf{T}Q_3^\mathsf{T}$ yields the full QR decomposition.

How to correctly construct each Q_k isn't immediately obvious. The ingenious solution lies in one of the basic types of linear transformations: reflections.

[2]See Problem 3 of the Linear Systems lab for details on back substitution.

Householder Transformations

The *orthogonal complement* of a nonzero vector $\mathbf{v} \in \mathbb{R}^n$ is the set of all vectors $\mathbf{x} \in \mathbb{R}^n$ that are orthogonal to $\mathbf{v}$, denoted $\mathbf{v}^\perp = \{\mathbf{x} \in \mathbb{R}^n \mid \langle \mathbf{x}, \mathbf{v} \rangle = 0\}$. A *Householder transformation* is a linear transformation that reflects a vector $\mathbf{x}$ across the orthogonal complement $\mathbf{v}^\perp$ for some specified $\mathbf{v}$.

The matrix representation of the Householder transformation corresponding to $\mathbf{v}$ is given by $H_\mathbf{v} = I - 2\frac{\mathbf{v}\mathbf{v}^\mathsf{T}}{\mathbf{v}^\mathsf{T}\mathbf{v}}$. Since $H_\mathbf{v}^\mathsf{T} H_\mathbf{v} = I$, Householder transformations are orthonormal.

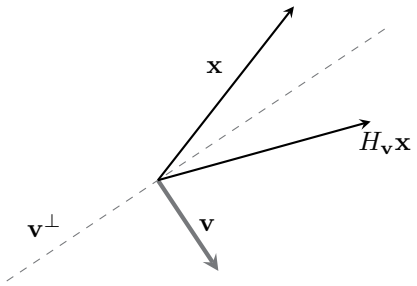


Figure 3.1: The vector $\mathbf{v}$ defines the orthogonal complement $\mathbf{v}^\perp$, which in this case is a line. Applying the Householder transformation $H_\mathbf{v}$ to $\mathbf{x}$ reflects $\mathbf{x}$ across $\mathbf{v}^\perp$.

Householder Triangularization

The *Householder algorithm* uses Householder transformations for the orthonormal transformations in the QR decomposition process described on the previous page. The goal in choosing Q_k is to send $\mathbf{x}_k$, the kth column of A, to the span of $\{\mathbf{e}_j\}_{j=1}^k$. In other words, if $Q_k\mathbf{x}_k = \mathbf{y}_k$, the last $m-k$ entries of $\mathbf{y}_k$ should be 0.

$$Q_k\mathbf{x}_k = Q_k \begin{bmatrix} z_1 \\ \vdots \\ z_k \\ z_{k+1} \\ \vdots \\ z_m \end{bmatrix} = \begin{bmatrix} y_1 \\ \vdots \\ y_k \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \mathbf{y}_k$$

To begin, decompose $\mathbf{x}_k$ into $\mathbf{x}_k = \mathbf{x}_k' + \mathbf{x}_k''$, where $\mathbf{x}_k'$ and $\mathbf{x}_k''$ are of the form

$$\mathbf{x}_k' = [z_1 \quad \cdots \quad z_{k-1} \quad 0 \quad \cdots \quad 0]^\mathsf{T} \qquad \text{and} \qquad \mathbf{x}_k'' = [0 \quad \cdots \quad 0 \quad z_k \quad \cdots \quad z_m]^\mathsf{T}.$$

Because $\mathbf{x}_k'$ represents elements of A that lie above the diagonal, only $\mathbf{x}_k''$ needs to be altered by the reflection.

The two vectors $\mathbf{x}_k'' \pm \|\mathbf{x}_k''\|\mathbf{e}_k$ both yield Householder transformations that send $\mathbf{x}_k''$ to the span of $\mathbf{e}_k$ (see Figure 3.2). Between the two, the one that reflects $\mathbf{x}_k''$ further is more numerically stable. This reflection corresponds to

$$\mathbf{v}_k = \mathbf{x}_k'' + \operatorname{sign}(z_k)\|\mathbf{x}_k''\|\mathbf{e}_k,$$

where z_k is the first nonzero component of $\mathbf{x}_k''$ (the kth component of $\mathbf{x}_k$).

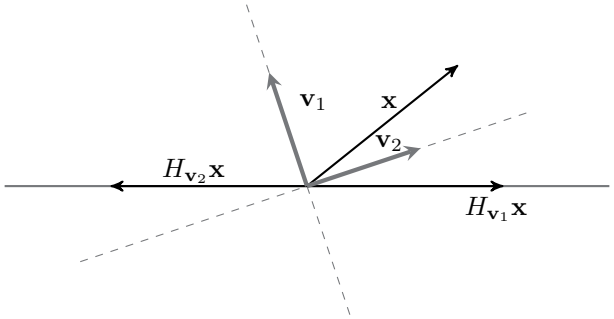


Figure 3.2: There are two possible reflections that map $\mathbf{x}$ into the span of $\mathbf{e}_1$, defined by the vectors $\mathbf{v}_1$ and $\mathbf{v}_2$. In this illustration, $H_{\mathbf{v}_2}$ is the more stable transformation since it reflects $\mathbf{x}$ further than $H_{\mathbf{v}_1}$.

After choosing $\mathbf{v}_k$, set $\mathbf{u}_k = \frac{\mathbf{v}_k}{\|\mathbf{v}_k\|}$. Then $H_{\mathbf{v}_k} = I - 2\frac{\mathbf{v}_k\mathbf{v}_k^\mathsf{T}}{\|\mathbf{v}_k\|^2} = I - 2\mathbf{u}_k\mathbf{u}_k^\mathsf{T}$, and hence Q_k is given by the following block matrix.

$$Q_k = \begin{bmatrix} I_{k-1} & \mathbf{0} \\ \mathbf{0} & H_{\mathbf{v}_k} \end{bmatrix} = \begin{bmatrix} I_{k-1} & \mathbf{0} \\ \mathbf{0} & I_{m-k+1} - 2\mathbf{u}_k\mathbf{u}_k^\mathsf{T} \end{bmatrix}$$

Here I_p denotes the $p \times p$ identity matrix, and thus each Q_k is $m \times m$.

It is apparent from its form that Q_k does not affect the first $k-1$ rows and columns of any matrix that it acts on. Then by starting with $R = A$ and $Q = I$, at each step of the algorithm we need only multiply the entries in the lower right $(m-k+1) \times (m-k+1)$ submatrices of R and Q by $I - 2\mathbf{u}_k\mathbf{u}_k^\mathsf{T}$. This completes the Householder algorithm, detailed below.

Algorithm 3.2

procedure HOUSEHOLDER(A)
  $m, n \leftarrow \text{shape}(A)$
  $R \leftarrow \text{copy}(A)$
  $Q \leftarrow I_m$ ▷ The $m \times m$ identity matrix.
  for $k = 0 \dots n-1$ **do**
    $\mathbf{u} \leftarrow \text{copy}(R_{k:,k})$
    $u_0 \leftarrow u_0 + \text{sign}(u_0)\|\mathbf{u}\|$ ▷ u_0 is the first entry of $\mathbf{u}$.
    $\mathbf{u} \leftarrow \mathbf{u}/\|\mathbf{u}\|$ ▷ Normalize $\mathbf{u}$.
    $R_{k:,k:} \leftarrow R_{k:,k:} - 2\mathbf{u}\left(\mathbf{u}^\mathsf{T}R_{k:,k:}\right)$ ▷ Apply the reflection to R.
    $Q_{k:,:} \leftarrow Q_{k:,:} - 2\mathbf{u}\left(\mathbf{u}^\mathsf{T}Q_{k:,:}\right)$ ▷ Apply the reflection to Q.
  return Q^T, R

Problem 4. Write a function that accepts as input a $m \times n$ matrix A of rank n. Use Algorithm 3.2 to compute the full QR decomposition of A.

Consider the following implementation details.

- NumPy's `np.sign()` is an easy way to implement the sign() operation in step 7. However, `np.sign(0)` returns 0, which will cause a problem in the rare case that $u_0 = 0$ (which is possible if the top left entry of A is 0 to begin with). The following code defines a function that returns the sign of a single number, counting 0 as positive.

```
sign = lambda x: 1 if x >= 0 else -1
```

- In steps 9 and 10, the multiplication of $\mathbf{u}$ and $(\mathbf{u}^\mathsf{T}X)$ is an *outer product* ($\mathbf{x}\mathbf{y}^\mathsf{T}$ instead of the usual $\mathbf{x}^\mathsf{T}\mathbf{y}$). Use `np.outer()` instead of `np.dot()` to handle this correctly.

  Use NumPy and SciPy to generate test cases and validate your function.

```
>>> A = np.random.random((5, 3))
>>> Q,R = la.qr(A)                  # Get the full QR decomposition.
>>> print(A.shape, Q.shape, R.shape)
(5,3) (5,5) (5,3)
>>> np.allclose(Q @ R, A)
True
```

Upper Hessenberg Form

An *upper Hessenberg matrix* is a square matrix that is nearly upper triangular, with zeros below the first subdiagonal. Every $n \times n$ matrix A can be written $A = QHQ^\mathsf{T}$ where Q is orthonormal and H, called the *Hessenberg form* of A, is an upper Hessenberg matrix. Putting a matrix in upper Hessenberg form is an important first step to computing its eigenvalues numerically.

This algorithm also uses Householder transformations. To find orthogonal Q and upper Hessenberg H such that $A = QHQ^\mathsf{T}$, it suffices to find such matrices that satisfy $Q^\mathsf{T}AQ = H$. Thus, the strategy is to multiply A on the left and right by a series of orthonormal matrices until it is in Hessenberg form.

Using the same Q_k as in the kth step of the Householder algorithm introduces $n-k$ zeros in the kth column of A, but multiplying Q_kA on the right by Q_k^T destroys all of those zeros. Instead, choose a Q_1 that fixes $\mathbf{e}_1$ and reflects the first column of A into the span of $\mathbf{e}_1$ and $\mathbf{e}_2$. The product Q_1A then leaves the first row of A alone, and the product $(Q_1A)Q_1^\mathsf{T}$ leaves the first column of (Q_1A) alone.

$$\begin{bmatrix} * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \end{bmatrix} \xrightarrow{Q_1} \begin{bmatrix} * & * & * & * & * \\ * & * & * & * & * \\ 0 & * & * & * & * \\ 0 & * & * & * & * \\ 0 & * & * & * & * \end{bmatrix} \xrightarrow{Q_1^\mathsf{T}} \begin{bmatrix} * & * & * & * & * \\ * & * & * & * & * \\ 0 & * & * & * & * \\ 0 & * & * & * & * \\ 0 & * & * & * & * \end{bmatrix}$$
$$A \qquad\qquad Q_1A \qquad\qquad (Q_1A)Q_1^\mathsf{T}$$

Continuing the process results in the upper Hessenberg form of A.

$$Q_3Q_2Q_1AQ_1^\mathsf{T}Q_2^\mathsf{T}Q_3^\mathsf{T} = \begin{bmatrix} * & * & * & * & * \\ * & * & * & * & * \\ 0 & * & * & * & * \\ 0 & 0 & * & * & * \\ 0 & 0 & 0 & * & * \end{bmatrix}$$

This implies that $A = Q_1^\mathsf{T} Q_2^\mathsf{T} Q_3^\mathsf{T} H Q_3 Q_2 Q_1$, so setting $Q = Q_1^\mathsf{T} Q_2^\mathsf{T} Q_3^\mathsf{T}$ results in the desired factorization $A = QHQ^\mathsf{T}$.

Constructing the Reflections

Constructing the Q_k uses the same approach as in the Householder algorithm, but shifted down one element. Let $\mathbf{x}_k = \mathbf{y}'_k + \mathbf{y}''_k$ where $\mathbf{y}'_k$ and $\mathbf{y}''_k$ are of the form

$$\mathbf{y}'_k = [z_1 \quad \cdots \quad z_k \quad 0 \quad \cdots \quad 0]^\mathsf{T} \qquad \text{and} \qquad \mathbf{y}''_k = [0 \quad \cdots \quad 0 \quad z_{k+1} \quad \cdots \quad z_m]^\mathsf{T}.$$

Because $\mathbf{y}'_k$ represents elements of A that lie above the first subdiagonal, only $\mathbf{y}''_k$ needs to be altered. This suggests using the following reflection.

$$\mathbf{v}_k = \mathbf{y}''_k + \operatorname{sign}(z_k)\|\mathbf{y}''_k\|\mathbf{e}_k \qquad\qquad \mathbf{u}_k = \frac{\mathbf{v}_k}{\|\mathbf{v}_k\|}$$

$$Q_k = \begin{bmatrix} I_k & \mathbf{0} \\ \mathbf{0} & H_{\mathbf{v}_k} \end{bmatrix} = \begin{bmatrix} I_k & \mathbf{0} \\ \mathbf{0} & I_{m-k} - 2\mathbf{u}_k\mathbf{u}_k^\mathsf{T} \end{bmatrix}$$

The complete algorithm is given below. Note how similar it is to Algorithm 3.2.

Algorithm 3.3

procedure HESSENBERG(A)
  $m, n \leftarrow \text{shape}(A)$
  $H \leftarrow \text{copy}(A)$
  $Q \leftarrow I_m$
  for $k = 0 \ldots n-3$ **do**
    $\mathbf{u} \leftarrow \text{copy}(H_{k+1:,k})$
    $u_0 \leftarrow u_0 + \text{sign}(u_0)\|\mathbf{u}\|$
    $\mathbf{u} \leftarrow \mathbf{u}/\|\mathbf{u}\|$
    $H_{k+1:,k:} \leftarrow H_{k+1:,k:} - 2\mathbf{u}(\mathbf{u}^\mathsf{T} H_{k+1:,k:})$ ▷ Apply Q_k to H.
    $H_{:,k+1:} \leftarrow H_{:,k+1:} - 2(H_{:,k+1:}\mathbf{u})\mathbf{u}^\mathsf{T}$ ▷ Apply Q_k^T to H.
    $Q_{k+1:,:} \leftarrow Q_{k+1:,:} - 2\mathbf{u}(\mathbf{u}^\mathsf{T} Q_{k+1:,:})$ ▷ Apply Q_k to Q.
  return H, Q^T

Problem 5. Write a function that accepts a nonsingular $n \times n$ matrix A. Use Algorithm 3.3 to compute the upper Hessenberg H and orthogonal Q satisfying $A = QHQ^\mathsf{T}$.

Compare your results to `scipy.linalg.hessenberg()`.

```
# Generate a random matrix and get its upper Hessenberg form via SciPy.
>>> A = np.random.random((8,8))
>>> H, Q = la.hessenberg(A, calc_q=True)

# Verify that H has all zeros below the first subdiagonal and QHQ^T = A.
>>> np.allclose(np.triu(H, -1), H)
True
>>> np.allclose(Q @ H @ Q.T, A)
```

```
True
```

Additional Material

Complex QR Decomposition

The QR decomposition also exists for matrices with complex entries. The standard inner product in $\mathbb{R}^m$ is $\langle \mathbf{x}, \mathbf{y} \rangle = \mathbf{x}^\mathsf{T}\mathbf{y}$, but the (more general) standard inner product in $\mathbb{C}^m$ is $\langle \mathbf{x}, \mathbf{y} \rangle = \mathbf{x}^\mathsf{H}\mathbf{y}$. The $^\mathsf{H}$ stands for the *Hermitian conjugate*, the conjugate of the transpose. Making a few small adjustments in the implementations of Algorithms 3.1 and 3.2 accounts for using the complex inner product.

1. Replace any transpose operations with the conjugate of the transpose.

```
>>> A = np.reshape(np.arange(4) + 1j*np.arange(4), (2,2))
>>> print(A)
[[ 0.+0.j  1.+1.j]
 [ 2.+2.j  3.+3.j]]

>>> print(A.T)                      # Regular transpose.
[[ 0.+0.j  2.+2.j]
 [ 1.+1.j  3.+3.j]]

>>> print(A.conj().T)               # Hermitian conjugate.
[[ 0.-0.j  2.-2.j]
 [ 1.-1.j  3.-3.j]]
```

2. Conjugate the first entry of vector or matrix multiplication before multiplying with `np.dot()`.

```
>>> x = np.arange(2) + 1j*np.arange(2)
>>> print(x)
[ 0.+0.j  1.+1.j]

>>> np.dot(x, x)                    # Standard real inner product.
2j

>>> np.dot(x.conj(), y)             # Standard complex inner product.
(2 + 0j)
```

3. In the complex plane, there are infinitely many reflections that map a vector $\mathbf{x}$ into the span of $\mathbf{e}_k$, not just the two displayed in Figure 3.2. Using $\text{sign}(z_k)$ to choose one is still a valid method, but it requires updating the `sign()` function so that it can handle complex numbers.

```
sign = lambda x: 1 if np.real(x) >= 0 else -1
```

QR with Pivoting

The LU decomposition can be improved by employing Gaussian elimination with partial pivoting, where the rows of A are strategically permuted at each iteration. The QR factorization can be similarly improved by permuting the columns of A at each iteration. The result is the factorization $AP = QR$, where P is a permutation matrix that encodes the column swaps. To compute the pivoted QR decomposition with `scipy.linalg.qr()`, set the keyword `pivoting` to `True`.

```
# Get the decomposition AP = QR for a random matrix A.
>>> A = np.random.random((8,10))
>>> Q,R,P = la.qr(A, pivoting=True)

# P is returned as a 1-D array that encodes column ordering,
# so A can be reconstructed with fancy indexing.
>>> np.allclose(Q @ R, A[:,P])
True
```

QR via Givens

The Householder algorithm uses reflections to triangularize A. However, A can also be made upper triangular using rotations. To illustrate the idea, recall that the following matrix represents a counterclockwise rotation of θ radians.

$$R_\theta = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}$$

This transformation is orthonormal. Given $\mathbf{x} = [a, b]^\mathsf{T}$, if θ is the angle between $\mathbf{x}$ and $\mathbf{e}_1$, then $R_{-\theta}$ maps $\mathbf{x}$ to the span of $\mathbf{e}_1$.

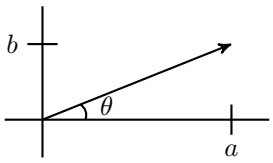


Figure 3.3: Rotating clockwise by θ sends the vector $[a, b]^\mathsf{T}$ to the span of $\mathbf{e}_1$.

In terms of a and b, $\cos\theta = \frac{a}{\sqrt{a^2+b^2}}$ and $\sin\theta = \frac{b}{\sqrt{a^2+b^2}}$. Therefore,

$$R_{-\theta}\mathbf{x} = \begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} \frac{a}{\sqrt{a^2+b^2}} & \frac{b}{\sqrt{a^2+b^2}} \\ -\frac{b}{\sqrt{a^2+b^2}} & \frac{a}{\sqrt{a^2+b^2}} \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} \sqrt{a^2+b^2} \\ 0 \end{bmatrix}.$$

The matrix R_θ above is an example of a 2×2 *Givens rotation matrix*. In general, the Givens matrix $G(i, j, \theta)$ represents the orthonormal transformation that rotates the 2-dimensional span of $\mathbf{e}_i$ and $\mathbf{e}_j$ by θ radians. The matrix representation of this transformation is a generalization of R_θ.

$$G(i, j, \theta) = \begin{bmatrix} I & 0 & 0 & 0 & 0 \\ 0 & c & 0 & -s & 0 \\ 0 & 0 & I & 0 & 0 \\ 0 & s & 0 & c & 0 \\ 0 & 0 & 0 & 0 & I \end{bmatrix}$$

Here I represents the identity matrix, $c = \cos\theta$, and $s = \sin\theta$. The c's appear on the i^{th} and j^{th} diagonal entries.

Givens Triangularization

As demonstrated, θ can be chosen such that $G(i, j, \theta)$ rotates a vector so that its jth-component is 0. Such a transformation will only affect the i^{th} and j^{th} entries of any vector it acts on (and thus the i^{th} and j^{th} rows of any matrix it acts on).

To compute the QR decomposition of A, iterate through the subdiagonal entries of A in the order depicted by Figure 3.4. Zero out the ij^{th} entry with a rotation in the plane spanned by $\mathbf{e}_{i-1}$ and $\mathbf{e}_i$, represented by the Givens matrix $G(i-1, i, \theta)$.

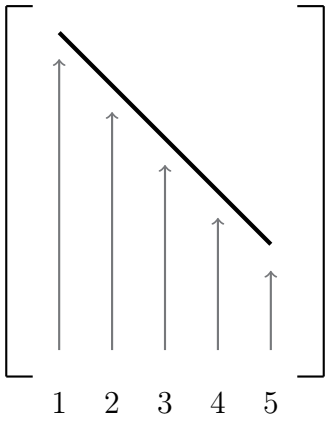


Figure 3.4: The order in which to zero out subdiagonal entries in the Givens triangularization algorithm. The heavy black line is the main diagonal of the matrix. Entries should be zeroed out from bottom to top in each column, beginning with the leftmost column.

On a 2×3 matrix, the process can be visualized as follows.

$$\begin{bmatrix} * & * \\ * & * \\ * & * \end{bmatrix} \xrightarrow{G(2,3,\theta_1)} \begin{bmatrix} * & * \\ \boxed{*} & \boxed{*} \\ \boxed{0} & \boxed{*} \end{bmatrix} \xrightarrow{G(1,2,\theta_2)} \begin{bmatrix} \boxed{*} & \boxed{*} \\ \boxed{0} & \boxed{*} \\ 0 & * \end{bmatrix} \xrightarrow{G(2,3,\theta_3)} \begin{bmatrix} * & * \\ 0 & \boxed{*} \\ 0 & \boxed{0} \end{bmatrix}$$

At each stage, the boxed entries are those modified by the previous transformation. The final transformation $G(2, 3, \theta_3)$ operates on the bottom two rows, but since the first two entries are zero, they are unaffected.

Assuming that at the ij^{th} stage of the algorithm a_{ij} is nonzero, Algorithm 3.4 computes the Givens triangularization of a matrix. Notice that the algorithm does not actually form the entire matrices $G(i, j, \theta)$; instead, it modifies only those entries of the matrix that are affected by the transformation.

Algorithm 3.4

procedure GIVENS TRIANGULARIZATION(A)
  $m, n \leftarrow \text{shape}(A)$
  $R \leftarrow \text{copy}(A)$
  $Q \leftarrow I_m$
  for $j = 0 \dots n-1$ **do**
    for $i = m-1 \dots j+1$ **do**
      $a, b \leftarrow R_{i-1,j}, R_{i,j}$
      $G \leftarrow [[a, b], [-b, a]]/\sqrt{a^2+b^2}$
      $R_{i-1:i+1,j:} \leftarrow GR_{i-1:i+1,j:}$
      $Q_{i-1:i+1,:} \leftarrow GQ_{i-1:i+1,:}$
  return Q^T, R

QR of a Hessenberg Matrix via Givens

The Givens algorithm is particularly efficient for computing the QR decomposition of a matrix that is already in upper Hessenberg form, since only the first subdiagonal needs to be zeroed out. Algorithm 3.5 details this process.

Algorithm 3.5

procedure GIVENS TRIANGULARIZATION OF HESSENBERG(H)
  $m, n \leftarrow \text{shape}(H)$
  $R \leftarrow \text{copy}(H)$
  $Q \leftarrow I_m$
  for $j = 0 \dots \min\{n-1, m-1\}$ **do**
    $i = j + 1$
    $a, b \leftarrow R_{i-1,j}, R_{i,j}$
    $G \leftarrow [[a, b], [-b, a]]/\sqrt{a^2+b^2}$
    $R_{i-1:i+1,j:} \leftarrow GR_{i-1:i+1,j:}$
    $Q_{i-1:i+1,:i+1} \leftarrow GQ_{i-1:i+1,:i+1}$
  return Q^T, R

> **NOTE**
>
> When A is symmetric, its upper Hessenberg form is a *tridiagonal* matrix, meaning its only nonzero entries are on the main diagonal, the first subdiagonal, and the first superdiagonal. This is because the Q_k's zero out everything below the first subdiagonal of A and the Q_k^T's zero out everything to the right of the first superdiagonal. Tridiagonal matrices make computations fast, so computing the Hessenberg form of a symmetric matrix is very useful.

4 Least Squares and Computing Eigenvalues

Lab Objective: *Because of its numerical stability and convenient structure, the QR decomposition is the basis of many important and practical algorithms. In this lab, we introduce linear least squares problems, tools in Python for computing least squares solutions, and two fundamental algorithms for computing eigenvalue. The QR decomposition makes solving several of these problems quick and numerically stable.*

Least Squares

A linear system $A\mathbf{x} = \mathbf{b}$ is *overdetermined* if it has more equations than unknowns. In this situation, there is no true solution, and $\mathbf{x}$ can only be approximated.

The *least squares solution* of $A\mathbf{x} = \mathbf{b}$, denoted $\widehat{\mathbf{x}}$, is the "closest" vector to a solution, meaning it minimizes the quantity $\|A\widehat{\mathbf{x}} - \mathbf{b}\|_2$. In other words, $\widehat{\mathbf{x}}$ is the vector such that $A\widehat{\mathbf{x}}$ is the projection of $\mathbf{b}$ onto the range of A, and can be calculated by solving the *normal equations*:[1]

$$A^\mathsf{T}A\widehat{\mathbf{x}} = A^\mathsf{T}\mathbf{b}$$

If A is full rank (which it usually is in applications) its QR decomposition provides an efficient way to solve the normal equations. Let $A = \widehat{Q}\widehat{R}$ be the reduced QR decomposition of A, so $\widehat{Q}$ is $m \times n$ with orthonormal columns and $\widehat{R}$ is $n \times n$, invertible, and upper triangular. Since $\widehat{Q}^\mathsf{T}\widehat{Q} = I$, and since $\widehat{R}^\mathsf{T}$ is invertible, the normal equations can be reduced as follows (we omit the hats on $\widehat{Q}$ and $\widehat{R}$ for clarity):

$$\begin{aligned}
A^\mathsf{T}A\widehat{\mathbf{x}} &= A^\mathsf{T}\mathbf{b} \\
(QR)^\mathsf{T}QR\widehat{\mathbf{x}} &= (QR)^\mathsf{T}\mathbf{b} \\
R^\mathsf{T}Q^\mathsf{T}QR\widehat{\mathbf{x}} &= R^\mathsf{T}Q^\mathsf{T}\mathbf{b} \\
R^\mathsf{T}R\widehat{\mathbf{x}} &= R^\mathsf{T}Q^\mathsf{T}\mathbf{b} \\
R\widehat{\mathbf{x}} &= Q^\mathsf{T}\mathbf{b}
\end{aligned} \tag{4.1}$$

Thus $\widehat{\mathbf{x}}$ is the least squares solution to $A\mathbf{x} = \mathbf{b}$ if and only if $\widehat{R}\widehat{\mathbf{x}} = \widehat{Q}^\mathsf{T}\mathbf{b}$. Since $\widehat{R}$ is upper triangular, this equation can be solved quickly with back substitution.

[1] See Chapter 3 of Volume I for a formal derivation of the normal equations.

Problem 1. Write a function that accepts an $m \times n$ matrix A of rank n and a vector $\mathbf{b}$ of length n. Use the QR decomposition and (4.1) to solve the normal equations corresponding to $A\mathbf{x} = \mathbf{b}$.

You may use either SciPy's QR routine or one of your own QR routines. In addition, you may use `la.solve_triangular()`, SciPy's optimized routine for solving triangular systems.

Fitting a Line

The least squares solution can be used to find the best fit curve of a chosen type to a set of points. Consider the problem of finding the line $y = ax + b$ that best fits a set of m points $\{(x_k, y_k)\}_{k=1}^m$. Ideally, we seek a and b such that $y_k = ax_k + b$ for all k. The following linear system simultaneously represents all of these equations.

$$A\mathbf{x} = \begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ x_3 & 1 \\ \vdots & \vdots \\ x_m & 1 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_m \end{bmatrix} = \mathbf{b} \tag{4.2}$$

Note that A has full column rank as long as not all of the x_k values are the same.

Because this system has two unknowns, it is guaranteed to have a solution if it has two or fewer equations. However, if there are more than two data points, the system is overdetermined if any set of three points is not collinear. We therefore seek a least squares solution, which in this case means finding the slope $\widehat{a}$ and y-intercept $\widehat{b}$ such that the line $y = \widehat{a}x + \widehat{b}$ best fits the data.

Figure 4.1 is a typical example of this idea where $\widehat{a} \approx \frac{1}{2}$ and $\widehat{b} \approx -3$.

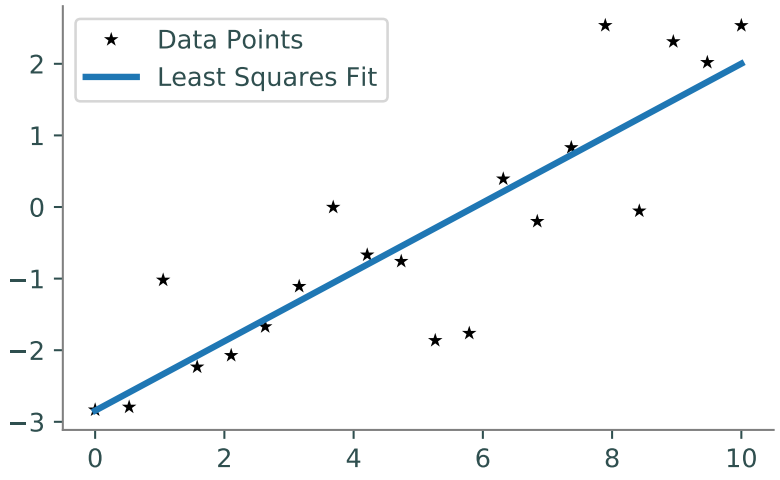


Figure 4.1

Problem 2. The file `housing.npy` contains the purchase-only housing price index, a measure of how housing prices are changing, for the United States from 2000 to 2010.[a] Each row in the array is a separate measurement; the columns are the year and the price index, in that order. To avoid large numerical computations, the year measurements start at 0 instead of 2000.

Find the least squares line that relates the year to the housing price index (i.e., let year be the x-axis and index the y-axis).

1. Construct the matrix A and the vector $\mathbf{b}$ described by (4.2).
   (Hint: `np.vstack()`, `np.column_stack()`, and/or `np.ones()` may be helpful.)
2. Use your function from Problem 1 to find the least squares solution.
3. Plot the data points as a scatter plot.
4. Plot the least squares line with the scatter plot.

[a] See `http://www.fhfa.gov/DataTools/Downloads/Pages/House-Price-Index.aspx`.

Note

The least squares problem of fitting a line to a set of points is often called *linear regression*, and the resulting line is called the *linear regression line*. SciPy's specialized tool for linear regression is `scipy.stats.linregress()`. This function takes in an array of x-coordinates and a corresponding array of y-coordinates, and returns the slope and intercept of the regression line, along with a few other statistical measurements.

For example, the following code produces Figure 4.1.

```
>>> import numpy as np
>>> from scipy.stats import linregress

# Generate some random data close to the line y = .5x - 3.
>>> x = np.linspace(0, 10, 20)
>>> y = .5*x - 3 + np.random.randn(20)

# Use linregress() to calculate m and b, as well as the correlation
# coefficient, p-value, and standard error. See the documentation for
# details on each of these extra return values.
>>> a, b, rvalue, pvalue, stderr = linregress(x, y)

>>> plt.plot(x, y, 'k*', label="Data Points")
>>> plt.plot(x, a*x + b, label="Least Squares Fit")
>>> plt.legend(loc="upper left")
>>> plt.show()
```

Fitting a Polynomial

Least squares can also be used to fit a set of data to the best fit polynomial of a specified degree. Let $\{(x_k, y_k)\}_{k=1}^m$ be the set of m data points in question. The general form for a polynomial of degree n is as follows:

$$p_n(x) = c_n x^n + c_{n-1}x^{n-1} + \cdots + c_2 x^2 + c_1 x + c_0$$

Note that the polynomial is uniquely determined by its $n+1$ coefficients $\{c_k\}_{k=0}^n$. Ideally, then, we seek the set of coefficients $\{c_k\}_{k=0}^n$ such that

$$y_k = c_n x_k^n + c_{n-1}x_k^{n-1} + \cdots + c_2 x_k^2 + c_1 x_k + c_0$$

for all values of k. These m linear equations yield the following linear system:

$$A\mathbf{x} = \begin{bmatrix} x_1^n & x_1^{n-1} & \cdots & x_1^2 & x_1 & 1 \\ x_2^n & x_2^{n-1} & \cdots & x_2^2 & x_2 & 1 \\ x_3^n & x_3^{n-1} & \cdots & x_3^2 & x_3 & 1 \\ \vdots & \vdots & & \vdots & \vdots & \vdots \\ x_m^n & x_m^{n-1} & \cdots & x_m^2 & x_m & 1 \end{bmatrix} \begin{bmatrix} c_n \\ c_{n-1} \\ \vdots \\ c_2 \\ c_1 \\ c_0 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_m \end{bmatrix} = \mathbf{b} \tag{4.3}$$

If $m > n+1$ this system is overdetermined, requiring a least squares solution.

Working with Polynomials in NumPy

The $m \times (n+1)$ matrix A of (4.3) is called a *Vandermonde matrix*.[2] NumPy's `np.vander()` is a convenient tool for quickly constructing a Vandermonde matrix, given the values $\{x_k\}_{k=1}^m$ and the number of desired columns.

```
>>> print(np.vander([2, 3, 5], 2))
[[2 1]                              # [[2**1, 2**0]
 [3 1]                              #  [3**1, 3**0]
 [5 1]]                             #  [5**1, 5**0]]

>>> print(np.vander([2, 3, 5, 4], 3))
[[ 4  2  1]                         # [[2**2, 2**1, 2**0]
 [ 9  3  1]                         #  [3**2, 3**1, 3**0]
 [25  5  1]                         #  [5**2, 5**1, 5**0]
 [16  4  1]]                        #  [4**2, 4**1, 4**0]
```

NumPy also has powerful tools for working efficiently with polynomials. The class `np.poly1d` represents a 1-dimensional polynomial. Instances of this class are callable like a function.[3] The constructor accepts the polynomial's coefficients, from largest degree to smallest.

Table 4.1 lists some attributes and methods of the `np.poly1d` class.

[2] Vandermonde matrices have many special properties and are useful for many applications, including polynomial interpolation and discrete Fourier analysis.

[3] Class instances can be made callable by implementing the `__call__()` magic method.

Attribute	Description
`coeffs`	The $n+1$ coefficients, from greatest degree to least.
`order`	The polynomial degree (n).
`roots`	The $n-1$ roots.
Method	Returns
`deriv()`	The coefficients of the polynomial after being differentiated.
`integ()`	The coefficients of the polynomial after being integrated (with $c_0 = 0$).

Table 4.1: Attributes and methods of the `np.poly1d` class.

```
# Create a callable object for the polynomial f(x) = (x-1)(x-2) = x^2 - 3x + 2.
>>> f = np.poly1d([1, -3, 2])
>>> print(f)
   2
1 x - 3 x + 2

# Evaluate f(x) for several values of x in a single function call.
>>> f([1, 2, 3, 4])
array([0, 0, 2, 6])
```

Problem 3. The data in `housing.npy` is nonlinear, and might be better fit by a polynomial than a line.

Write a function that uses (4.3) to calculate the polynomials of degree 3, 6, 9, and 12 that best fit the data. Plot the original data points and each least squares polynomial together in individual subplots.
(Hint: define a separate, refined domain with `np.linspace()` and use this domain to smoothly plot the polynomials.)

Instead of using Problem 1 to solve the normal equations, you may use SciPy's least squares routine, `scipy.linalg.lstsq()`.

```
>>> from scipy import linalg as la

# Define A and b appropriately.

# Solve the normal equations using SciPy's least squares routine.
# The least squares solution is the first of four return values.
>>> x = la.lstsq(A, b)[0]
```

Compare your results to `np.polyfit()`. This function receives an array of x values, an array of y values, and an integer for the polynomial degree, and returns the coefficients of the best fit polynomial of that degree.

ACHTUNG!

Having more parameters in a least squares model is not always better. For a set of m points, the best fit polynomial of degree $m-1$ *interpolates* the data set, meaning that $p(x_k) = y_k$ exactly for each k. In this case there are enough unknowns that the system is no longer overdetermined. However, such polynomials are highly subject to numerical errors and are unlikely to accurately represent true patterns in the data.

Choosing to have too many unknowns in a fitting problem is (fittingly) called *overfitting*, and is an important issue to avoid in any statistical model.

Fitting a Circle

Suppose the set of m points $\{(x_k, y_k)\}_{k=1}^m$ are arranged in a nearly circular pattern. The general equation of a circle with radius r and center (c_1, c_2) is as follows:

$$(x-c_1)^2 + (y-c_2)^2 = r^2. \tag{4.4}$$

The circle is uniquely determined by r, c_1, and c_2, so these are the parameters that should be solved for in a least squares formulation of the problem. However, (4.4) is not linear in any of these variables.

$$\begin{aligned} (x-c_1)^2 + (y-c_2)^2 &= r^2 \\ x^2 - 2c_1x + c_1^2 + y^2 - 2c_2y + c_2^2 &= r^2 \\ x^2 + y^2 &= 2c_1x + 2c_2y + r^2 - c_1^2 - c_2^2 \end{aligned} \tag{4.5}$$

The quadratic terms x^2 and y^2 are acceptable because the points $\{(x_k, y_k)\}_{k=1}^m$ are given. To eliminate the nonlinear terms in the unknown parameters r, c_1, and c_2, define a new variable $c_3 = r^2 - c_1^2 - c_2^2$. Then for each point (x_k, y_k), (4.5) becomes the following:

$$2c_1x_k + 2c_2y_k + c_3 = x_k^2 + y_k^2$$

These m equations are linear in c_1, c_2, and c_3, and can be written as a linear system.

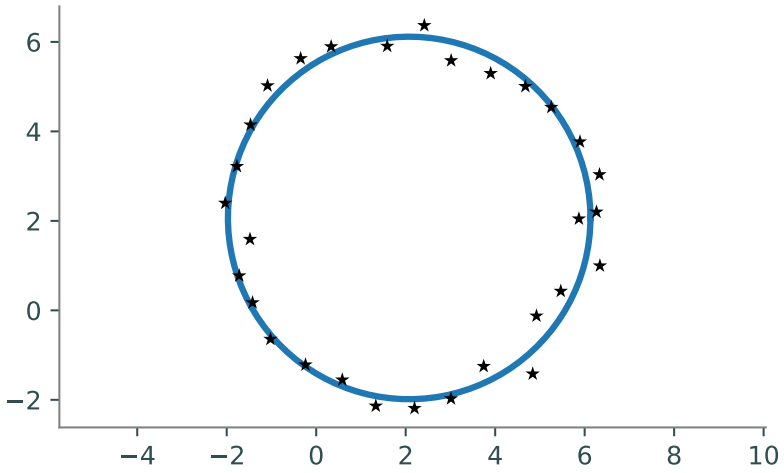
$$\begin{bmatrix} 2x_1 & 2y_1 & 1 \\ 2x_2 & 2y_2 & 1 \\ \vdots & \vdots & \vdots \\ 2x_m & 2y_m & 1 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix} = \begin{bmatrix} x_1^2 + y_1^2 \\ x_2^2 + y_2^2 \\ \vdots \\ x_m^2 + y_m^2 \end{bmatrix} \tag{4.6}$$

After solving for the least squares solution, r can be recovered with the relation $r = \sqrt{c_1^2 + c_2^2 + c_3}$. Finally, plotting a circle is best done with polar coordinates. Using the same variables as before, the circle can be represented in polar coordinates.

$$x = r\cos(\theta) + c_1, \qquad y = r\sin(\theta) + c_2, \qquad \theta \in [0, 2\pi] \tag{4.7}$$

To plot the circle, solve the least squares system for c_1, c_2, and r, define an array for θ, then use (4.7) to calculate the coordinates of the points the circle.

```
# Load some data and construct the matrix A and the vector b.
>>> xk, yk = np.load("circle.npy").T
>>> A = np.column_stack((2*xk, 2*yk, np.ones_like(xk)))
>>> b = xk**2 + yk**2

# Calculate the least squares solution and solve for the radius.
>>> c1, c2, c3 = la.lstsq(A, b)[0]
>>> r = np.sqrt(c1**2 + c2**2 + c3)

# Plot the circle using polar coordinates.
>>> theta = np.linspace(0, 2*np.pi, 200)
>>> x = r*np.cos(theta) + c1
>>> y = r*np.sin(theta) + c2
>>> plt.plot(x, y)                  # Plot the circle.
>>> plt.plot(xk, yk, 'k*')          # Plot the data points.
>>> plt.axis("equal")
```



Problem 4. The general equation for an ellipse is

$$ax^2 + bx + cxy + dy + ey^2 = 1.$$

Write a function that calculates the parameters for the ellipse that best fits the data in the file `ellipse.npy`. Plot the original data points and the ellipse together, using the following function to plot the ellipse.

```
def plot_ellipse(a, b, c, d, e):
    """Plot an ellipse of the form ax^2 + bx + cxy + dy + ey^2 = 1."""
    theta = np.linspace(0, 2*np.pi, 200)
    cos_t, sin_t = np.cos(theta), np.sin(theta)
```

```
    A = a*(cos_t**2) + c*cos_t*sin_t + e*(sin_t**2)
    B = b*cos_t + d*sin_t
    r = (-B + np.sqrt(B**2 + 4*A)) / (2*A)
    plt.plot(r*cos_t, r*sin_t, lw=2)
    plt.gca().set_aspect("equal", "datalim")
```

Computing Eigenvalues

The eigenvalues of an $n \times n$ matrix A are the roots of its characteristic polynomial $\det(A - \lambda I)$. Thus, finding the eigenvalues of A amounts to computing the roots of a polynomial of degree n. However, for $n \geq 5$, it is provably impossible to find an algebraic closed-form solution to this problem.[4] In addition, numerically computing the roots of a polynomial is a famously ill-conditioned problem, meaning that small changes in the coefficients of the polynomial (brought about by small changes in the entries of A) may yield wildly different results. Instead, eigenvalues must be computed with iterative methods.

The Power Method

The *dominant eigenvalue* of the $n \times n$ matrix A is the unique eigenvalue of greatest magnitude, if such an eigenvalue exists. The *power method* iteratively computes the dominant eigenvalue of A and its corresponding eigenvector.

Begin by choosing a vector $\mathbf{x}_0$ such that $\|\mathbf{x}_0\| = 1$, and define the following:

$$\mathbf{x}_{k+1} = \frac{A\mathbf{x}_k}{\|A\mathbf{x}_k\|}$$

If A has a dominant eigenvalue λ, and if the projection of $\mathbf{x}_0$ onto the subspace spanned by the eigenvectors corresponding to λ is nonzero, then the sequence of vectors $\{\mathbf{x}_k\}_{k=0}^{\infty}$ converges to an eigenvector $\mathbf{x}$ of A corresponding to λ.

Since $\mathbf{x}$ is an eigenvector of A, $A\mathbf{x} = \lambda\mathbf{x}$. Left multiplying by $\mathbf{x}^\mathsf{T}$ on each side gives $\mathbf{x}^\mathsf{T}A\mathbf{x} = \lambda\mathbf{x}^\mathsf{T}\mathbf{x}$, and hence $\lambda = \frac{\mathbf{x}^\mathsf{T}A\mathbf{x}}{\mathbf{x}^\mathsf{T}\mathbf{x}}$. This ratio is called the *Rayleigh quotient*. However, since each $\mathbf{x}_k$ is normalized, $\mathbf{x}^\mathsf{T}\mathbf{x} = \|\mathbf{x}\|^2 = 1$, so $\lambda = \mathbf{x}^\mathsf{T}A\mathbf{x}$.

The entire algorithm is summarized below.

Algorithm 4.1

```
procedure POWER METHOD(A)
    m, n ← shape(A)                          ▷ A is square so m = n.
    x_0 ← random(n)                          ▷ A random vector of length n
    x_0 ← x_0/‖x_0‖                          ▷ Normalize x_0
    for k = 1, 2, ..., N − 1 do
        x_{k+1} ← A x_k
        x_{k+1} ← x_{k+1}/‖x_{k+1}‖
    return x_N^T A x_N, x_N
```

[4] This result, called *Abel's impossibility theorem*, was first proven by Niels Heinrik Abel in 1824.

The power method is limited by a few assumptions. First, not all square matrices A have a dominant eigenvalue. However, the Perron-Frobenius theorem guarantees that if all entries of A are positive, then A has a dominant eigenvalue. Second, there is no way to choose an $\mathbf{x}_0$ that is guaranteed to have a nonzero projection onto the span of the eigenvectors corresponding to λ, though a random $\mathbf{x}_0$ will almost surely satisfy this condition. Even with these assumptions, a rigorous proof that the power method converges is most convenient with tools from spectral calculus.

Problem 5. Write a function that accepts an $n \times n$ matrix A, a maximum number of iterations N, and a stopping tolerance `tol`. Use Algorithm 4.1 to compute the dominant eigenvalue of A and a corresponding eigenvector. Continue the loop in step 5 until either $\|\mathbf{x}_{k+1} - \mathbf{x}_k\|$ is less than the tolerance `tol`, or until iterating the maximum number of times N.

Test your function on square matrices with all positive entries, verifying that $A\mathbf{x} = \lambda\mathbf{x}$. Use SciPy's eigenvalue solver, `scipy.linalg.eig()`, to compute all of the eigenvalues and corresponding eigenvectors of A and check that λ is the dominant eigenvalue of A.

```
# Construct a random matrix with positive entries.
>>> A = np.random.random((10,10))

# Compute the eigenvalues and eigenvectors of A via SciPy.
>>> eigs, vecs = la.eig(A)

# Get the dominant eigenvalue and eigenvector of A.
# The eigenvector of the kth eigenvalue is the kth column of 'vecs'.
>>> loc = np.argmax(eigs)
>>> lamb, x = eigs[loc], vecs[:,loc]

# Verify that Ax = lambda x.
>>> np.allclose(A @ x, lamb * x)
True
```

The QR Algorithm

An obvious shortcoming of the power method is that it only computes one eigenvalue and eigenvector. The QR algorithm, on the other hand, attempts to find all eigenvalues of A.

Let $A_0 = A$, and for arbitrary k let $Q_k R_k = A_k$ be the QR decomposition of A_k. Since A is square, so are Q_k and R_k, so they can be recombined in reverse order.

$$A_{k+1} = R_k Q_k$$

This recursive definition establishes an important relation between the A_k.

$$Q_k^{-1} A_k Q_k = Q_k^{-1}(Q_k R_k)Q_k = (Q_k^{-1}Q_k)(R_k Q_k) = A_{k+1}$$

Thus A_k is orthonormally similar to A_{k+1}, and similar matrices have the same eigenvalues. The series of matrices $\{A_k\}_{k=0}^{\infty}$ converges to the following block matrix.

$$S = \begin{bmatrix} S_1 & * & \cdots & * \\ \mathbf{0} & S_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & * \\ \mathbf{0} & \cdots & \mathbf{0} & S_m \end{bmatrix} \qquad \text{for example, } S = \begin{bmatrix} s_1 & * & * & \cdots & * \\ 0 & s_{2,1} & s_{2,2} & \cdots & * \\ & s_{2,3} & s_{2,4} & \cdots & * \\ & & & \ddots & \vdots \\ & & & & s_m \end{bmatrix}$$

Each S_i is either a 1×1 or 2×2 matrix.[5] In the example above on the right, since the first subdiagonal entry is zero, S_1 is the 1×1 matrix with a single entry, s_1. But as $s_{2,3}$ is not zero, S_2 is 2×2.

Since S is block upper triangular, its eigenvalues are the eigenvalues of its diagonal S_i blocks. Then because A is similar to each A_k, those eigenvalues of S are the eigenvalues of A.

When A has real entries but complex eigenvalues, 2×2 S_i blocks appear in S. Finding eigenvalues of a 2×2 matrix is equivalent to finding the roots of a 2nd degree polynomial, which has a closed form solution via the quadratic equation. This implies that complex eigenvalues come in conjugate pairs.

$$\begin{aligned} \det(S_i - \lambda I) = \begin{vmatrix} a-\lambda & b \\ c & d-\lambda \end{vmatrix} &= (a-\lambda)(d-\lambda) - bc \\ &= \lambda^2 - (a+d)\lambda + (ad-bc) \end{aligned} \tag{4.8}$$

Hessenberg Preconditioning

The QR algorithm works more accurately and efficiently on matrices that are in upper Hessenberg form, as upper Hessenberg matrices are already close to triangular. Furthermore, if $H = QR$ is the QR decomposition of upper Hessenberg H then RQ is also upper Hessenberg, so the almost-triangular form is preserved at each iteration. Putting a matrix in upper Hessenberg form before applying the QR algorithm is called *Hessenberg preconditioning*.

With preconditioning in mind, the entire QR algorithm is as follows.

Algorithm 4.2

```
1: procedure QR Algorithm(A, N)
2:     m, n ← shape(A)
3:     S ← hessenberg(A)                    ▷ Put A in upper Hessenberg form.
4:     for k = 0, 1, ..., N − 1 do
5:         Q, R ← qr(S)                     ▷ Get the QR decomposition of A_k.
6:         S ← RQ                           ▷ Recombine R_k and Q_k into A_{k+1}.
7:     eigs ← []                            ▷ Initialize an empty list of eigenvalues.
8:     i ← 0
9:     while i < n do
10:        if S_i is 1 × 1 then
11:            Append the only entry s_i of S_i to eigs
12:        else if S_i is 2 × 2 then
13:            Calculate the eigenvalues of S_i
14:            Append the eigenvalues of S_i to eigs
15:            i ← i + 1
16:        i ← i + 1                        ▷ Move to the next S_i.
17:    return eigs
```

[5] If all of the S_i are 1×1 matrices, then the upper triangular S is called the *Schur form* of A. If some of the S_i are 2×2 matrices, then S is called the *real Schur form* of A.

Problem 6. Write a function that accepts an $n \times n$ matrix A, a number of iterations N, and a tolerance `tol`. Use Algorithm 4.2 to implement the QR algorithm with Hessenberg preconditioning, returning the eigenvalues of A.

Consider the following implementation details.

- Use `scipy.linalg.hessenberg()` or your own Hessenburg algorithm to reduce A to upper Hessenberg form in step 3.
- The loop in step 4 should run for N total iterations.
- Use `scipy.linalg.qr()` or one of your own QR factorization routines to compute the QR decomposition of S in step 5. Note that since S is in upper Hessenberg form, Givens rotations are the most efficient way to produce Q and R.
- Assume that S_i is 1×1 in step 10 if one of two following criteria hold:
  - S_i is the last diagonal entry of S.
  - The absolute value of element below the ith main diagonal entry of S (the lower left element of the 2×2 block) is less than `tol`.
- If S_i is 2×2, use the quadratic formula and (4.8) to compute its eigenvalues. Use the function `cmath.sqrt()` to correctly compute the square root of a negative number.

Test your function on small random symmetric matrices, comparing your results to SciPy's `scipy.linalg.eig()`. To construct a random symmetric matrix, note that $A + A^\mathsf{T}$ is always symmetric.

Note

Algorithm 4.2 is theoretically sound, but can still be greatly improved. Most modern computer packages instead use the *implicit QR algorithm*, an improved version of the QR algorithm, to compute eigenvalues.

For large matrices, there are other iterative methods besides the power method and the QR algorithm for efficiently computing eigenvalues. They include the Arnoldi iteration, the Jacobi method, the Rayleigh quotient method, and others.

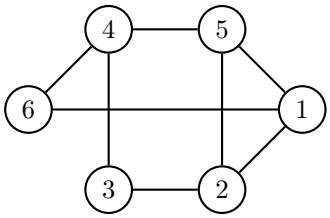
5 Image Segmentation

Lab Objective: *Graph theory has a variety of applications. A graph (or network) can be represented in many ways on a computer. In this lab, we study a common matrix representation for graphs and show how certain properties of the matrix representation correspond to inherent properties of the original graph. We also introduce tools for working with images in Python, and conclude with an application of using graphs and linear algebra to segment images.*

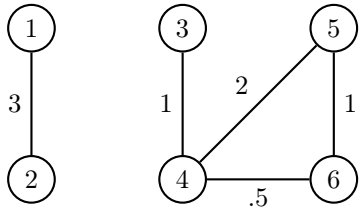
Graphs as Matrices

A *graph* is a mathematical structure that represents relationships between objects. Graphs are defined by $G = (V, E)$, where V is a set of *vertices* (or *nodes*) and E is a set of *edges*, each of which connects one node to another. A graph can be classified in several ways.

- The edges of an *undirected* graph are bidirectional: if an edge goes from node A to node B, then that same edge also goes from B to A. For example, the graphs G_1 and G_2 in Figure 5.1 are both undirected. In a *directed graph*, edges only go one way, usually indicated by an arrow pointing from one node to another. In this lab, we focus on undirected graphs.
- The edges of a *weighted* graph have a weight assigned to them, such as G_2. A weighted graph could represent a collection of cities with roads connecting them: each vertex would represent a city, and the edges would represent roads between the cities. The length of each road could be the weight of the corresponding edge. An *unweighted* graph like G_1 does not have weights assigned to its edges, but any unweighted graph can be thought of as a weighted graph by assigning a weight of 1 to every edge.



(a) G_1, an unweighted undirected graph.



(b) G_2, a weighted undirected graph.

Figure 5.1

Adjacency, Degree, and Laplacian Matrices

For computation and analysis, graphs are commonly represented by a few special matrices. For these definitions, let G be a graph with N nodes and let w_{ij} be the weight of the edge connecting node i to node j (if such an edge exists).

1. The *adjacency matrix* of G is the $N \times N$ matrix A with entries

$$a_{ij} = \begin{cases} w_{ij} & \text{if an edge connects node i and node j} \\ 0 & \text{otherwise.} \end{cases}$$

   The adjacency matrices A_1 of G_1 and A_2 of G_2 are as follows.

$$A_1 = \begin{bmatrix} 0 & 1 & 0 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 \end{bmatrix} \qquad A_2 = \begin{bmatrix} 0 & 3 & 0 & 0 & 0 & 0 \\ 3 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 2 & .5 \\ 0 & 0 & 0 & 2 & 0 & 1 \\ 0 & 0 & 0 & .5 & 1 & 0 \end{bmatrix}$$

   Notice that these adjacency matrices are symmetric. This is always the case for undirected graphs since the edges are bidirectional.

2. The *degree matrix* of G is the $N \times N$ diagonal matrix D whose ith diagonal entry is

$$d_{ii} = \sum_{j=1}^{N} w_{ij}. \tag{5.1}$$

   The degree matrices D_1 of G_1 and D_2 of G_2 are given below.

$$D_1 = \begin{bmatrix} 3 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 \end{bmatrix} \qquad D_2 = \begin{bmatrix} 3 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3.5 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1.5 \end{bmatrix}$$

   The ith diagonal entry of D is called the *degree* of node i, the sum of the weights of the edges leaving node i.

3. The *Laplacian matrix* of G is the $N \times N$ matrix L given by

$$L = D - A, \tag{5.2}$$

   where D is the degree matrix of G and A is the adjacency matrix of G. For G_1 and G_2, the Laplacian matrices L_1 and L_2 are given below.

$$L_1 = \begin{bmatrix} 3 & -1 & 0 & 0 & -1 & -1 \\ -1 & 3 & -1 & 0 & -1 & 0 \\ 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & -1 & 3 & -1 & -1 \\ -1 & -1 & 0 & -1 & 3 & 0 \\ -1 & 0 & 0 & -1 & 0 & 2 \end{bmatrix} \qquad L_2 = \begin{bmatrix} 3 & -3 & 0 & 0 & 0 & 0 \\ -3 & 3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & -1 & 3.5 & -2 & -.5 \\ 0 & 0 & 0 & -2 & 3 & -1 \\ 0 & 0 & 0 & -.5 & -1 & 1.5 \end{bmatrix}$$

Problem 1. Write a function that accepts the adjacency matrix A of a graph G. Use (5.1) and (5.2) to compute the Laplacian matrix L of G.
(Hint: The diagonal entries of D can be computed in one line by summing A over an axis.)

Test your function on the graphs G_1 and G_2 from Figure 5.1 and validate your results with `scipy.sparse.csgraph.laplacian()`.

Connectivity

A *connected graph* is a graph where every vertex is connected to every other vertex by at least one path. For example, G_1 is connected, whereas G_2 is not because there is no path from node 1 (or node 2) to node 3 (or nodes 4, 5, or 6). The naïve brute-force algorithm for determining if a graph is connected is to check that there is a path from each edge to every other edge. While this may work for very small graphs, most interesting graphs have thousands of vertices, and for such graphs this approach is prohibitively expensive. Luckily, an interesting result from algebraic graph theory relates the connectivity of a graph to its Laplacian matrix.

If L is the Laplacian matrix of a graph, then the definition of D and the construction $L = D - A$ guarantees that the rows (and columns) of L must each sum to 0. Therefore L cannot have full rank, so $\lambda = 0$ must be an eigenvalue of L. Furthermore, if L represents a graph that is **not** connected, more than one of the eigenvalues of L must be zero. To see this, let $J \subset \{1, 2, \dots, N\}$ such that the vertices $\{v_j\}_{j \in J}$ form a connected component of the graph, meaning that there is a path between each pair of vertices in the set. Next, let $\mathbf{x}$ be the vector with entries

$$x_k = \begin{cases} 1, & k \in J \\ 0, & k \notin J. \end{cases}$$

Then $\mathbf{x}$ is an eigenvector of L corresponding to the eigenvalue $\lambda = 0$.

For example, the example graph G_2 has two connected components.

1. $J_1 = \{1, 2\}$ so that $\mathbf{x}_1 = [1, 1, 0, 0, 0, 0]^\mathsf{T}$. Then

$$L_2\mathbf{x}_1 = \begin{bmatrix} 3 & -3 & 0 & 0 & 0 & 0 \\ -3 & 3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & -1 & 3.5 & -2 & -.5 \\ 0 & 0 & 0 & -2 & 3 & -1 \\ 0 & 0 & 0 & -.5 & -1 & 1.5 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \mathbf{0}.$$

2. $J_2 = \{3, 4, 5, 6\}$ and hence $\mathbf{x}_2 = [0, 0, 1, 1, 1, 1]^\mathsf{T}$. Then

$$L_2\mathbf{x}_2 = \begin{bmatrix} 3 & -3 & 0 & 0 & 0 & 0 \\ -3 & 3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & -1 & 3.5 & -2 & -.5 \\ 0 & 0 & 0 & -2 & 3 & -1 \\ 0 & 0 & 0 & -.5 & -1 & 1.5 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \mathbf{0}.$$

In fact, it can be shown that the number of zero eigenvalues of the Laplacian exactly equals the number of connected components. This makes calculating how many connected components are in a graph only as hard as calculating the eigenvalues of its Laplacian.

A Laplacian matrix L is always a positive semi-definite matrix when all weights in the graph are positive, meaning that its eigenvalues are each nonnegative. The second smallest eigenvalue of L is called the *algebraic connectivity* of the graph. It is clearly 0 for non-connected graphs, but for a connected graph, the algebraic connectivity provides useful information about its sparsity or "connectedness." A higher algebraic connectivity indicates that the graph is more strongly connected.

Problem 2. Write a function that accepts the adjacency matrix A of a graph G and a small tolerance value `tol`. Compute the number of connected components in G and its algebraic connectivity. Consider all eigenvalues that are less than the given `tol` to be zero.

Use `scipy.linalg.eig()` or `scipy.linalg.eigvals()` to compute the eigenvalues of the Laplacian matrix. These functions return complex eigenvalues (with negligible imaginary parts); use `np.real()` to extract the real parts.

Images as Matrices

Computer images are stored as arrays of integers that indicate pixel values. Most $m \times n$ grayscale (black and white) images are stored in Python as a $m \times n$ NumPy arrays, while most $m \times n$ color images are stored as 3-dimensional $m \times n \times 3$ arrays. Color image arrays can be thought of as a stack of three $m \times n$ arrays, one each for red, green, and blue values. The datatype for an image array is `np.uint8`, unsigned 8-bit integers that range from 0 to 255. A 0 indicates a black pixel while a 255 indicates a white pixel.

Use `scipy.misc.imread()` to read an image from a file. Matplotlib's `plt.imshow()` displays an image array, but it displays arrays of floats between 0 and 1 more cleanly than arrays of 8-bit integers. Therefore it is customary to scale the array by dividing each entry by 255 before processing or showing the image. In this case, a 0 still indicates a black pixel, but now a 1 indicates pure white.

```
>>> from scipy.misc import imread
>>> from matplotlib import pyplot as plt

>>> image = imread("dream.png")      # Read a (very) small image.
>>> print(image.shape)               # Since the array is 3-dimensional,
(48, 48, 3)                          # this is a color image.

# The image is read in as integers from 0 to 255.
>>> print(image.min(), image.max(), image.dtype)
0 254 uint8

# Scale the image to floats between 0 and 1 for Matplotlib.
>>> scaled = image / 255.
>>> print(scaled.min(), scaled.max(), scaled.dtype)
0.0 0.996078431373 float64

# Display the scaled image.
>>> plt.imshow(scaled)
>>> plt.axis("off")
>>> plt.show()
```

A color image can be converted to grayscale by averaging the RGB values of each pixel, resulting in a 2-D array called the *brightness* of the image. To properly display a grayscale image, specify the keyword argument `cmap="gray"` in `plt.imshow()`.

```
# Average the RGB values of a colored image to obtain a grayscale image.
>>> brightness = scaled.mean(axis=2)        # Average over the last axis.
>>> print(brightness.shape)                 # Note that the array is now 2-D.
(48, 48)

# Display the image in gray.
>>> plt.imshow(brightness, cmap="gray")
>>> plt.axis("off")
>>> plt.show()
```

Finally, it is often important in applications to flatten an image matrix into a large 1-D array. Use `np.ravel()` to convert a $m \times n$ array into a 1-D array with mn entries.

```
>>> import numpy as np
>>> A = np.random.randint(0, 10, (3,4))
>>> print(A)
[[4 4 7 7]
 [8 1 2 0]
 [7 0 0 9]]

# Unravel the 2-D array (by rows) into a 1-D array.
>>> np.ravel(A)
array([4, 4, 7, 7, 8, 1, 2, 0, 7, 0, 0, 9])

# Unravel a grayscale image into a 1-D array and check its size.
>>> M,N = brightness.shape
>>> flat_brightness = np.ravel(brightness)
>>> M*N == flat_brightness.size
True
>>> print(flat_brightness.shape)
(2304,)
```

Problem 3. Define a class called `ImageSegmenter`.

1. Write the constructor so that it accepts the name of an image file. Read the image, scale it so that it contains floats between 0 and 1, then store it as an attribute. If the image is in color, compute its brightness matrix by averaging the RGB values at each pixel (if it is a grayscale image, the image array itself is the brightness matrix). Flatten the brightness matrix into a 1-D array and store it as an attribute.

2. Write a method called `show_original()` that displays the original image. If the original image is grayscale, remember to use `cmap="gray"` as part of `plt.imshow()`.

ACHTUNG!

Matplotlib's `plt.imread()` also reads image files. However, this function automatically scales PNG image entries to floats between 0 and 1, but it still reads non-PNG image entries as 8-bit integers. To avoid this inconsistent behavior, always use `scipy.misc.imread()` to read images and divide by 255 when scaling is desired.

Graph-based Image Segmentation

Image segmentation is the process of finding natural boundaries in an image and partitioning the image along those boundaries (see Figure 5.2). Though humans can easily pick out portions of an image that "belong together," it takes quite a bit of work to teach a computer to recognize boundaries and sections in an image. However, segmenting an image often makes it easier to analyze, so image segmentation is ongoing area of research in computer vision and image processing.

Figure 5.2: The image `dream.png` and its segments.

There are many ways to approach image segmentation. The following algorithm, developed by Jianbo Shi and Jitendra Malik in 2000 **[Shi2000]**, converts the image to a graph and "cuts" it into two connected components.

Constructing the Image Graph

Let G be a graph whose vertices are the mn pixels of an $m \times n$ image (either grayscale or color). Each vertex i has a brightness $B(i)$, the grayscale or average RGB value of the pixel, as well as a coordinate location $X(i)$, the indices of the pixel in the original image array.

Define w_{ij}, the weight of the edge between pixels i and j, by

$$w_{ij} = \begin{cases} \exp\left(-\frac{|B(i)-B(j)|}{\sigma_B^2} - \frac{\|X(i)-X(j)\|}{\sigma_X^2}\right) & \text{if } \|X(i)-X(j)\| < r \\ 0 & \text{otherwise,} \end{cases} \tag{5.3}$$

where r, σ_B^2 and σ_X^2 are constants for tuning the algorithm. In this context, $\|\cdot\|$ is the standard *euclidean norm*, meaning that $\|X(i) - X(j)\|$ is the physical distance between vertices i and j, measured in pixels.

With this definition for w_{ij}, pixels that are farther apart than the radius r are not connected at all in G. Pixels within r of each other are more strongly connected if they are similar in brightness and close together (the value in the exponential is negative but close to zero). On the other hand, highly contrasting pixels where $|B(i) - B(j)|$ is large have weaker connections (the value in the exponential is highly negative).

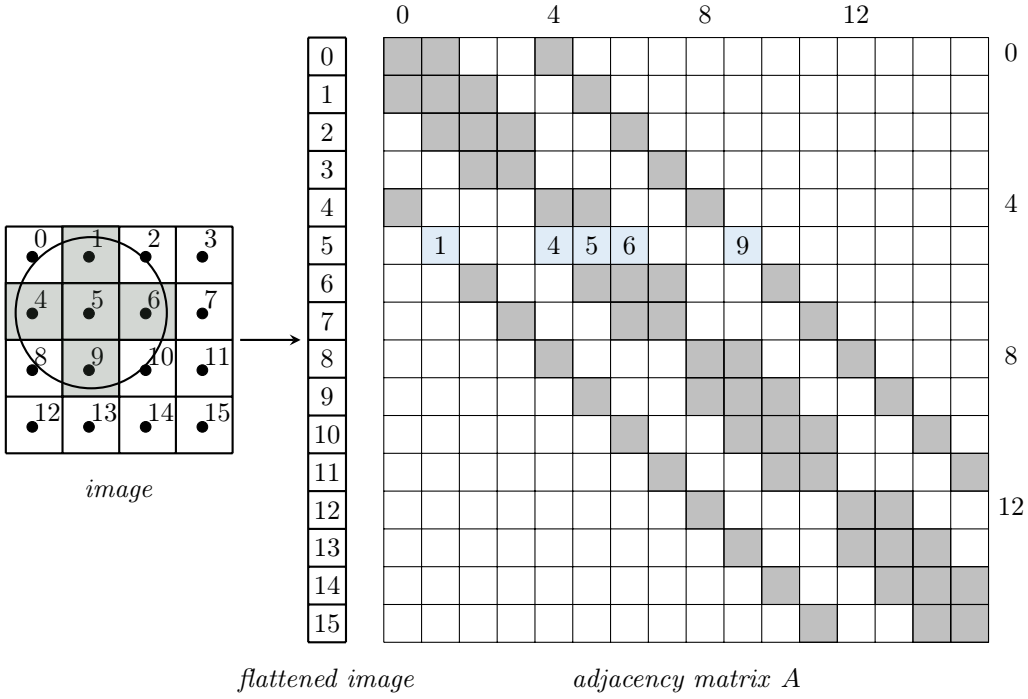


Figure 5.3: The grid on the left represents a 4×4 ($m \times n$) image with 16 pixels. On the right is the corresponding 16×16 ($mn \times mn$) adjacency matrix with all nonzero entries shaded. For example, in row 5, entries 1, 4, 5, 6, and 9 are nonzero because those pixels are within radius $r = 1.2$ of pixel 5.

Since there are mn total pixels, the adjacency matrix A of G with entries w_{ij} is $mn \times mn$. With a relatively small radius r, A is relatively sparse, and should therefore be constructed and stored as a sparse matrix. The degree matrix D is diagonal, so it can be stored as a regular 1-dimensional NumPy array. The procedure for constructing these matrices can be summarized in just a few steps.

1. Initialize A as a sparse $mn \times mn$ matrix and D as a vector with mn entries.
2. For each vertex i ($i = 0, 1, \ldots, mn - 1$),
   (a) Find the set of all vertices J_i such that $\|X(i) - X(j)\| < r$ for each $j \in J_i$. For example, in Figure 5.3 $i = 5$ and $J_i = \{1, 4, 5, 6, 9\}$.
   (b) Calculate the weights w_{ij} for each $j \in J_i$ according to (5.3) and store them in A.
   (c) Set the ith element of D to be the sum of the weights, $d_i = \sum_{j \in J_i} w_{ij}$.

The most difficult part to implement efficiently is step 2a, computing the neighborhood J_i of the current pixel i. However, the computation only requires knowing the current index i, the radius r, and the height and width m and n of the original image. The following function takes advantage of this fact and returns (as NumPy arrays) both J_i and the distances $\|X(i) - X(j)\|$ for each $j \in J_i$.

```
def get_neighbors(index, radius, height, width):
    """Calculate the flattened indices of the pixels that are within the given
    distance of a central pixel, and their distances from the central pixel.

    Parameters:
        index (int): The index of a central pixel in a flattened image array
            with original shape (radius, height).
        radius (float): Radius of the neighborhood around the central pixel.
        height (int): The height of the original image in pixels.
        width (int): The width of the original image in pixels.

    Returns:
        (1-D ndarray): the indices of the pixels that are within the specified
            radius of the central pixel, with respect to the flattened image.
        (1-D ndarray): the euclidean distances from the neighborhood pixels to
            the central pixel.
    """
    # Calculate the original 2-D coordinates of the central pixel.
    row, col = index // width, index % width

    # Get a grid of possible candidates that are close to the central pixel.
    r = int(radius)
    x = np.arange(max(col - r, 0), min(col + r + 1, width))
    y = np.arange(max(row - r, 0), min(row + r + 1, height))
    X, Y = np.meshgrid(x, y)

    # Determine which candidates are within the given radius of the pixel.
    R = np.sqrt(((X - col)**2 + (Y - row)**2))
    mask = R < radius
    return (X[mask] + Y[mask]*width).astype(np.int), R[mask]
```

To see how this works, consider Figure 5.3 where the original image is 4×4 and the goal is to compute the neighborhood of the pixel $i = 5$.

```
# Compute the neighbors and corresponding distances from the figure.
>>> neighbors_1, distances_1 = get_neighbors(5, 1.2, 4, 4)
>>> print(neighbors_1, distances_1, sep='\n')
[1 4 5 6 9]
[ 1.  1.  0.  1.  1.]

# Increasing the radius from 1.2 to 1.5 results in more neighbors.
>>> neighbors_2, distances_2 = get_neighbors(5, 1.5, 4, 4)
>>> print(neighbors_2, distances_2, sep='\n')
[ 0  1  2  4  5  6  8  9 10]
[ 1.41421356  1.          1.41421356  1.          0.          1.
  1.41421356  1.          1.41421356]
```

Problem 4. Write a method for the `ImageSegmenter` class that accepts floats r defaulting to 5, σ_B^2 defaulting to .02, and σ_X^2 defaulting to 3. Compute the adjacency matrix A and the degree matrix D according to the weights specified in (5.3).

Initialize A as a `scipy.sparse.lil_matrix`, which is optimized for incremental construction. Fill in the nonzero elements of A one row at a time. Use `get_neighbors()` at each step to help compute the weights.
(Hint: Try to compute and store an entire row of weights at a time. What does the command `A[5, np.array([1, 4, 5, 6, 9])] = weights` do?)

Finally, convert A to a `scipy.sparse.csc_matrix`, which is faster for computations. Then return A and D.

Segmenting the Graph

With an image represented as a graph G, the goal is to now split G into two distinct connected components by removing edges from the existing graph. This is called *cutting* G, and the set of edges that are removed is called the *cut*. The cut with the least weight will best segment the image.

Let D be the degree matrix and L be the Laplacian matrix of G. Shi and Malik proved that the eigenvector corresponding to the second smallest[1] eigenvalue of $D^{-1/2}LD^{-1/2}$ can be used to minimize the cut: the indices of its positive entries are the indices of the pixels in the flattened image which belong to one segment, and the indices of its negative entries are the indices of the pixels which belong to the other segment. In this context $D^{-1/2}$ refers to element-wise exponentiation, so the (i,j)th entry of $D^{-1/2}$ is $1/\sqrt{d_{ij}}$.

Because A is $mn \times mn$, the desired eigenvector has mn entries. Reshaping the eigenvector to be $m \times n$ allows it to align with the original image. Use the reshaped eigenvector to create a boolean mask that indexes one of the segments. That is, construct a $m \times n$ array where the entries belonging to one segment are `True` and the other entries are `False`.

```
>>> x = np.arange(-5,5).reshape((5,2)).T
>>> print(x)
[[-5 -3 -1  1  3]
 [-4 -2  0  2  4]]

# Construct a boolean mask of x describing which entries of x are positive.
>>> mask = x > 0
>>> print(mask)
[[False False False  True  True]
 [False False False  True  True]]

# Use the mask to zero out all of the nonpositive entries of x.
>>> x * mask
array([[0, 0, 0, 1, 3],
       [0, 0, 0, 2, 4]])
```

[1]Both D and L are symmetric matrices, so all eigenvalues of $D^{-1/2}LD^{-1/2}$ are real, and therefore "the second smallest one" is well-defined.

Problem 5. Write a method for the `ImageSegmenter` class that accepts an adjacency matrix A as a `scipy.sparse.csc_matrix` and a degree matrix D as a 1-D NumPy array. Construct an $m \times n$ boolean mask describing the segments of the image.

1. Compute the Laplacian L with `scipy.sparse.csgraph.laplacian()` or by converting D to a sparse diagonal matrix and computing $L = D - A$ (do not use your function from Problem 1 unless it works correctly and efficiently for sparse matrices).
2. Construct $D^{-1/2}$ as a sparse diagonal matrix using D and `scipy.sparse.diags()`, then compute $D^{-1/2}LD^{-1/2}$. Use `@` or the `dot()` method of the sparse matrix for the matrix multiplication, **not** `np.dot()`.
3. Use `scipy.spase.linalg.eigsh()` to compute the eigenvector corresponding to the second-smallest eigenvalue of $D^{-1/2}LD^{-1/2}$. Set the keyword arguments `which="SM"` and `k=2` to compute only the two smallest eigenvalues and their eigenvectors.
4. Reshape the eigenvector as a $m \times n$ matrix and use this matrix to construct the desired boolean mask. Return the mask.

Multiplying the boolean mask component-wise by the original image array produces the *positive segment*, a copy of the original image where the entries that aren't in the segment are set to 0. Computing the *negative segment* requires inverting the boolean mask, then multiplying the inverted mask with the original image array. Finally, if the original image is a $m \times n \times 3$ color image, the mask must be stacked into a $m \times n \times 3$ array to facilitate entry-wise multiplication.

```
>>> mask = np.arange(-5,5).reshape((5,2)).T > 0
>>> print(mask)
[[False False False  True  True]
 [False False False  True  True]]

# The mask can be negated with the tilde operator ~.
>>> print(~mask)
[[ True  True  True False False]
 [ True  True  True False False]]

# Stack a mask into a 3-D array with np.dstack().
>>> print(mask.shape, np.dstack((mask, mask, mask)).shape)
(2, 5) (2, 5, 3)
```

Problem 6. Write a method for the `ImageSegmenter` class that accepts floats r, σ_B^2, and σ_X^2, with the same defaults as in Problem 4. Call your methods from Problems 4 and 5 to obtain the segmentation mask. Plot the original image, the positive segment, and the negative segment side-by-side in subplots. Your method should work for grayscale or color images.

Use `dream.png` as a test file and compare your results to Figure 5.2.

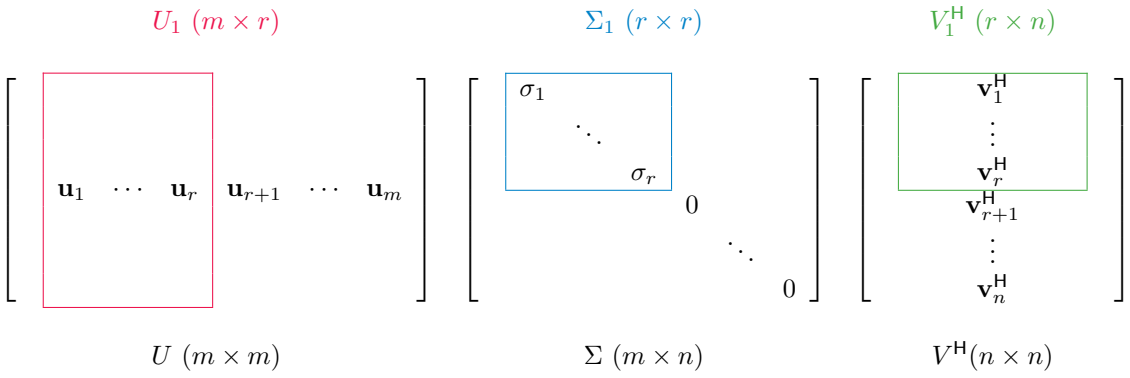
6 The SVD and Image Compression

Lab Objective: *The Singular Value Decomposition (SVD) is an incredibly useful matrix factorization that is widely used in both theoretical and applied mathematics. The SVD is structured in a way that makes it easy to construct low-rank approximations of matrices, and it is therefore the basis of several data compression algorithms. In this lab we learn to compute the SVD and use it to implement a simple image compression routine.*

The SVD of a matrix A is a factorization $A = U\Sigma V^\mathsf{H}$ where U and V have orthonormal columns and Σ is diagonal. The diagonal entries of Σ are called the *singular values* of A and are the square roots of the eigenvalues of $A^\mathsf{H}A$. Since $A^\mathsf{H}A$ is always positive semidefinite, its eigenvalues are all real and nonnegative, so the singular values are also real and nonnegative. The singular values σ_i are usually sorted in decreasing order so that $\Sigma = \text{diag}(\sigma_1, \sigma_2, \dots, \sigma_n)$ with $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_n \geq 0$. The columns $\mathbf{u}_i$ of U, the columns $\mathbf{v}_i$ of V, and the singular values of A satisfy $A\mathbf{v}_i = \sigma_i \mathbf{u}_i$.

Every $m \times n$ matrix A of rank r has an SVD with exactly r nonzero singular values. Like the QR decomposition, the SVD has two main forms.

- **Full SVD**: Denoted $A = U\Sigma V^\mathsf{H}$. U is $m \times m$, V is $n \times n$, and Σ is $m \times n$. The first r columns of U span $\mathscr{R}(A)$, and the remaining $n - r$ columns span $\mathscr{N}(A^\mathsf{H})$. Likewise, the first r columns of V span $\mathscr{R}(A^\mathsf{H})$, and the last $m - r$ columns span $\mathscr{N}(A)$.
- **Compact (Reduced) SVD**: Denoted $A = U_1\Sigma_1 V_1^\mathsf{H}$. U_1 is $m \times r$ (the first r columns of U), V_1 is $n \times r$ (the first r columns of V), and Σ_1 is $r \times r$ (the first $r \times r$ block of Σ). This smaller version of the SVD has all of the information needed to construct A and nothing more. The zero singular values and the correpsonding columns of U and V are neglected.



Finally, the SVD yields an *outer product expansion* of A in terms of the singular values and the columns of U and V.

$$A = \sum_{i=1}^{r} \sigma_i \mathbf{u}_i \mathbf{v}_i^H \tag{6.1}$$

Note that only terms from the compact SVD are needed for this expansion.

Computing the Compact SVD

It is difficult to compute the SVD from scratch because it is an eigenvalue-based decomposition. However, given an eigenvalue solver such as `scipy.linalg.eig()`, the algorithm becomes much simpler. First, obtain the eigenvalues and eigenvectors of A^HA, and use these to compute Σ. Since A^HA is normal, it has an orthonormal eigenbasis, so set the columns of V to be the eigenvectors of A^HA. Then, since $A\mathbf{v}_i = \sigma_i \mathbf{u}_i$, construct U by setting its columns to be $\mathbf{u}_i = \frac{1}{\sigma_i} A\mathbf{v}_i$.

The key is to sort the singular values and the corresponding eigenvectors in the same manner. In addition, it is computationally inefficient to keep track of the entire matrix Σ since it is a matrix of mostly zeros, so we need only store the singular values as a vector $\boldsymbol{\sigma}$. The entire procedure for computing the compact SVD is given below.

Algorithm 6.1

1: **procedure** COMPACT_SVD(A)
2: $\boldsymbol{\lambda}, V \leftarrow \text{eig}(A^HA)$ ▷ Calculate the eigenvalues and eigenvectors of A^HA.
3: $\boldsymbol{\sigma} \leftarrow \sqrt{\boldsymbol{\lambda}}$ ▷ Calculate the singular values of A.
4: $\boldsymbol{\sigma} \leftarrow \text{sort}(\boldsymbol{\sigma})$ ▷ Sort the singular values **from greatest to least**.
5: $V \leftarrow \text{sort}(V)$ ▷ Sort the eigenvectors **the same way** as in the previous step.
6: $r \leftarrow \text{count}(\boldsymbol{\sigma} \neq 0)$ ▷ Count the number of nonzero singular values (the rank of A).
7: $\boldsymbol{\sigma}_1 \leftarrow \boldsymbol{\sigma}_{:r}$ ▷ Keep only the positive singular values.
8: $V_1 \leftarrow V_{:,:r}$ ▷ Keep only the corresponding eigenvectors.
9: $U_1 \leftarrow AV_1/\boldsymbol{\sigma}_1$ ▷ Construct U with array broadcasting.
10: **return** $U_1, \boldsymbol{\sigma}_1, V_1^H$

Problem 1. Write a function that accepts a matrix A and a small error tolerance `tol`. Use Algorithm 6.1 to compute the compact SVD of A. In step 6, compute r by counting the number of singular values that are greater than `tol`.

Consider the following tips for implementing the algorithm.

- The Hermitian A^H can be computed with `A.conj().T`.
- In step 4, the way that $\boldsymbol{\sigma}$ is sorted needs to be stored so that the columns of V can be sorted the same way. Consider using `np.argsort()` and fancy indexing to do this, but remember that by default it sorts from least to greatest (not greatest to least).
- Step 9 can be done by looping over the columns of V, but it can be done more easily and efficiently with array broadcasting.

Test your function by calculating the compact SVD for random matrices. Verify that U and V are orthonormal, that $U\Sigma V^H = A$, and that the number of nonzero singular values is the rank of A. You may also want to compre your results to SciPy's SVD algorithm.

```
>>> import numpy as np
>>> from scipy import linalg as la

# Generate a random matrix and get its compact SVD via SciPy.
>>> A = np.random.random((10,5))
>>> U,s,Vh = la.svd(A, full_matrices=False)
>>> print(U.shape, s.shape, Vh.shape)
(10, 5) (5,) (5, 5)

# Verify that U is orthonormal, U Sigma Vh = A, and the rank is correct.
>>> np.allclose(U.T @ U, np.identity(5))
True
>>> np.allclose(U @ np.diag(s) @ Vh, A)
True
>>> np.linalg.matrix_rank(A) == len(s)
True
```

Visualizing the SVD

An $m \times n$ matrix A defines a linear transformation that sends points from $\mathbb{R}^n$ to $\mathbb{R}^m$. The SVD decomposes a matrix into two rotations and a scaling, so that any linear transformation can be easily described geometrically. Specifically, V^H represents a rotation, Σ a rescaling along the principal axes, and U another rotation.

Problem 2. Write a function that accepts a 2×2 matrix A. Generate a 2×200 matrix S representing a set of 200 points on the unit circle, with x-coordinates on the top row and y-coordinates on the bottom row (recall the equation for the unit circle in polar coordinates: $x = \cos(\theta)$, $y = \sin(\theta)$, $\theta \in [0, 2\pi]$). Also define the matrix

$$E = \left[\begin{array}{c|c|c} \mathbf{e}_1 & \mathbf{0} & \mathbf{e}_2 \end{array}\right] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

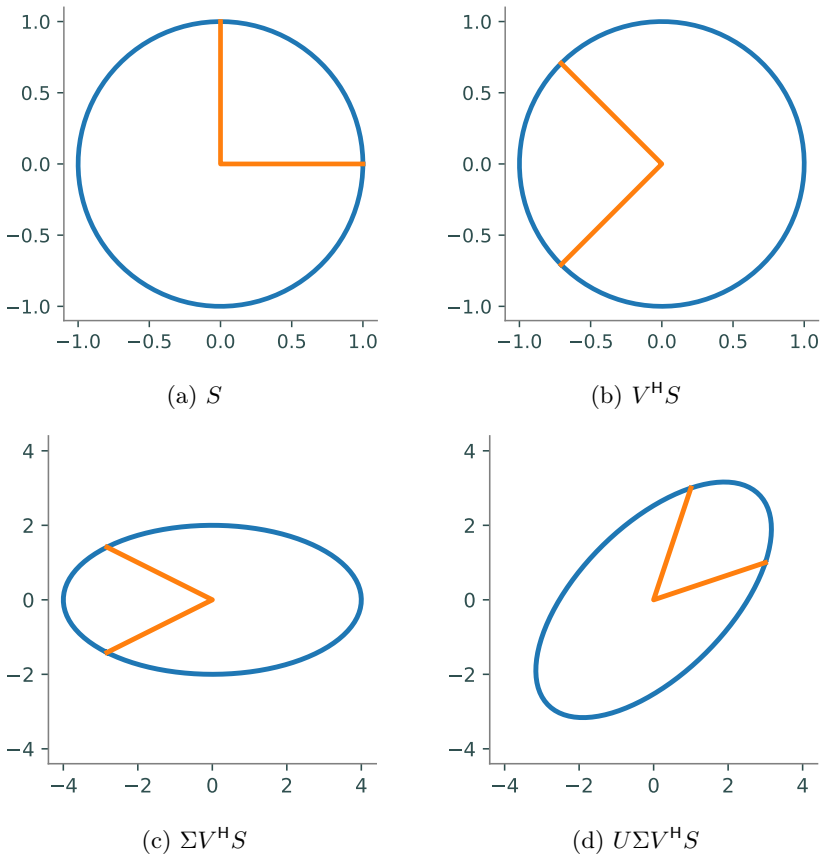
so that plotting the first row of S against the second row of S displays the unit circle, and plotting the first row of E against its second row displays the standard basis vectors in $\mathbb{R}^2$.

Compute the full SVD $A = U\Sigma V^\mathsf{H}$ using `scipy.linalg.svd()`. Plot four subplots to demonstrate each step of the transformation, plotting S and E, $V^\mathsf{H}S$ and $V^\mathsf{H}E$, $\Sigma V^\mathsf{H}S$ and $\Sigma V^\mathsf{H}E$, then $U\Sigma V^\mathsf{H}S$ and $U\Sigma V^\mathsf{H}E$.

For the matrix

$$A = \begin{bmatrix} 3 & 1 \\ 1 & 3 \end{bmatrix},$$

your function should produce Figure 6.1.
(Hint: Use `plt.axis("equal")` to fix the aspect ratio so that the circles don't appear elliptical.)



(a) S (b) $V^{\mathsf{H}}S$

(c) $\Sigma V^{\mathsf{H}}S$ (d) $U\Sigma V^{\mathsf{H}}S$

Figure 6.1: Each step in transforming the unit circle and two unit vectors using the matrix A.

Using the SVD for Data Compression

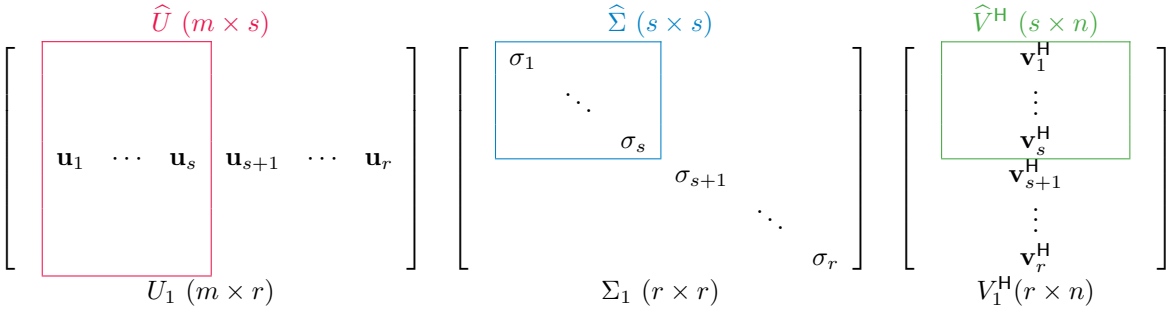
Low-Rank Matrix Approximations

If A is a $m \times n$ matrix of rank $r < \min\{m, n\}$, then the compact SVD offers a way to store A with less memory. Instead of storing all mn values of A, storing the matrices U_1, Σ_1 and V_1 only requires saving a total of $mr + r + nr$ values. For example, if A is 100×200 and has rank 20, then A has $20,000$ values, but its compact SVD only has total $6,020$ entries, a significant decrease.

The *truncated SVD* is an approximation to the compact SVD that allows even greater efficiency at the cost of a little accuracy. Instead of keeping all of the nonzero singular values, the truncated SVD only keeps the first $s < r$ singular values, plus the corresponding columns of U and V. In this case, (6.1) becomes the following.

$$A_s = \sum_{i=1}^{s} \sigma_i \mathbf{u}_i \mathbf{v}_i^{\mathsf{H}}$$

More precisely, the truncated SVD of A is $A_s = \widehat{U}\widehat{\Sigma}\widehat{V}^{\mathsf{H}}$, where $\widehat{U}$ is $m \times s$, $\widehat{V}$ is $n \times s$, and $\widehat{\Sigma}$ is $s \times s$. The resulting matrix A_s has rank s and is only an approximation to A, since $r - s$ nonzero singular values are neglected.



The beauty of the SVD is that it makes it easy to select the information that is most important. Larger singular values correspond to columns of U and V that contain more information, so dropping the smallest singular values retains as much information as possible. In fact, given a matrix A, its rank-s truncated SVD approximation A_s is the *best rank s approximation* of A with respect to both the induced 2-norm and the Frobenius norm. This result is called the *Schmidt, Mirsky, Eckhart-Young Theorem*, a very significant concept that appears in signal processing, statistics, machine learning, semantic indexing (search engines), and control theory.

Problem 3. Write a function that accepts a matrix A and a positive integer s.

1. Use your function from Problem 1 or `scipy.linalg.svd()` to compute the compact SVD of A, then form the truncated SVD by stripping off the appropriate columns and entries from U_1, Σ_1, and V_1. Return the best rank s approximation A_s of A (with respect to the induced 2-norm and Frobenius norm).

2. Also return the number of entries required to store the truncated form $\widehat{U}\widehat{\Sigma}\widehat{V}^{\mathsf{H}}$ (where $\widehat{\Sigma}$ is stored as a one-dimensional array, not the full diagonal matrix). The number of entries stored in NumPy array can be accessed by its `size` attribute.

   ```
   >>> A = np.random.random((20, 20))
   >>> A.size
   400
   ```

3. If s is greater than the number of nonzero singular values of A (meaning $s > \text{rank}(A)$), raise a `ValueError`.

Use `np.linalg.matrix_rank()` to verify the rank of your approximation.

Error of Low-Rank Approximations

Another result of the Schmidt, Mirsky, Eckhart-Young Theorem is that the exact 2-norm error of the best rank-s approximation A_s for the matrix A is the $(s+1)$th singular value of A.

$$\|A - A_s\|_2 = \sigma_{s+1} \tag{6.2}$$

This offers a way to approximate A within a desired error tolerance ϵ: choose s such that σ_{s+1} is the largest singular value that is less than ϵ, then compute A_s. This A_s throws away as much information as possible without violating the property $\|A - A_s\|_2 < \epsilon$.

Problem 4. Write a function that accepts a matrix A and an error tolerance ϵ.

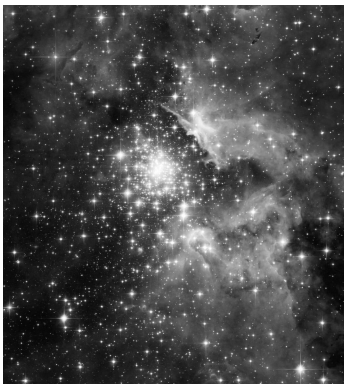
1. Compute the compact SVD of A, then use (6.2) to compute the lowest rank approximation A_s of A with 2-norm error less than ϵ. Avoid calculating the SVD more than once. (Hint: `np.argmax()`, `np.where()`, and/or fancy indexing may be useful.)
2. As in the previous problem, also return the number of entries needed to store the resulting approximation A_s via the truncated SVD.
3. If ϵ is less than or equal to the smallest singular value of A, raise a `ValueError`; in this case, A cannot be approximated within the tolerance by a matrix of lesser rank.

This function should be close to identical to the function from Problem 3, but with the extra step of identifying the appropriate s. Construct test cases to validate that $\|A - A_s\|_2 < \epsilon$.

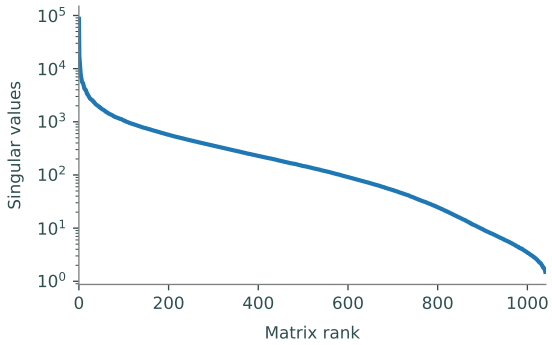
Image Compression

Images are stored on a computer as matrices of pixel values. Sending an image over the internet or a text message can be expensive, but computing and sending a low-rank SVD approximation of the image can considerably reduce the amount of data sent while retaining a high level of image detail. Successive levels of detail can be sent after the inital low-rank approximation by sending additional singular values and the corresponding columns of V and U.

Examining the singular values of an image gives us an idea of how low-rank the approximation can be. Figure 6.2 shows the image in `hubble_gray.jpg` and a log plot of its singular values. The plot in 6.2b is typical for a photograph—the singular values start out large but drop off rapidly. In this rank 1041 image, 913 of the singular values are 100 or more times smaller than the largest singular value. By discarding these relatively small singular values, we can retain all but the finest image details, while storing only a rank 128 image. This is a **huge** reduction in data size.



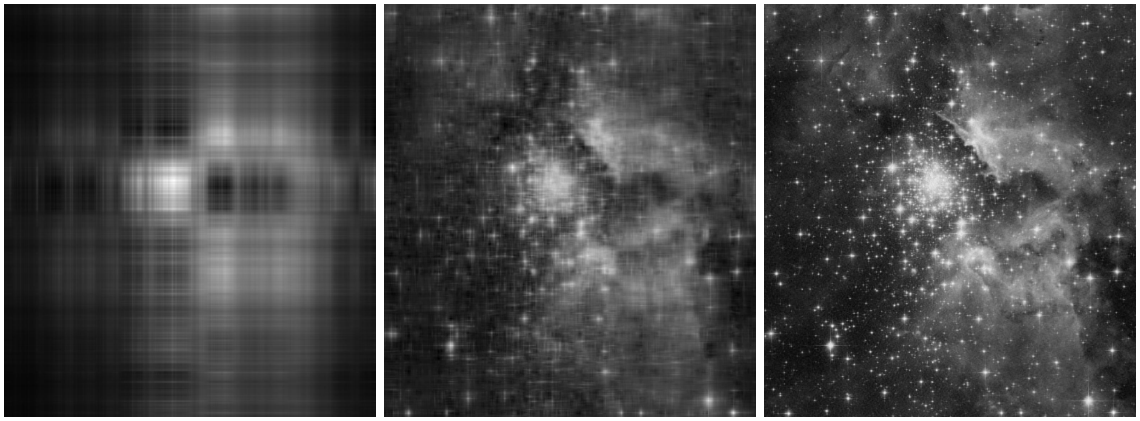
(a) NGC 3603 (Hubble Space Telescope).



(b) Singular values on a log scale.

Figure 6.2

Figure 6.3 shows several low-rank approximations of the image in Figure 6.2a. Even at a low rank the image is recognizable. By rank 120, the approximation differs very little from the original.



(a) Rank 2 (b) Rank 20 (c) Rank 120

Figure 6.3

Grayscale images are stored on a computer as 2-dimensional arrays, while color images are stored as 3-dimensional arrays—one layer each for red, green, and blue arrays. To read and display images, use `scipy.misc.imread()` and `plt.imshow()`. Images are read in as integer arrays with entries between 0 and 255 (`dtype=np.uint8`), but `plt.imshow()` works better if the image is an array of floats in the interval $[0, 1]$. Scale the image properly by dividing the array by 255.

```
>>> from matplotlib import pyplot as plt

# Send the RGB values to the interval (0,1).
>>> image_gray = plt.imread("hubble_gray.jpg") / 255.
>>> image_gray.shape            # Grayscale images are 2-d arrays.
(1158, 1041)

>>> image_color = plt.imread("hubble.jpg") / 255.
>>> image_color.shape           # Color images are 3-d arrays.
(1158, 1041, 3)

# The final axis has 3 layers for red, green, and blue values.
>>> red_layer = image_color[:,:,0]
>>> red_layer.shape
(1158, 1041)

# Display a gray image.
>>> plt.imshow(red_layer, cmap="gray")
>>> plt.axis("off")             # Turn off axis ticks and labels.
>>> plt.show()

# Display a color image.
>>> plt.imshow(image_color)     # cmap=None by default.
>>> plt.axis("off")
>>> plt.show()
```

Problem 5. Write a function that accepts the name of an image file and an integer s. Use your function from Problem 3, to compute the best rank-s approximation of the image. Plot the original image and the approximation in separate subplots. In the figure title, report the difference in number of entries required to store the original image and the approximation (use `plt.suptitle()`).

Your function should be able to handle both grayscale and color images. Read the image in and check its dimensions to see if it is color or not. Grayscale images can be approximated directly since they are represented by 2-dimensional arrays. For color images, let R, G, and B be the matrices for the red, green, and blue layers of the image, respectively. Calculate the low-rank approximations R_s, G_s, and B_s separately, then put them together in a new 3-dimensional array of the same shape as the original image.
(Hint: `np.dstack()` may be useful for putting the color layers back together.)

Finally, it is possible for the low-rank approximations to have values slightly outside the valid range of RGB values. Set any values outside of the interval $[0, 1]$ to the closer of the two boundary values.
(Hint: fancy indexing or `np.clip()` may be useful here.)

To check, compressing `hubble_gray.jpg` with a rank 20 approximation should appear similar to Figure 6.3b and save $1,161,478$ matrix entries.

Additional Material

More on Computing the SVD

For an $m \times n$ matrix A of rank $r < \min\{m, n\}$, the compact SVD of A neglects last $m - r$ columns of U and the last $n - r$ columns of V. The remaining columns of each matrix can be calculated by using Gram-Schmidt orthonormalization. If $m < r < n$ or $n < r < m$, only one of U_1 and V_1 will need to be filled in to construct the full U or V. Computing these extra columns is one way to obtain a basis for $\mathscr{N}(A^H)$ or $\mathscr{N}(A)$.

Algorithm 6.1 begins with the assumption that we have a way to compute the eigenvalues and eigenvectors of $A^H A$. Computing eigenvalues is a notoriously difficult problem, and computing the SVD from scratch without an eigenvalue solver is much more difficult than the routine described by Algorithm 6.1. The procedure involves two phases:

1. Factor A into $A = U_a B V_a^H$ where B is bidiagonal (only nonzero on the diagonal and the first superdiagonal) and U_a and V_a are orthonormal. This is usually done via *Golub-Kahan Bidiagonalization*, which uses Householder reflections, or *Lawson-Hanson-Chan bidiagonalization*, which relies on the QR decomposition.

2. Factor B into $B = U_b \Sigma V_b^H$ by the QR algorithm or a divide-and-conquer algorithm. Then the SVD of A is given by $A = (U_a U_b)\Sigma(V_a V_b)^H$.

For more details, see Lecture 31 of *Numerical Linear Algebra* by Lloyd N. Trefethen and David Bau III, or Section 5.4 of *Applied Numerical Linear Algebra* by James W. Demmel.

Animating Images with Matplotlib

Matplotlib can be used to animate images that change over time. For instance, we can show how the low-rank approximations of an image change as the rank s increases, showing how the image is recovered as more ranks are added. Try using the following code to create such an animation.

```
from matplotlib import pyplot as plt
from matplotlib.animation import FuncAnimation

def animate_images(images):
    """Animate a sequence of images. The input is a list where each
    entry is an array that will be one frame of the animation.
    """
    fig = plt.figure()
    plt.axis("off")
    im = plt.imshow(images[0], animated=True)

    def update(index):
        plt.title("Rank {} Approximation".format(index))
        im.set_array(images[index])
        return im,              # Note the comma!

    a = FuncAnimation(fig, update, frames=len(images), blit=True)
    plt.show()
```

See `https://matplotlib.org/examples/animation/dynamic_image.html` for another example.

7 Facial Recognition

Lab Objective: *A facial recognition algorithm attempts to match a person's portrait to a database of many portraits. Facial recognition is becoming increasingly important in security, law enforcement, artificial intelligence, and other areas. Though humans can easily match pictures to people, computers are beginning to surpass humans at facial recognition. In this lab, we implement a basic facial recognition system that relies on eigenvectors and the SVD to efficiently determine the difference between faces.*

Preparing an Image Database

The `faces94` face image dataset[1] contains several photographs of 153 people, organized into folders by person. To perform facial recognition on this dataset, select one image per person and convert these images into a database. For this particular facial recognition algorithm, the entire database can be stored in just a few NumPy arrays.

Digital images are stored on computers as arrays of pixels. Therefore, an $m \times n$ image can be stored in memory as an $m \times n$ matrix or, equivalently, as an mn-vector by concatenating the rows of the matrix. Then a collection of k images can be stored as a single $mn \times k$ matrix F, where each column of F represents a single image. That is, if

$$F = \begin{bmatrix} \mathbf{f}_1 & \mathbf{f}_2 & \cdots & \mathbf{f}_k \end{bmatrix},$$

then each $\mathbf{f}_i$ is a mn-vector representing a single image.

The following function obtains one image for each person in the `faces94` dataset and converts the collection of images into an $mn \times k$ matrix F described above.

```
import numpy as np
from os import walk
from scipy.misc import imread

def get_faces(path="./faces94"):
    # Traverse the directory and get one image per subdirectory.
```

[1] See `http://cswww.essex.ac.uk/mv/allfaces/faces94.html`.

```
    faces = []
    for (dirpath, dirnames, filenames) in walk(path):
        for fname in filenames:
            if fname[-3:]=="jpg":       # Only get jpg images.
                # Load the image, convert it to grayscale,
                # and flatten it into a vector.
                faces.append(np.ravel(imread(dirpath+"/"+fname, flatten=True)))
                break
    # Put all the face vectors column-wise into a matrix.
    return np.transpose(faces)
```

Problem 1. Write a function that accepts an image as a flattened mn-vector, along with its original dimensions m and n. Use `np.reshape()` to convert the flattened image into its original $m \times n$ shape and display the result with `plt.imshow()`.
(Hint: use `cmap='gray'` in `plt.imshow()` to display images in grayscale.)

Unzip the `faces94.zip` archive and use `get_faces()` to construct F. Each `faces94` image is 200×180, and there are 153 people in the dataset, so F should be 36000×153. Use your function to display one of the images stored in F.

The Eigenfaces Method

With the image database F, we could construct a simple facial recognition system with the following strategy. Let $\mathbf{g}$ be an mn-vector representing an unknown face that is not part of the database F. Then the $\mathbf{f}_i$ that minimizes $\|\mathbf{g}-\mathbf{f}_i\|_2$ is the matching face. Unfortunately, computing $\|\mathbf{g}-\mathbf{f}_i\|_2$ for each i is very computationally expensive, especially if the images are high-resolution and/or the database contains a large number of images. The *eigenfaces method* is a way to reduce the computational cost of finding the closest matching face by focusing on only the most important features of each face. Because the method ignores less significant facial features, it is also usually more accurate than the naïve method.

The first step of the algorithm is to shift the images by the *mean face*. Shifting a set of data by the mean exaggerates the distinguishing features of each entry. In the context of facial recognition, shifting by the mean accentuates the unique features of each face. For the images vectors stored in F, the mean face $\boldsymbol{\mu}$ is the defined to be the element-wise average of the $\mathbf{f}_i$.

$$\boldsymbol{\mu} = \frac{1}{k}\sum_{i=1}^{k} \mathbf{f}_i$$

Hence, the ith mean-shifted face vector $\bar{\mathbf{f}}_i$ is given by

$$\bar{\mathbf{f}}_i = \mathbf{f}_i - \boldsymbol{\mu}.$$

Next, define $\bar{F}$ as the $mn \times k$ matrix whose columns are given by the mean-shifted face vectors:

$$\bar{F} = \left[\begin{array}{c|c|c|c} \bar{\mathbf{f}}_1 & \bar{\mathbf{f}}_2 & \cdots & \bar{\mathbf{f}}_k \end{array}\right].$$

(a) The mean face. (b) An original face. (c) A mean-shifted face.

Figure 7.1

Problem 2. Write a class called `FacialRec` whose constructor accepts a path to a directory of images. In the constructor, use `get_faces()` to construct F, then compute the mean face $\boldsymbol{\mu}$ and the shifted faces $\bar{F}$. Store each array as an attribute.
(Hint: Both $\boldsymbol{\mu}$ and $\bar{F}$ can be computed in a single line of code by using NumPy functions and/or array broadcasting.)

Use your function from Problem 1 to visualize the mean face, and compare it to Figure 7.1a. Also display an original face and its corresponding mean-shifted face. Compare your results with Figures 7.1b and 7.1c.

To increase computational efficiency and minimize storage, the face vectors can be represented with fewer values by projecting $\bar{F}$ onto a lower-dimensional subspace. Let s be a natural number such that $s < r$, where r is the rank of $\bar{F}$. By projecting $\bar{F}$ onto an s-dimensional subspace, each face can be stored with only s values.

Specifically, let $U\Sigma V^{\mathsf{H}}$ be the compact SVD of $\bar{F}$ with rank r, which can also be represented by

$$\bar{F} = \sum_{i=1}^{r} \sigma_i \mathbf{u}_i \mathbf{v}_i^{\mathsf{H}}.$$

The first r columns of U form a basis for the range of $\bar{F}$. Recall that the Schmidt, Mirsky, Eckart-Young Theorem states that the matrix

$$\bar{F}_s = \sum_{i=1}^{s} \sigma_i \mathbf{u}_i \mathbf{v}_i^{\mathsf{H}}$$

is the best rank-s approximation of $\bar{F}$ for each $s < r$. This means that $\|\bar{F} - \bar{F}_s\|$ is minimized against all other $\|\bar{F} - B\|$ where B has rank s. As a consequence of this theorem, the first s columns of U form a basis that provides the "best" s-dimensional subspace for approximating $\bar{F}$.

The s basis vectors $\mathbf{u}_1, \ldots, \mathbf{u}_s$ are are commonly called the *eigenfaces* because they are eigenvectors of $\bar{F}\bar{F}^{\mathsf{T}}$ and because they resemble face images. Each original face image can be efficiently represented in terms of these eigenfaces. See Figure 7.2 for visualizations of the some of the eigenfaces for the `facesd94` data set.

Figure 7.2: The first, 50th, and 100th eigenfaces.

In general, the lower eigenfaces provide a more general information of a face and higher-ordered eigenfaces provide the details necessary to distinguish particular faces.[2] These eigenfaces will be used to construct the face images in the dataset. The more eigenfaces used, the more detailed the resulting image will be.

Next, let U_s be the matrix with the first s eigenfaces as columns. Since the eigenfaces $\{\mathbf{u}_i\}_{i=1}^s$ form an orthonormal set, U_s is an orthonormal matrix (independent of s) and hence $U_s^\mathsf{T}U_s = I$. The matrix $P_s = U_sU_s^\mathsf{T}$ projects vectors in $\mathbb{R}^{mn}$ to the subspace spanned by the orthonormal basis $\{\mathbf{u}_i\}_{i=1}^s$, and the change of basis matrix U_s^T puts the projection in terms of the basis of eigenfaces. Thus the projection $\widehat{\mathbf{f}}_i$ of $\bar{\mathbf{f}}_i$ in terms of the basis of eigenfaces is given by

$$\widehat{\mathbf{f}}_i = U_s^\mathsf{T}P_s\bar{\mathbf{f}}_i = U_s^\mathsf{T}U_sU_s^\mathsf{T}\bar{\mathbf{f}}_i = U_s^\mathsf{T}\bar{\mathbf{f}}_i. \tag{7.1}$$

Note carefully that though the shifted image $\bar{\mathbf{f}}_i$ has mn entries, the projection $\widehat{\mathbf{f}}_i$ has only s entries since U_s is $mn \times s$. Likewise, the matrix $\widehat{F}$ that has the projections $\widehat{\mathbf{f}}_i$ as columns is $s \times k$, and

$$\widehat{F} = U_s^\mathsf{T}F. \tag{7.2}$$

Problem 3. In the constructor of `FacialRec`, calculate the compact SVD of $\bar{F}$ and save the matrix U as an attribute. Compare the computed eigenfaces (the columns of U) to Figure 7.2.

Also write a method that accepts a vector of length mn or an $mn \times l$ matrix, as well as an integer s. Construct U_s by taking the first s columns of U, then use (7.1) or (7.2) to calculate the projection of the input vector or matrix onto the span of the first s eigenfaces.
(Hint: this method should be implemented with a single line of code.)

Reducing the mean-shifted face image $\bar{\mathbf{f}}_i$ to the lower-dimensional projection $\widehat{\mathbf{f}}_i$ drastically reduces the computational cost of the facial recognition algorithm, but this efficiency gain comes at a price. A projection image only approximates the corresponding original image, but as long as s isn't too small, the approximation is usually good enough for the algorithm to work well. Before completing the facial recognition system, we reconstruct some of these projections to visualize the amount of information lost.

[2]Neil Muller, Lourenco Magaia, and B. M. Herbst. *Singular Value Decomposition, Eigenfaces, and 3D Reconstructions.* SIAM Review. 2004. 46:3, 518-545.

From (7.1), since U_s^T projects $\bar{\mathbf{f}}_i$ and performs a change of basis to get $\widehat{\mathbf{f}}_i$, its transpose U_s puts $\widehat{\mathbf{f}}_i$ back into the original basis with as little error as possible. That is,

$$U_s\widehat{\mathbf{f}}_i \approx \bar{\mathbf{f}}_i = \mathbf{f}_i - \boldsymbol{\mu},$$

so that we have the approximation

$$\widetilde{\mathbf{f}}_i = U_s\widehat{\mathbf{f}}_i + \boldsymbol{\mu} \approx \mathbf{f}_i. \tag{7.3}$$

This $\widetilde{\mathbf{f}}_i$ is called the *reconstruction* of $\mathbf{f}_i$.

(a) A reconstruction with $s = 5$. (b) A reconstruction with $s = 19$. (c) A reconstruction with $s = 75$.

Figure 7.3: An image rebuilt with various numbers of eigenfaces. The image is already recognizable when it is reconstructed with only 19 eigenfaces—less than an eighth of the 153 eigenfaces! Note the similarities between this method and regular image compression via the truncated SVD.

Problem 4. Instantiate a `FacialRec` object that draws from the `faces94` dataset. Select one of the shifted images $\bar{\mathbf{f}}_i$. For at least 4 values of s, use your method from Problem 3 to compute the corresponding s-projection $\widehat{\mathbf{f}}_i$, then use (7.3) to compute the reconstruction $\widetilde{\mathbf{f}}_i$. Display the various reconstructions and the original image. Compare your results to Figure 7.3

Matching Faces

Let $\mathbf{g}$ be a vector representing an unknown face that is not part of the database. We determine which image in the database is most like $\mathbf{g}$ by comparing $\widehat{\mathbf{g}}$ to each of the $\widehat{\mathbf{f}}_i$. Fist, shift $\mathbf{g}$ by the mean to obtain $\bar{\mathbf{g}}$, then project $\bar{\mathbf{g}}$ using a given number of eigenfaces.

$$\widehat{\mathbf{g}} = U_s^\mathsf{T}\bar{\mathbf{g}} = U_s^\mathsf{T}(\mathbf{g} - \boldsymbol{\mu}) \tag{7.4}$$

Next, determine which $\widehat{\mathbf{f}}_i$ is closest to $\widehat{\mathbf{g}}$. Since the columns of U_s are an orthonormal basis, the computation in this basis yields the same result as computing in the standard Euclidean basis would. Then setting

$$j = \operatorname*{argmin}_i \|\widehat{\mathbf{f}}_i - \widehat{\mathbf{g}}\|_2, \tag{7.5}$$

we have that the jth face image $\mathbf{f}_j$ is the best match for $\mathbf{g}$. Again, since $\widehat{\mathbf{f}}_i$ and $\widehat{\mathbf{g}}_i$ only have s entries, the computation in (7.5) is much cheaper than comparing the raw $\mathbf{f}_i$ to $\mathbf{g}$.

Problem 5. Write a method for the `FacialRec` class that accepts an image vector $\mathbf{g}$ and an integer s. Use your method from Problem 3 to compute $\widehat{F}$ and $\widehat{\mathbf{g}}$ for the given s, then use (7.5) to determine the best matching face in the database. Return the index of the matching face. (Hint: `scipy.linalg.norm()` and `np.argmin()` may be useful.)

Note

This facial recognition system works by solving a *nearest neighbor search*, since the goal is to find the $\mathbf{f}_i$ that is "nearest" to the input image $\mathbf{g}$. Nearest neighbor searches can be performed more efficiently with the use of a *k-d tree*, a binary search tree for storing vectors. The system could also be called a *k-neighbors classifier* with $k = 1$.

Problem 6. Write a method for the `FacialRec` class that accepts an flat image vector $\mathbf{g}$, an integer s, and the original dimensions of $\mathbf{g}$. Use your method from Problem 5 to find the index j of the best matching face, then display the original face $\mathbf{g}$ alongside the best match $\mathbf{f}_j$.

The following generator yields random faces from `faces94` that can be used as test cases.

```
def sample_faces(num_faces, path="./faces94"):
    # Get the list of possible images.
    files = []
    for (dirpath, dirnames, filenames) in walk(path):
        for fname in filenames:
            if fname[-3:]=="jpg":       # Only get jpg images.
                files.append(dirpath+"/"+fname)

    # Get a subset of the image names and yield the images one at a time.
    test_files = np.random.choice(files, num_faces, replace=False)
    for fname in test_files:
        yield np.ravel(imread(fname, flatten=True))
```

The `yield` keyword is like a `return` statement, but the next time the generator is called, it will resume immediately after the last `yield` statement.[a]

Use `sample_faces()` to get at least 5 random faces from `faces94`, and match each random face to the database with $s = 38$. Iterate through the random faces with the following syntax.

```
for test_image in sample_faces(5):
    # 'test_image' is a now flattened face vector.
```

[a] See the Python Essentials lab on Profiling for more on generators.

Although there are other approaches to facial recognition that utilize more complex techniques, the method of eigenfaces remains a wonderfully simple and effective solution.

Additional Material

Improvements on the Facial Recognition System with Eigenfaces

The `FacialRec` class does its job well, but it could be improved in several ways. Here are a few ideas.

- The most computationally intensive part of the algorithm is computing $\widehat{F}$. Instead of recomputing $\widehat{F}$ every time the method from Problem 5 is called, store $\widehat{F}$ and s as attributes the first time the method is called. In subsequent calls, only recompute $\widehat{F}$ if the user specifies a different value for s.
- Load a `scipy.spatial.KDTree` object with $\widehat{F}$ and use its `query()` method to compute (7.5). Building a kd-tree is expensive, so be sure to only build a new tree when necessary (i.e., the user specifies a new value for s).
- Include an error tolerance ϵ in the method for Problem 5. If $\|\mathbf{f}_j - \mathbf{g}\| > \epsilon$, print a message or raise an exception to indicate that there is no suitable match for $\mathbf{g}$ in the database. In this case, add $\mathbf{g}$ to the database for future reference.
- Generalize the system by turning it into a k-neighbors classifier. In the constructor, add several faces per person to the database (this requires modifying `get_faces()`). Assign each individual a unique ID so that the system knows which faces correspond to the same person. Modify the method from Problem 5 so that it also accepts an integer k, then use `scipy.spatial.KDTree` to find the k nearest images to $\mathbf{g}$. Choose the ID that belongs to the most nearest neighbors, then return an index that corresponds to an individual with that ID.

  In other words, choose the k faces $\mathbf{f}_i$ that give the smallest values of $\|\mathbf{f}_i - \widehat{\mathbf{g}}\|_2$. These faces then get to vote on which person $\mathbf{g}$ belongs to.
- Improve the user interface of the class by modifying the method from Problem 6 so that it accepts a file name to read from instead of an array. A few lines of code from `get_faces()` or `sample_faces()` might be helpful for this.

Other Methods for Facial Recognition

The method of facial recognition presented here is more formally called *principal component analysis (PCA) using eigenfaces*. Several other machine learning and optimization techniques, such as linear discriminant analysis (LDA), elastic matching, dynamic link matching, and Hidden Markov Models (HMMs) have also been applied to the facial recognition problem. Other techniques focus on getting better information about the faces in the first place, the most prevalent being 3-dimensional recognition and thermal imaging. See `https://en.wikipedia.org/wiki/Facial_recognition_system` for a good survey of different approaches to the facial recognition problem.

8 Numerical Differentiation

Lab Objective: *The derivative is exceptionally useful in many applications, but we often do not know the original function or the derivative may be too difficult to compute. In these situations, finite difference quotients are beneficial to use to approximate the derivative. In this lab, we will implement several methods for approximating the derivative of a function numerically. Additionally, we will explore the accuracy of these approximations with respect to: the number of points used, the value of h and the number of dimensions.*

Derivative Approximations in One Dimension

The derivative of a function f at a point x_0 is

$$f'(x_0) = \lim_{h \to 0} \frac{f(x_0 + h) - f(x_0)}{h}. \tag{8.1}$$

In this lab, we will investigate one way a computer can calculate $f'(x_0)$.

Forward Difference Quotient

Suppose that in Equation (8.1), instead of taking a limit, we just pick a small value for h. $f'(x_0)$ is expected to be close to the quantity

$$\frac{f(x_0 + h) - f(x_0)}{h}. \tag{8.2}$$

This quotient is called the *first order forward difference approximation* of the derivative. Using the points x_0 and $x_0 - h$ in place of $x_0 + h$ and x_0 respectively is called the *first order backwards difference quotient*. Because $f'(x_0)$ is the limit of such quotients, this quotient is close to $f'(x_0)$ when h is small. Taylor's formula shows just how close it is. By Taylor's formula,

$$f(x_0 + h) = f(x_0) + f'(x_0)h + R_2(h)$$

where $R_2(h) = \left(\int_0^1 (1-t)f''(x_0 + th)dt\right) h^2$ (this is the integral form of the remainder for Taylor's Theorem; see Volume 1 Chapter 6). When we solve this equation for $f'(x_0)$, we get

$$f'(x_0) = \frac{f(x_0 + h) - f(x_0)}{h} - \frac{R_2(h)}{h}. \tag{8.3}$$

Thus, the error in using the first order forward difference quotient to approximate $f'(x_0)$ is

$$\left|\frac{R_2(h)}{h}\right| \leq |h| \int_0^1 |1-t||f''(x_0+th)|dt.$$

If we assume f'' is continuous, then for any δ, set $M = \sup_{x\in(x_0-\delta,x_0+\delta)} f''(x)$. Then if $|h| < \delta$, we have

$$\left|\frac{R_2(h)}{h}\right| \leq |h| \int_0^1 M dt = M|h| \in O(h).$$

Similarly, the backward quotient is also in $O(h)$. The *second order forward difference quotient*, which uses three points ($x, x+h$, and $x+2h$) instead of two, is given by:

$$f'(x_0) \approx \frac{-3f(x_0)+4f(x_0+h)-f(x_0+2h)}{2h}. \tag{8.4}$$

And the *second order backwards difference quotient*:

$$f'(x_0) \approx \frac{3f(x_0)-4f(x_0-h)+f(x_0-2h)}{2h}. \tag{8.5}$$

Centered Difference Quotient

A finite difference quotient that is in $O(h^2)$, and consequently has a smaller error when $|h| < 1$, is called the *centered difference quotient*. It is defined for the second and fourth order respectively as:

$$f'(x_0) \approx \frac{f(x_0+h)-f(x_0-h)}{2h} \tag{8.6}$$

$$f'(x_0) \approx \frac{f(x_0-2h)-8f(x_0-h)+8f(x_0+h)-f(x_0+2h)}{12h}. \tag{8.7}$$

For a derivation of the second order centered difference quotient, please refer to the additional materials section.

Problem 1. In separate functions implement the

1. first order forward difference quotient,
2. second order backward difference quotient,
3. second order centered difference quotient, and the
4. fourth order centered difference quotient.

Each function should accept a callable function f, an array of points, and a float representing h that defaults to 10^{-5}. Return an array of the difference quotients.

To test your function, you can define a polynomial and calculate its derivative analytically. Then pass your array of points into the analytically computed derivative and into your functions and verify that the returned arrays are close to one another.

Accuracy of Approximations

It is important to pick an appropriate step size h when approximating a derivative by finite difference quotients. The step size should be small but not too small, as dividing by very small numbers causes errors in floating point arithmetic. This means that as we decrease $|h|$, the error $|f'(x_0) - \tilde{f}(x_0)|$ (where $\tilde{f}$ is the numerical approximation) will first decrease but then will increase as $|h|$ gets too small.

Problem 2. For the function $f(x) = (\sin(x) + 1)^x$, calculate and plot the errors of the

1. second order backward difference quotient,
2. second order centered difference quotient, and the
3. fourth order centered difference quotient

using your functions from Problem 1 to get the numerical approximations. Do this for at least 6 evenly-spaced values of $h \in [10^{-8}, 1]$. Use a `loglog()` plot, include a legend and put a dot on the graph for each value of h. Your function should accept a float value where the derivative is being approximated at.

Hints: Define f and analytically compute its derivative. For each value of h, calculate and plot $|f'(x_0) - \tilde{f}(x_0)|$. Consider using the NumPy function `logspace()` to define your h-values. To include a point on your graph, put `'-o'` as an argument in your `loglog()` function call.

Evaluated at $x_0 = 1$, the plot of just the fourth order centered difference quotient should resemble Figure 8.1. You should notice a bend in each of the graphs, where the h-value is getting too small.

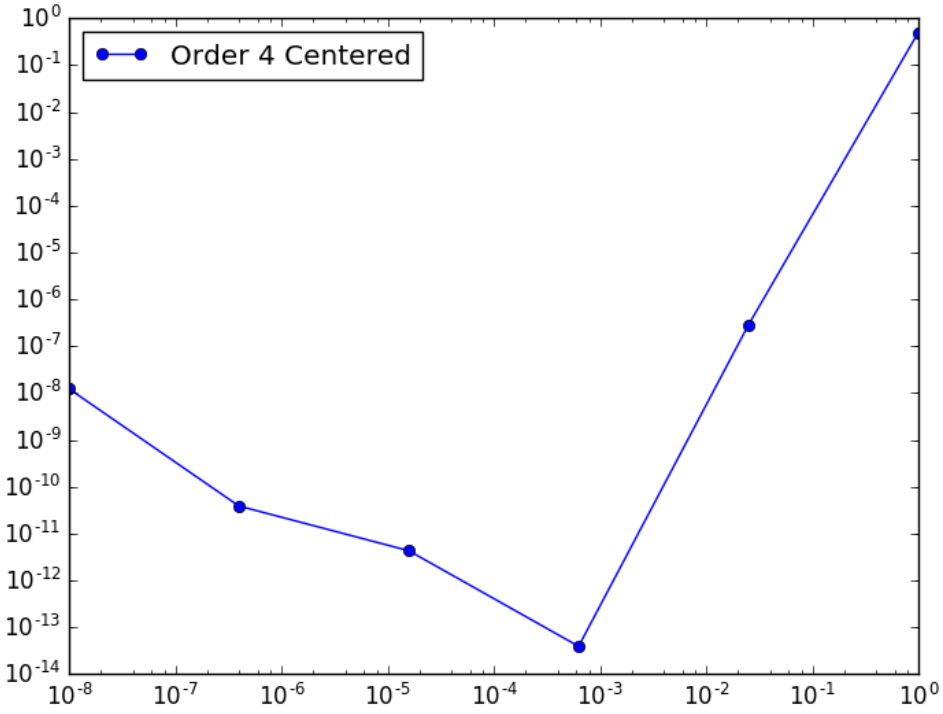


Figure 8.1: The plotted errors of fourth order centered difference quotient for the function $f(x) = (\sin(x) + 1)^x$ evaluated at $x = 1$.

Achtung!

Mathematically, choosing smaller h values results in smaller errors. On a computer however, values of h that are too small result in imprecise computations due to *catastrophic cancellation*, which we will discuss in Conditioning and Stability. Consequently, the optimal value of h is one that is small but not too small, such as 10^{-5}.

Although the centered difference quotient gives a more accurate approximation of the derivative, there are some functions that do not behave well under centered difference quotients. Additionally, information on both sides of the point x_0 may not be available. In these cases, one must use the forward or backward difference quotient to approximate the derivative.

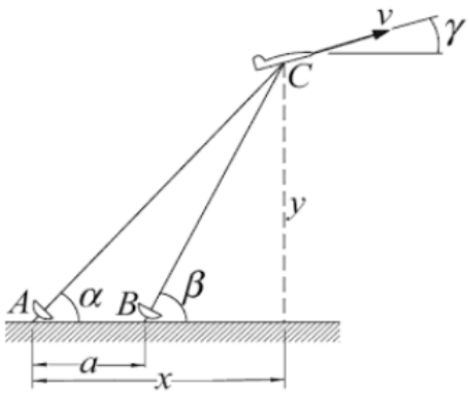


Figure 8.2: Radar stations in relation to plane

Problem 3. The radar stations A and B, separated by the distance a = 500 km, track a plane C by recording the angles α and β at one-second intervals (See figure 8.2). Successive readings for α and β at integer times $t \in [7, 14]$ are given in the textfile `plane.txt`. The first column contains the integer values of t, the second contains the float values of α in degrees and the third contains the float values β in degrees. Use finite difference quotients to calculate the velocity of the plane for each value of t in the file. The coordinates of the plane are

$$x = a\frac{\tan(\beta)}{\tan(\beta) - \tan(\alpha)} \tag{8.8}$$

$$y = a\frac{\tan(\beta)\tan(\alpha)}{\tan(\beta) - \tan(\alpha)}. \tag{8.9}$$

Use these functions to find the coordinates of the plane at each point in time and plot the trajectory (note that NumPy trigometric functions only accept angles in radians). Then approximate $x'(t)$ and $y'(t)$ at each point (using the forward difference quotient on $t = 7$, the backward on $t = 14$ and the centered on all other points). Plot the values of the velocity $\sqrt{x'(t)^2 + y'(t)^2}$ at each point in time and then return them in an array.

The trajectory of the plane will be constantly increasing. And the values of the speed will vary between .265 and .285 km/sec which is approximately equivalent to $592 - 637$ mph.

(Kiusalaas, Jaan. Numerical Methods in Engineering with Python 3)

Note

Finite difference quotients can be used to approximate higher-order derivatives of f. However, taking derivatives is an unstable operation which can amplify the arithmetic error in your computation. For this reason, difference quotients are not generally used to approximate derivatives higher than second order.

Derivative Approximations in Multiple Dimensions

Finite difference methods can also be used to calculate derivatives in higher dimensions. Recall that the Jacobian of a function $f : \mathbb{R}^n \to \mathbb{R}^m$ at a point $x_0 \in \mathbb{R}^n$ is the $m \times n$ matrix $J = (J_{ij})$ defined component-wise by

$$J_{ij} = \frac{\partial f_i}{\partial x_j}(x_0).$$

For example, the Jacobian for a function $f : \mathbb{R}^3 \to \mathbb{R}^2$ is defined by

$$J = \begin{pmatrix} \frac{\partial f}{\partial x_1} & \frac{\partial f}{\partial x_2} & \frac{\partial f}{\partial x_3} \end{pmatrix} = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \frac{\partial f_1}{\partial x_3} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \frac{\partial f_2}{\partial x_3} \end{pmatrix}.$$

The Jacobian is useful in many applications. For example, the Jacobian can be used to find zeros of functions in multiple variables.

The forward difference quotient for approximating a partial derivative is

$$\frac{\partial f}{\partial x_j}(x_0) \approx \frac{f(x_0 + he_j) - f(x_0)}{h},$$

where e_j is the j^{th} standard basis vector. Similarly, the centered difference approximation is

$$\frac{\partial f}{\partial x_j}(x_0) \approx \frac{\frac{1}{2}f(x_0 + he_j) - \frac{1}{2}f(x_0 - he_j)}{h}.$$

Problem 4. Return the approximate Jacobian matrix of a function at a specific point using the centered difference quotient. Your function should accept:

1. a callable function f,
2. an integer n that is the dimension of the domain of f,
3. an integer m that is the dimension of the range of f,
4. an (1 x n)-dimensional NumPy array `pt` representing a point in $\mathbb{R}^n$, and
5. a keyword argument h that defaults to 10^{-5}.

You can test your function with the following code:

```
>>> f = lambda x: np.array([x[0]**2+x[1]**2, np.sin(x[0])+np.exp(x[1])])
>>> pt = np.array([1., -1.])
>>> jacobian(f, 2, 2, pt, 1e-5)
array([[2.,-2.],[0.54030231, 0.36787944]])
```

Problem 5.

Let $f : \mathbb{R}^2 \to \mathbb{R}^2$ be defined by

$$f(x, y) = \begin{bmatrix} e^x \sin(y) + y^3 \\ 3y - \cos(x) \end{bmatrix}$$

Find the error between your Jacobian function and the analytically computed derivative on the square $[-1, 1] \times [-1, 1]$ using ten thousand grid points (100 per side). You may apply your Jacobian function to the points one at a time using a double `for` loop. Once you get the error matrix for a given point, calculate the Frobenius norm of this matrix (`la.norm()` defaults to the Frobenius norm). This norm will be your total error for that point. Return the maximum error of your Jacobian function over all points in the square.

Hint: The following code defines the function $f(x, y) = \begin{bmatrix} x^2 \\ x + y \end{bmatrix}$.

```
# f accepts a length-2 NumPy array
>>> f = lambda x: np.array([x[0]**2, x[0]+x[1]])
```

Additional Material

Derivations

$f'(x_0)$ can be approximated to the second order with another difference quotient, called the centered difference quotient. We begin by trying to find the backward difference quotient. Evaluate Taylor's formula at $x_0 - h$ to derive

$$f'(x_0) = \frac{f(x_0) - f(x_0 - h)}{h} + \frac{R_2(-h)}{h}. \tag{8.10}$$

The first term on the right hand side of (8.10) is called the *backward difference quotient.* This quotient also approximates $f'(x_0)$ to the first order. When we add (8.3) and (8.10) and solve for $f'(x_0)$, we get

$$f'(x_0) = \frac{\frac{1}{2}f(x_0 + h) - \frac{1}{2}f(x_0 - h)}{h} + \frac{R_2(-h) - R_2(h)}{2h} \tag{8.11}$$

The *centered difference quotient* is the first term of the right hand side of (8.11). Let us investigate the remainder term to see how accurate this approximation is. Recall from the proof of Taylor's theorem that $R_k = \frac{f^{(k)}(x_0)}{k!}h^k + R_{k+1}$. Therefore,

$$\begin{aligned}
\frac{R_2(-h) - R_2(h)}{2h} &= \frac{1}{2h}\left(\frac{f''(x_0)}{2!}h^2 + R_3(-h) - \frac{f''(x_0)}{2!}h^2 - R_3(h)\right) \\
&= \frac{1}{2h}(R_3(-h) - R_3(h)) \\
&= \frac{1}{2h}\left(\left(\int_0^1 \frac{(1-t)^2}{2}f'''(x_0 + th)dt\right)h^3 - \left(\int_0^1 \frac{(1-t)^2}{2}f'''(x_0 - th)dt\right)h^3\right) \\
&= \left(\int_0^1 \frac{(1-t)^2}{4}(f'''(x_0 + th) - f'''(x_0 - th))\right)h^2 \\
&\in O(h^2)
\end{aligned}$$

once we restrict h to some δ-neighborhood of 0. So the error in using the centered difference quotient is smaller than using the forward and backward difference quotients when $|h| < 1$.

9 Symbolic and Automatic Differentiation

Lab Objective: *Python can compute derivatives symbolically and automatically. SymPy uses symbolic computations to calculate exact derivatives. Autograd automatically differentiates Python and NumPy code. In this lab, we learn how to use these packages for differentiation. We will also compare the computation cost and accuracy of differentiating between SymPy, Autograd, and numerical differentiation.*

SymPy

Symbolic Manipulation

It is simple to numerically compute $2x^5 + 4xy + 3x$ given any specific values of x and y. In some circumstances, however, getting the entire algebraic expression is more desirable. We can use SymPy to create symbolic representations of expressions.

To symbolically represent expressions, symbolic variables must first be defined. To define the symbol x, we write `x = sy.symbols('x')`. Multiple variables can also be defined at once with `sy.symbols('x,y,z')`. Combining symbolic objects results in a SymPy *expression*.

```
>>> import sympy as sy

# Define the symbolic variables x and y.
>>> x, y  = sy.symbols('x, y')

# Create the expression 2x^5 + 4xy + 3x.
>>> expr = 2*x**5 + 4*x*y + 3*x
>>> print(expr)
2*x**5 + 4*x*y + 3*x
```

Be careful that the function `sy.symbols()` is spelled correctly. The command `sy.Symbol()` will still work for a single symbolic variable, but `sy.symbol` is a submodule and cannot be called at all.

ACHTUNG!

Beware of integer division: the expression `(3/4)*sy.sin(x)` will evaluate to 0. Be careful about using floating points as well. The expression `(1/3.)*sy.sin(x)` will evaluate to `0.333333333333333*sy.sin(x)`.

To keep $\frac{3}{4}$ symbolic, use `3*sy.sin(x)/4` or `sy.Rational(3,4)*sy.sin(x)` instead.

Problem 1. Write a function that creates the expression $\frac{2}{5}e^{x^2-y}\cosh(x+y) + \frac{3}{7}\log(xy+1)$ symbolically with SymPy. The Sympy syntax for $\cosh(x)$ and $\log(x)$ are`sy.cosh(x)` and `sy.log(x)`, respectively. Make sure that your constants are not floating point numbers.

SymPy can be used to solve difficult expressions for given variables. Consider the following equation:

$$\frac{w}{w-x} + \frac{x}{x-y} + \frac{y}{y-w} = 0$$

The explicit solution of w,written in terms of x and y, would be tedious to compute by hand but SymPy can solve for this explicit solution.

```
>>> w, x, y = sy.symbols('w, x, y')
>>> expr = w/(w-x) + x/(x-y) + y/(y-w)

# Solve for the expression in terms of w.
>>> sy.solve(expr,w)
[(x**2 + 3*x*y - 2*y**2 + (-x + y)*sqrt(x**2 - 8*x*y + 4*y**2))/(2*(2*x - y)), ↩
      (x**2 + 3*x*y - 2*y**2 + (x - y)*sqrt(x**2 - 8*x*y + 4*y**2))/(2*(2*x - y↩
    ))]
```

Note that `sy.solve()` returns a list of expressions that solves for w. To use the expression solved, one must take that expression from the list.

```
# Take the first expression that solves for w in terms of x and y.
>>> sy.solve(expr,w)[0]
(x**2 + 3*x*y - 2*y**2 + (-x + y)*sqrt(x**2 - 8*x*y + 4*y**2))/(2*(2*x - y))
```

In the example above, a symbolic expression is used instead of an equation. This is because SymPy automatically sets the expression equal to zero, solves for the indicated variable, and then returns the result. If there is an equation given, subtract everything to one side of the equality.

Another way to use `sy.solve()` is to declare an equation. An equation can be defined using `sy.Eq`. To represent the equation $y = 3x + 2$, declare `equation = sy.Eq(3*x+2,y)`. To solve for x, use `sy.solve(equation,x)`.

Problem 2. Write a function that uses Sympy to solve the equation $y = \sqrt{5 - e^{x^2}}$ for x. Return the list of expressions that solves for x. The SymPy syntax for $\sqrt{x}$ is `sy.sqrt(x)`.

Symplify

SymPy can also be used to expand and simplify different symbolic expressions. As an example we will simplify the expression

$$\frac{wx^2y^2 - wx^2 - wy^2 + w - x^2y^2z + 2x^2y^2 + x^2z - 2x^2 + y^2z - 2y^2 - z + 2}{wxy - wx - wy + w - xyz + 2xy + xz - 2x + yz - 2y - z + 2}.$$

```
>>> w, x, y, z=sy.symbols('w, x, y, z')
>>> expr = (w*x**2*y**2 - w*x**2 - w*y**2 + w - x**2*y**2*z + 2*x**2*y**2 + x↩
    **2*z - 2*x**2 + y**2*z - 2*y**2 - z + 2)/(w*x*y - w*x - w*y + w - x*y*z + ↩
    2*x*y + x*z - 2*x + y*z - 2*y - z + 2)
>>> expr.simplify()
x*y + x + y + 1
```

`simplify()` is the general simplification method for a SymPy expression. It can be called as a function from the module by using `sy.simplify()` or it can be used as a method for an object as in the example above. SymPy can compute specific types of simplification. For example, to factor an expression, use `factor()`. To expand an expression, use `expand()`. To focus purely on simplifying the trigonometric aspects of the expression, use `trigsimp()`. To cancel variable expressions in the numerator and denominator of all rational sub-expressions, use `cancel()`. There are several other kinds of algebraic manipulations in SymPy, see the documentation for a more comprehensive list. Many of these more important functions in SymPy are also available as methods to expressions. This is the case with all of the above examples.

Refer to the Additional Material or `http://docs.sympy.org/0.7.2/tutorial.html` for other useful features.

Differentiation using SymPy

SymPy can be used to take closed form derivatives without doing it by hand. Derivatives can be taken in Sympy using the `sy.Derivative()` function:

```
>>> x, y = sy.symbols('x,y')
>>> expr = sy.sin(x)*sy.cos(x)*sy.exp(y)*(x**3+y)**4
# Find the derivative of expr in terms of x.
>>> sy.Derivative(expr,x).doit()
12*x**2*(x**3 + y)**3*exp(y)*sin(x)*cos(x) - (x**3 + y)**4*exp(y)*sin(x)**2 + (↩
    x**3 + y)**4*exp(y)*cos(x)**2
```

The `.doit()` method tells SymPy to evaluate the derivative of the expression.

Equivalently, one can use the `.diff()` method of a SymPy expression.

```
>>> expr.diff(x)
```

```
12*x**2*(x**3 + y)**3*exp(y)*sin(x)*cos(x) - (x**3 + y)**4*exp(y)*sin(x)**2 + (↩
    x**3 + y)**4*exp(y)*cos(x)**2
```

To find the derivative of the expression above at $x = 0$, substitute a symbolic variable for a value by using the `.sub()` method shown below:

```
# Save the derivative as an expression named d_expr.
>>> d_expr = expr.diff(x)
# Substitute x with 0.
>>> d_expr.subs(x,0)
y**4*exp(y)
```

To substitute values in for multiple variables, either use a dictionary or a list of tuples for each variable and value.

```
# Substitute multiple variables with a dictionary.
>>> d_expr.subs({x:1.,y:2.})
839.384133011589
# Substitute multiple variables with a list of tuples.
>>> d_expr.subs([(x,1.),(y,2.)])
839.384133011589
```

Make sure that the substitutions you implemented are floating points. If they are not, Sympy will not evaluate the expression. You may use the method `.evalf( )` to evaluate the expression.

```
#  Replace y with the integer 2.
>>> d_expr.subs([(x,1.),(y,2)])
113.598289385442*exp(2)
# Use .evalf() to evaluate e^2.
>>> d_expr.subs([(x,1.),(y,2)]).evalf()
839.384133011589
```

Note that these methods return a modified version of the expression, but do not actually change the original expression.

Problem 3. Use SymPy to calculate the derivative of $e^{\sin(\cos(x))}$ at $x = 1$. Use the second order centered difference quotient from the previous lab to calculate the same derivative. Compare the performance of Sympy and the centered difference quotient. Print out the total time each method takes to compute the derivative as well as the error of the approximation.

The error is denoted as $|Df(x_0) - D\tilde{f}(x_0)|$ where $D\tilde{f}(x_0)$ is the approximated derivative and $Df(x_0) = -e^{\sin(cos(x))} \sin(x) \cos(\cos(x))$.

Return the SymPy approximation as a float.

Hint: Recall that the second order centered difference quotient is

$$f'(x_0) \approx \frac{f(x_0 + h) - f(x_0 - h)}{2h}.$$

For this approximation, let $h = 1 \times 10^{-5}$. The result should reveal that SymPy has an error of zero but the centered difference quotient will compute it faster.

From the previous problem, we could see that SymPy is very accurate in finding derivatives. However the cost of having accurate solutions is the time the method takes to compute the derivative. Finding the right method to compute differentiations will depend on which factor is more prominent. In cases where stability is more important, Sympy would be the better option. If accuracy is not as important but less computation time is important, then numerical differentiation (like centered difference quotient) might be the better choice. Later, in this lab, we will explore another differentiable tool called Autograd.

Useful tools for Differentiation with SymPy

When using `.diff()`, the method defaults to solving the first derivative of the function. Given a function that is differentiable n times, you can find the nth derivative of the function by having n as the second argument in `.diff()`.

The following equation takes the 20th partial derivative with respect to x of

$$\prod_{i=1}^{23} (x + iy)$$

```
>>> x, y, i = sy.symbols('x, y, i')
# Define the expression.
>>> expr = sy.product((x+i*y), (i, 1, 23))
# Expand the product.
>>> expr = expr.expand()
# Take the 20th derivative with respect to x.
>>> expr.diff(x, 20)
4308669456480829440000*(x**3 + 36*x**2*y + 426*x*y**2 + 1656*y**3)
```

Another effective tool in Sympy is to transform a sympy expression to a lambda function through `sy.lambdify()`. This can be used to calculate numerical values very fast. Consider the following example:

```
>>> x = sy.symbols('x')
# Assign the second derivative of sin(x)^2 to expr.
>>> expr = (sy.sin(x)**2).diff(x,2)
# Turn the expression into a lambda function with x as the variable.
>>> f = sy.lambdify(x,expr)
>>> f(0)
2.0
>>> f(np.pi/2)
-2.0
>>> f(np.pi)
2.0
```

There are many advantages of transforming a SymPy expression into a lambda function. Rather than substituting values by using the `.subs()` method, evaluating the lambda functions is cheaper to compute. According to the Lambdify documentation, using `sy.lambdify()` to do numerical evaluations "takes on the order of hundreds of nanoseconds, roughly two orders of magnitude faster than the `.subs()` method."

Problem 4. Compare the time it takes to evaluate the 3rd derivative of $\tanh(x)$ at 10,000 randomly generated points using the `.subs()` method versus turning a Sympy expression into a lambda function through `sy.lambdify()`. Print out the times it takes to evaluate the 3rd derivative of $\tanh(x)$ at 10,000 random points by `.subs()` and through `sy.lambdify()`.

By default, `sy.lambdify()` uses the `math` library. However, `sy.lambdify()` supports many other libraries including NumPy. By including `"numpy"` as the third argument of the function, the function generated by `sy.lambdify()` can have access to vectorized functions. Consider the following example:

```
#Generate an numpy array of points.
>>> points = np.linspace(0,2*np.pi,10)
>>> expr = sy.sin(2*x).diff(x,2)
# Turn expr in to a lambda function with the numpy attribute.
>>> f = sy.lambdify(x,expr,"numpy")
# Evaluate f with multiple points at once.
>>> f(points)
array([ -0.00000000e+00,  -3.93923101e+00,  -1.36808057e+00,
         3.46410162e+00,   2.57115044e+00,  -2.57115044e+00,
        -3.46410162e+00,   1.36808057e+00,   3.93923101e+00,
         1.95943488e-15])
```

SymPy can also be used to compute the Jacobian of a matrix using the `.jacobian()` method, which takes in either a list or a matrix of the variables. The Jacobian of $f(x,y) = \begin{bmatrix} x^2 \\ x+y \end{bmatrix}$ is found by doing the following:

```
# Create a matrix of symbolic variables.
>>> x,y = sy.symbols('x,y')
>>> F = sy.Matrix([x**2,x+y])

# Find the jacobian of the matrix with respect to x and y.
>>> F_jac = F.jacobian([x,y])
>>> F_jac
Matrix([
[2*x, 0],
[  1, 1]])

# Evaluate the Jacobian at (1,1).
>>> F_jac.subs([(x,1.),(y,1.)])
Matrix([
[2.0, 0],
```

```
[  1, 1]])
```

In addition, SymPy includes several integral transforms, such as the Laplace, Fourier, sine, and cosine transforms. SymPy also allows you to do simple separation of variables on PDEs, Taylor Series, Laurent Series, Fourier Series, and many, *many* other things.

Autograd

Autograd is a package that allows for efficient automatic differentiation using NumPy codes. Unlike SymPy ,which has many diverse applications, autograd is solely used in differentiation. Because Autograd works on ordinary NumPy code, it is very useful to calculate gradients automatically rather than deriving the code by hand. Due to this feature, it can be very useful in machine learning.

Autograd is installed by running the following command in the terminal:

```
pip install autograd
```

See `https://github.com/HIPS/autograd` for more complete installation instructions.

The following code computes the derivative of $e^{\sin(\cos(x))}$ at $x = 1$ using Autograd:

```
>>> from autograd import grad
>>> import autograd.numpy as anp        # Use autograd's own version of NumPy

>>> g = lambda x: anp.exp(anp.sin(anp.cos(x)))
>>> grad_g = grad(g)
>>> grad_g(1.)
-1.20697770398
```

To support most of the NumPy features[1], autograd uses a thinly-wrapped version of Numpy called `autograd.numpy`. This lab will denote the Autograd's version of Numpy as `anp`. Use `anp` the way NumPy is used.

The function `grad()` returns a function that computes the gradient of your original function. This new function, which returns the gradient, accepts the same parameters as the original function.

When there are multiple variables, the parameter `argnum` allows you to specify with respect to which variable you are computing the gradient.

```
>>> f = lambda x,y: 3*x*y + 2*y - x
>>> grad_f = grad(f, argnum=0) #gradient with respect to the first variable (x)
>>> grad_f(.25,.5)
0.5
>>> grad_f = grad(f, argnum=1) #gradient with respect to the second variable (y↩
    )
>>> grad_fun(.25,.5)
2.75
```

Finding the gradient with respect to multiple variables can by done using `multigrad()` by specifying which variables in the `argnums` parameter.

[1]For a list of Numpy features that Autograd does not support, please refer to `https://github.com/HIPS/autograd/blob/701ed8518140ffa4246e7ef18256a71ed639045b/docs/tutorial.md`.

```
>>> grad_fun = autograd.multigrad(function, argnums=[0,1])
>>> grad_fun(.25,.5)
(0.5, 2.75)
```

Problem 5. Use Autograd to compute the derivative of $f(x) = \ln\sqrt{\sin\left(\sqrt{x}\right)}$ at $x = \frac{\pi}{4}$. Compare how long it takes to compute this derivative among Autograd, SymPy, and the second order centered difference quotient and record the error each approximation. Print the computation time and error for each method.

The error is denoted as $|Df(x_0) - D\tilde{f}(x_0)|$ where $Df(x_0) = \frac{\cot\left(\sqrt{x}\right)}{4\sqrt{x}}$ and $D\tilde{f}(x_0)$ is the approximated derivative.

SymPy will have the exact derivative of the function yielding zero error. However, SymPy will also have the longest computation time. Centered difference quotient will have the least amount of time with the greatest error. Autograd will have shorter computation time than SymPy and a smaller error than centered difference quotient.

As shown in the previous problem, Autograd can be an efficient tool in differentiation. Although Autograd does not calculate exact derivatives, the resulting error is relatively small with less computational time than SymPy.

Autograd allows users to differentiate a function as many times as desired.

```
>>> f = lambda x: anp.sin(x) + 3**anp.cos(x)
# Calculate the first derivative.
>>> df = grad(f)
# Calculate the second derivative and so forth.
>>> df2 = grad(df)
>>> df3 = grad(df2)
>>> df3(1.)
2.6834458987503522
```

Although `grad()` is very efficient, it does not allow for array broadcasting. However, Autograd has another function `elementwise_grad()` that does.

```
>>> from autograd import elementwise_grad
>>> f = lambda x: anp.sin(x) + 3**anp.cos(x)
>>> f_grad = elementwise_grad(f)
>>> f_grad(np.array([1.,2.,3.,]))
array([-1.13338111, -1.04855565, -1.04224253])
```

Problem 6. Use `elementwise_grad()` to graph $f(x) = \frac{1}{\cosh(x)}$ and it's next five derivatives where $x \in [-7, 7]$. Display the plots in multiple subplots.

While the `grad()` function can only output scalar-valued functions, `jacobian()` can allow you to find the gradient of vectors. The following shows how to find the Jacobian of $f(x,y) = \begin{bmatrix} x^2 \\ x+y \end{bmatrix}$ evaluated at (1,1).

```
from autograd import jacobian
>>> f = lambda x: anp.array([x[0]**2, x[0]+x[1]])
>>> jacobian_f = jacobian(f)
>>> jacobian_f(anp.array([1.,1.]))
array([[ 2.,  0.],
       [ 1.,  1.]])
```

Problem 7.

Let $f : \mathbb{R}^2 \to \mathbb{R}^2$ be defined by

$$f(x,y) = \begin{bmatrix} e^x \sin(y) + y^3 \\ 3y - \cos(x) \end{bmatrix}$$

Find the Jacobian function using SymPy and Autograd. Print out the time it takes to compute each Jacobian at $(x,y) = (1,1)$.

Notice that Autograd computes the Jacobian a lot faster than SymPy.

To learn more about Autograd visit `https://github.com/HIPS/autograd`.

Additional Materials

Displaying SymPy Expressions

SymPy includes a simplified plotting wrapper around Matplotlib.

```
>>> x = sy.symbols('x')
>>> expr = sy.sin(x) * sy.exp(x)
>>> sy.plot(expr, (x, -3, 3))
```

The code above plots $\sin(x)e^x$ for values of x from -3 to 3.

SymPy also has several nice options for printing equations. To know what the equation looks like use `sy.pprint()`. It can interface with the IPython Notebook to display the formula more clearly as well. IPython Notebook can enable pretty printing by loading the extension that comes with SymPy. In SymPy 7.2, this is done as follows:

```
%load_ext sympy.interactive.ipythonprinting
```

The syntax is written a little differently in SymPy 7.3.

```
import sympy as sy
sy.init_printing()
```

Figure 9.1 shows a screenshot of SymPy's special printing in the IPython notebook. If at some point you need to write a formula in LaTeX, the function `sy.latex()` can convert a SymPy symbolic expression to LaTeX.

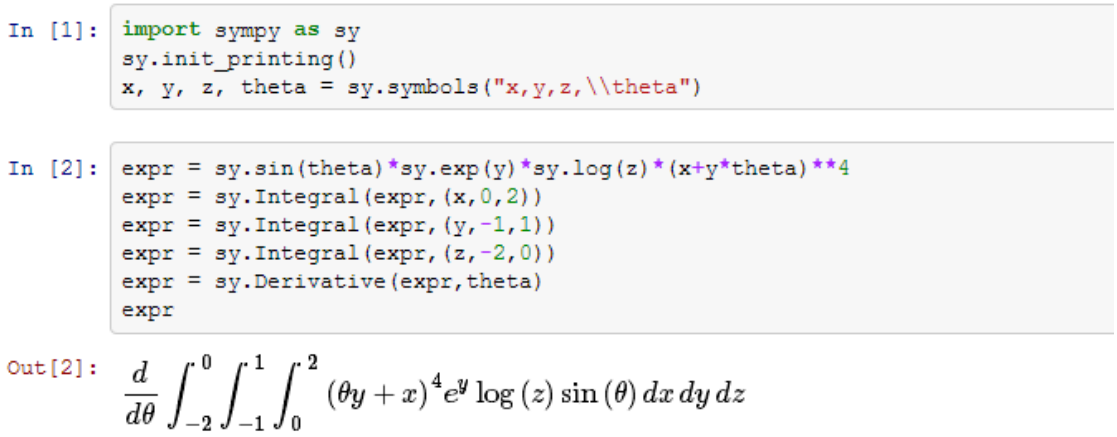


Figure 9.1: A screenshot showing how SymPy can interface with the IPython Notebook to display equations.

Basic Number Types

SymPy has some good built in datatypes which can be used to represent rational numbers and arbitrary precision floating point numbers. Arbitrary precision floating point operations are supported through the package `mpmath`. These can be useful if computation to a very high precision is needed. It can also avoid possible overflow error in computation. They are, however, much more costly to compute.

You can declare a rational number $\frac{a}{b}$ using `sy.Rational(a, b)`. A real number r of precision n can be declared using `sy.Float(r,n)`.

A nice example of the use of these datatypes is the following function which computes π to the nth digit.

```
def mypi(n):
    #Calculates pi to n decimal points.
    tot = sy.Rational(0, 1)
    term = 1
    bound = sy.Rational(1, 10)**(n+1)
    i = 0
    while bound <= term:
        term = 6 * sy.Rational(sy.factorial(2*i), 4**i*(sy.factorial(i))**2*(2*↩
            i+1)*2**(2*i+1))
        tot += term
        i += 1
    return sy.Float(tot, n)
```

This function works by evaluating the Taylor series for $6 \arcsin\left(\frac{1}{2}\right)$. We used a rather crude error estimate to ensure that we were close enough to break the loop.

More Sympy Substitution

Substitution also can be used (to some extent) to substitute one expression for another. For example, if you want to apply the double angle identity to replace products of sines and cosines, you could use the following:

```
>>> expr.subs(sy.sin(x) * sy.cos(x), sy.sin(2*x)/2)
(x**3 + y)**4*exp(y)*sin(2*x)/2
```

To eliminate higher powers of a variable in an expression, use something like:

```
>>> expr.subs(x**3, 0)
y**4*exp(y)*sin(x)*cos(x)
```

which will eliminate all terms of the expression involving x^3. At present time, this will not eliminate terms involving x^4 or higher powers of x that are not divisible by 3.

Integrals in SymPy

SymPy can integrate two different variables along two different bounds.

```
sy.integrate(y**2*x**2, (x, -1, 1), (y, -1, 1))
```

It can also integrate with respect to multiple variables.

```
sy.integrate(y**2 * x**2, x, y)
```

Integrate a difficult expression like $e^x \sin(x) \sinh(x)$ can be done with one line in SymPy.

```
sy.Integral(sy.sin(x) * sy.exp(x) * sy.sinh(x), x).doit()
```

Differential Equations in SymPy

SymPy can be used to solve some sorts of basic ordinary differential equations. This will solve the equation $y_{xx} - 2 * y_x + y = \sin(x)$.

```
x = sy.symbols('x')
f = sy.Function('f')
eq = sy.Eq(f(x).diff(x, 2) - 2*f(x).diff(x) + f(x), sy.sin(x))
sy.dsolve(eq)
```

or, equivalently,

```
x = sy.symbols('x')
f = sy.Function('f')
expr = f(x).diff(x, 2) - 2*f(x).diff(x) + f(x) - sy.sin(x)
sy.dsolve(expr)
```

10 Newton's Method

Lab Objective: *Newton's method finds the roots of functions; that is, it finds $\bar{x}$ such that $f(\bar{x}) = 0$. This method can be used in optimization to determine where the maxima and minima occur. In this lab, we use Newton's method to find zeros of a function. We also explore where an initial point converges based on basins of attraction.*

Newton's Method

Newton's method begins with an initial guess x_0. Successive approximations of a root are found with the recursive sequence

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}.$$

In other words, Newton's method approximates the root of a function by finding the x-intercept of the tangent line at $(x_n, f(x_n))$ (see Figure **??**).

The sequence $\{x_n\}$ will converge to the zero $\overline{x}$ of f if

1. f and f' exist and are continuous,
2. $f'(\overline{x}) \neq 0$, and
3. x_0 is "sufficiently close" to $\overline{x}$.

When all three conditions hold, Newton's method converges quadratically. In applications, the first two conditions usually hold. However, if $\overline{x}$ and x_0 are not "sufficiently close", Newton's method may converge very slowly, or it may not converge at all.

Newton's method is powerful because given the three conditions above, it converges quickly. In these cases, the sequence $\{x_n\}$ converges to the actual root quadratically, meaning that the maximum error is squared at every iteration.

Let us do an example with $f(x) = x^2 - 1$. We define $f(x)$ and $f'(x)$ in Python as follows.

```
>>> import numpy as np
>>> f = lambda x : x**2 - 1
>>> Df = lambda x : 2*x
```

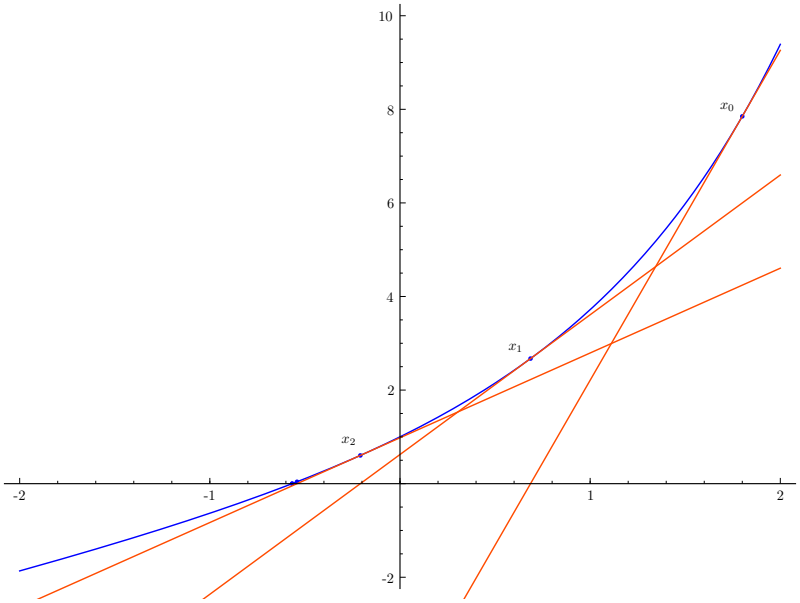


Figure 10.1: An illustration of how two iterations of Newton's method works with initial starting point x_0. Newton's method takes the tangent line (red) at the point $(x_n, f(x_n))$ and defines x_{n+1} to be the x-intercept of that line.

Now we set $x_0 = 1.5$ and iterate.

```
>>> xold = 1.5
>>> xnew = xold - f(xold)/Df(xold)
>>> xnew
1.0833333333333333
```

We can repeat this as many times as we desire.

```
>>> xold = xnew
>>> xnew = xold - f(xold)/Df(xold)
>>> xnew
1.0032051282051282
```

We have already computed the root 1 to two digits of accuracy.

Problem 1. Implement Newton's method with a function that accepts the following parameters: a function f, an initial x-value, the derivative of f, the maximum number of iterations for Newton's method to perform that defaults to 15, and a tolerance that defaults to 10^{-5}. The algorithm terminates when the difference between successive approximations is less than the tolerance or the maximum number of iterations has been reached. Return a tuple containing the last x-value computed, a Boolean telling whether or not Newton's method converged, and the number of iterations completed.

NOTE

Newton's method can be used to find zeros of functions that are hard to solve for analytically. Note that the function $f(x) = \frac{sin(x)}{x} - x$ is not continuous on any interval containing 0, but can be made continuous by defining $f(0) = 1$. Newton's method can be used to compute the zero of this function.

Problem 2. Suppose that an amount of P_1 dollars is put into an account at the beginning of years $1, 2, ..., N_1$ and that the account accumulates interest at a fractional rate r (for example, $r = .05$ corresponds to 5% interest). Suppose also that, at the beginning of years $N_1 + 1, N_1 + 2, ..., N_1 + N_2$, an amount of P_2 dollars is withdrawn from the account and that the account balance is exactly zero after the withdrawal at year $N_1 + N_2$. Then the variables satisfy the equation

$$P_1[(1 + r)^{N_1} - 1] = P_2[1 - (1 + r)^{-N_2}].$$

If $N_1 = 30, N_2 = 20, P_1 = 2000$, and $P_2 = 8000$, use Newton's method to determine r. (From Atkinson Page 118).

Backtracking

There are times when Newton's method may not converge due to the fact that the step from x_n to x_{n+1} was too large and the zero was stepped over completely. To combat this problem of overstepping, backtracking is a useful tool. Backtracking is simply taking a fraction of the full step from x_n to x_{n+1}. Define Newton's method with the recursive sequence

$$x_{n+1} = x_n - \alpha \frac{f(x_n)}{f'(x_n)}.$$

Note that setting $\alpha = 1$ results in the same Newton's method used up to this point in the lab. Backtracking uses $\alpha < 1$ in the above sequence and takes a fraction of the step at each iteration.

Problem 3. Modify your function from Problem 1 so that it accepts a parameter α that defaults to 1 to allow backtracking. Run the function on $f(x) = x^{1/3}$ with $x_0 = .01$ using the default value for α. What happens and why? Hint: The command `x**(1/3)` will not work when `x` is negative. Here is one way to define the function $f(x) = x^{1/3}$ in NumPy.

```
f = lambda x: np.sign(x)*np.power(np.abs(x), 1./3)
```

Now find an $\alpha < 1$ so that running the function on $f(x) = x^{1/3}$ with $x_0 = .01$ converges. Return the same results as in Problem 1; that is, return a tuple containing the last x-value computed, a Boolean telling whether or not Newton's method converged, and the number of iterations completed.

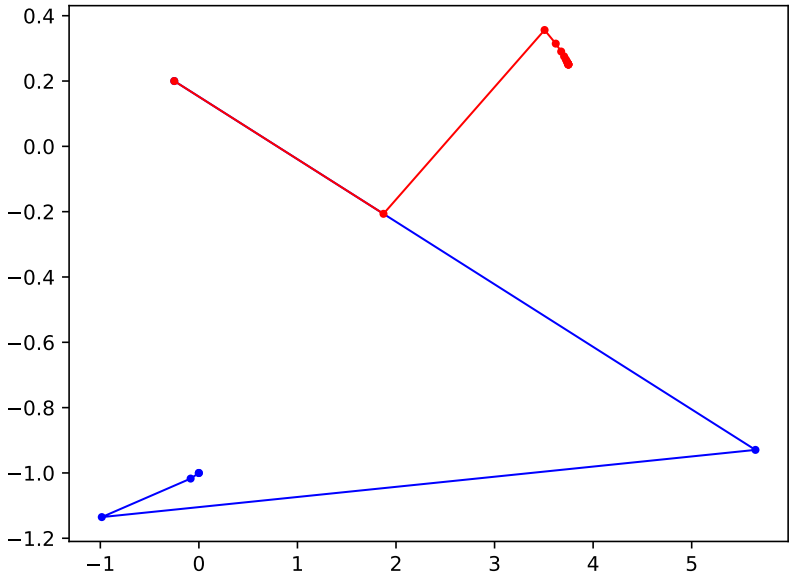


Figure 10.2: Starting at the same initial value results in convergence to two different solutions. The blue line converges to $(0, -1)$ (with $\alpha = 1$) in 5 iterations of Newton's method while the red line converges to $(3.75, .25)$ with $\alpha < 1$ in 15 iterations .

Newton's Method: Vector Version

Newton's method can be generalized from the single-variable case to multi-dimensional problems. We can solve the equation $f(\bar{\mathbf{x}}) = \mathbf{0}$ for $\bar{\mathbf{x}}$, where $f = (f_1, f_2, \ldots, f_n)$ is a vector of functions and $\bar{\mathbf{x}} = (\bar{x}_1, \bar{x}_2, \ldots, \bar{x}_n) \in \mathbb{R}^n$. The recursive sequence for the vector version of Newton's method is defined as

$$\mathbf{x}_{n+1} = \mathbf{x}_n - \alpha Df(\mathbf{x}_n)^{-1} f(\mathbf{x}_n).$$

Like the one-dimensional method, the vector version of Newton's method terminates when the difference between successive approximations is less than a predetermined tolerance ϵ; that is, $||\mathbf{x}_{n+1} - \mathbf{x}_n|| < \epsilon$, or the maximum number of iterations is reached.

Problem 4. 1. Create a function that performs Newton's method on vectors in $\mathbb{R}^2$ and accepts the following parameters: a function f, an initial guess $\mathbf{x_0}$, the derivative function of f, a maximum number of iterations that defaults to 15, a tolerance that defaults to 10^{-5}, and a backtracking factor α that defaults to 1. Return a tuple of lists containing the values of each component at each iteration.

2. Bioremediation involves the use of bacteria to consume toxic wastes. At a steady state, the bacterial density x and the nutrient concentration y satisfy the system of nonlinear equations

$$\gamma xy - x(1 + y) = 0,$$

$$-xy + (\delta - y)(1 + y) = 0,$$

where γ and δ are parameters that depend on various physical features of the system. For this problem, assume the typical values $\gamma = 5$ and $\delta = 1$, for which the system has solutions at $(x, y) = (0, 1), (0, -1)$, and $(3.75, .25)$. Solve the system using Newton's method and Newton's method with backtracking. Find an initial point where using $\alpha = 1$ converges to either $(0, 1)$ or $(0, -1)$ and using $\alpha < 1$ converges to $(3.75, .25)$. Plot the tracks used to find the solution (see Figure 10.2). Hint: use starting values within the rectangle

$$(x, y) : -.25 \leqslant x \leqslant 0, 0 \leqslant y \leqslant .25$$

and $\alpha \leq .75$.

(Adapted from problem 5.19 of M. T. Heath, Scientific Computing, an Introductory Survey, 2nd edition, McGraw Hill, 2002 and the Notes of Homer Walker).

Basins of Attraction: Newton Fractals

When $f(x)$ has many roots, the root that Newton's method converges to depends on the initial guess x_0. For example, the function $f(x) = x^2 - 1$ has roots at -1 and 1. If $x_0 < 0$, then Newton's method converges to -1; if $x_0 > 0$ then it converges to 1 (see Figure 10.3). We call the regions $(-\infty, 0)$ and $(0, \infty)$ *basins of attraction.*

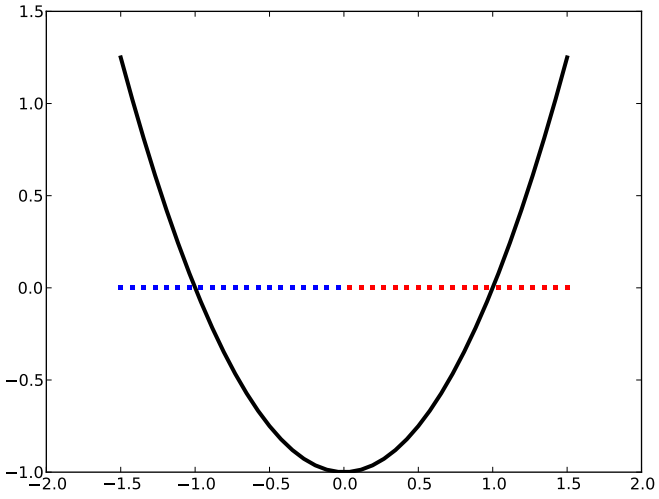


Figure 10.3: The plot of $f(x) = x^2 - 1$ along with some values for x_0. When Newton's method (with $\alpha = 1$) is initialized with a blue value for x_0 it converges to -1; when it is initialized with a red value it converges to 1.

When f is a polynomial of degree greater than 2, the basins of attraction are much more interesting. For example, if $f(x) = x^3 - x$, the basins are depicted in Figure 10.4.

We can extend these examples to the complex plane. Newton's method works in arbitrary Banach spaces with slightly stronger hypotheses (see Chapter 7 of Volume 1), and in particular it holds over $\mathbb{C}$.

Let us plot the basins of attraction for $f(x) = x^3 - 1$ on the domain $\{a+bi \mid (a,b) \in [-1.5, 1.5] \times [-1.5, 1.5]\}$ in the complex plane. We begin by creating a 700×700 grid of points in this domain. We create the real and imaginary parts of the points separately, and then use `np.meshgrid()` to turn them into a single grid of complex numbers.

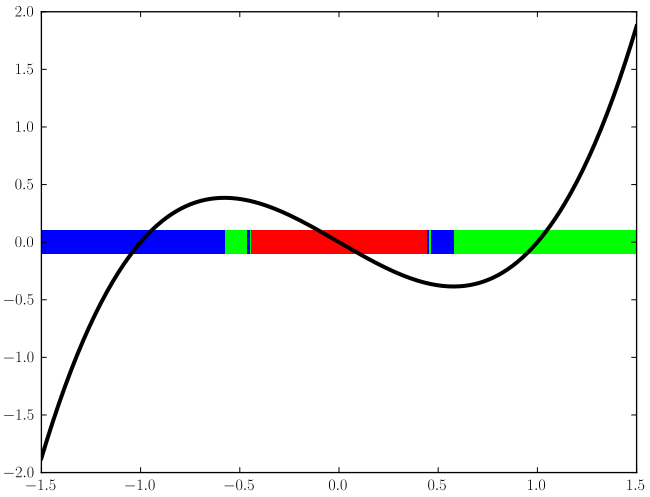


Figure 10.4: The plot of $f(x) = x^3 - x$ along with some values for x_0. With $\alpha = 1$, blue values converge to -1, red converge to 0, and green converge to 1.

```
>>> xreal = np.linspace(-1.5, 1.5, 700)
>>> ximag = np.linspace(-1.5, 1.5, 700)
>>> Xreal, Ximag = np.meshgrid(xreal, ximag)
>>> Xold = Xreal+1j*Ximag
```

Recall that `1j` is the complex number i in NumPy. The array `Xold` contains 700^2 complex points evenly spaced in the domain.

We may now perform Newton's method on the points in `Xold`.

```
>>> f = lambda x : x**3-1
>>> Df = lambda x : 3*x**2
>>> Xnew = Xold - f(Xold)/Df(Xold)
```

After iterating the desired number of times, we have an array `Xnew` whose entries are various roots of $x^3 - 1$.

Finally, we plot the array `Xnew`. The result is similar to Figure 10.5.

```
>>> plt.pcolormesh(Xreal, Ximag, Xnew)
```

Notice that in some portions of Figure 10.5, whenever red and blue try to come together, a patch of green appears in between. This behavior repeats on an infinitely small scale, producing a fractal. Because it arises from Newton's method, this fractal is called a *Newton fractal*.

Newton fractals tell us that the long-term behavior of the Newton method is extremely sensitive to the initial guess x_0. Changing x_0 by a small amount can change the output of Newton's method in a seemingly random way. This is an example of *chaos*.

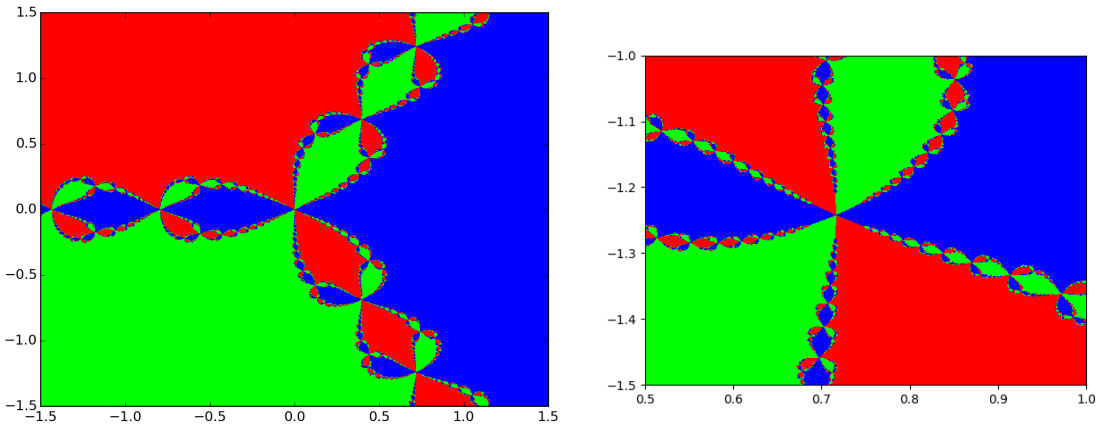


Figure 10.5: Basins of attraction for $x^3 - 1$ in the complex plane. The picture on the right is a close-up of a basin of the function.

Problem 5. Implement a method that plots the basins of attraction of a function in the complex plane. This method should take in a function f; the derivative of f; an array of the zeros of f; scalars `xmin, xmax, ymin, ymax` that define the domain for the plot; a scalar that determines the resolution of the plot that defaults to 1000; a maximum number of iterations; and a colormap to use in the plot that defaults to `brg`.

When the function `plt.pcolormesh()` is called on a complex array, it evaluates only on the real part of the complex numbers. This means that if two roots of `f` have the same real part, their basins will be the same color if you plot directly using `plt.pcolormesh()`.

One way to fix this problem is to compute `Xnew` as usual. Then iterate through the entries of `Xnew` and identify to which root each entry is closest using the input `roots`. Finally, create a new array whose entries are integers corresponding to the indices of these roots. Plot the array of integers to view the basins of attraction.

Test your function on the examples $f(x) = x^3 - 1$ above and $f(x) = x^3 - x$ below. The resulting plots should look like Figure 10.5 and Figure 10.6, respectively.
Hint: The roots of $f(x) = x^3 - x$ are 0, 1, and -1. The roots of $f(x) = x^3 - 1$ are the third roots of unity: 1, $-\frac{1}{2} + \frac{\sqrt{3}}{2}i$, and $-\frac{1}{2} - \frac{\sqrt{3}}{2}i$. Use the same domain for both plots: $[-1.5, 1.5] \times [-1.5, 1.5]$.

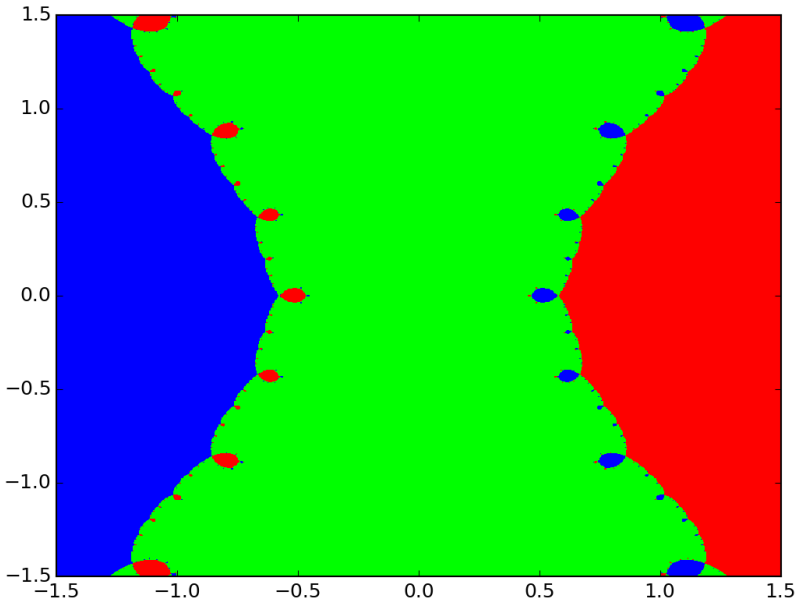


Figure 10.6: Basins of attraction for $x^3 - x$ in the complex plane.

11 Conditioning and Stability

Lab Objective: *The* condition number *of a function measures how sensitive that function is to changes in the input. On the other hand, the* stability *of an algorithm measures how accurately that algorithm computes the value of a function from exact input. In this lab, we examine the conditioning of common linear algebra problems, including computing polynomial roots and matrix eigenvalues. We also study several least squares algorithms to show that two algorithms for the same problem may not have the same level of stability.*

Condition Numbers

The *absolute condition number* of a function $f : \mathbb{R}^m \to \mathbb{R}^n$ at a point $\mathbf{x} \in \mathbb{R}^m$ is defined by

$$\hat{\kappa}(\mathbf{x}) = \lim_{\delta \to 0^+} \sup_{\|\mathbf{h}\| < \delta} \frac{\|f(\mathbf{x}+\mathbf{h}) - f(\mathbf{x})\|}{\|\mathbf{h}\|}. \tag{11.1}$$

In other words, the absolute condition number of f is the limit of the change in output over the change of input. Similarly, the *relative condition number* of f is the limit of the *relative* change in output over the *relative* change in input:

$$\kappa(\mathbf{x}) = \lim_{\delta \to 0^+} \sup_{\|\mathbf{h}\| < \delta} \left(\frac{\|f(\mathbf{x}+\mathbf{h}) - f(\mathbf{x})\|}{\|f(\mathbf{x})\|} \Big/ \frac{\|\mathbf{h}\|}{\|\mathbf{x}\|} \right) = \frac{\|\mathbf{x}\|}{\|f(\mathbf{x})\|} \hat{\kappa}(\mathbf{x}). \tag{11.2}$$

When a function's condition number is large, it is called *ill-conditioned*. Small changes to the input of an ill-conditioned function may produce large changes in output. In applications, it is important to know if a function is ill-conditioned because floating point representation almost always introduces input error.

The *condition number of a matrix* $\kappa(A) = \|A\|\|A^{-1}\|$ is an upper bound on the condition number for many of the common problems associated with the matrix, such as solving the system $A\mathbf{x} = \mathbf{b}$. If A is square but not invertible, then $\kappa(A) = \infty$ by convention. To compute $\kappa(A)$, we often use the matrix 2-norm, which is the largest singular value $\sigma_{\max}$ of A. Then since if σ is a singular value of A, $\frac{1}{\sigma}$ is a singular value of A^{-1}, we have

$$\kappa(A) = \frac{\sigma_{\max}}{\sigma_{\min}}, \tag{11.3}$$

which is also a valid equation for non-square matrices.

Problem 1. Write a function that accepts a matrix A and computes its condition number using (11.3). Use `scipy.linalg.svd()`, `scipy.linalg.svdvals()`, or `np.linalg.svd()` to compute the singular values of A, and avoid computing A^{-1}. If the smallest singular value is 0, return infinity (`np.inf`).

Test your function against `np.linalg.cond()`; you should expect the values to be within 10^{-7} of one another.

For large matrices where taking the SVD is difficult, the exact condition number of a matrix cannot always be computed and therefore must be estimated. Although not covered here, there exist many algorithms that can efficiently and accurately estimate the condition number of a matrix.

Example: The Wilkinson Polynomial

Let $f : \mathbb{C}^{n+1} \to \mathbb{C}^n$ be the function that maps the sequence of coefficients $(a_1, \dots, a_{n+1})$ to the roots of the polynomial $a_1x^n + a_2x^{n-1} + \dots + a_nx + a_{n+1}$. Finding the roots of polynomials is extremely ill-conditioned in general, so the condition number of f is likely very large.

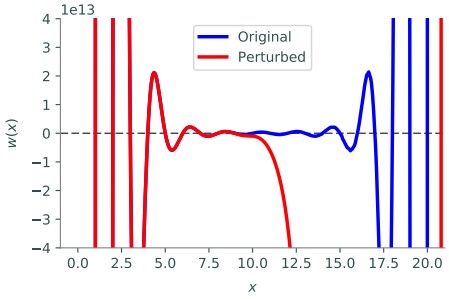
For instance, consider the Wilkinson polynomial.

$$w(x) = \prod_{r=1}^{20}(x - r) = x^{20} - 210x^{19} + 20615x^{18} - \dots$$

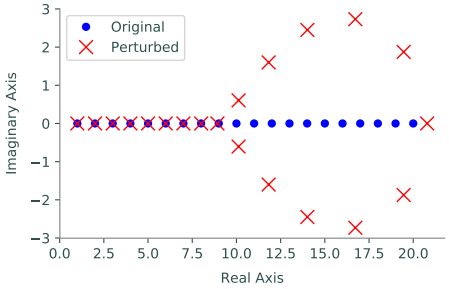
Let $\tilde{w}(x)$ be $w(x)$ where the coefficient on x^{19} is very slightly perturbed from -210 to -210.0000001. Below, we compute and compare the roots of $\tilde{w}(x)$ and $w(x)$ using NumPy and SymPy.

```
>>> import numpy as np
>>> import sympy as sy
>>> from scipy import linalg as la

# The roots of w are 1, 2, ..., 20.
>>> w_roots = np.arange(1, 21)

# Get the exact Wilkinson polynomial coefficients using SymPy.
>>> x, i = sy.symbols('x i')
>>> w, _ = sy.poly_from_expr(sy.product(x-i, (i, 1, 20)))
>>> w_coeffs = np.array(w.all_coeffs())

# Perturb one of the coefficients very slightly.
>>> perturb = np.zeros(21)
>>> perturb[1]=1e-7
>>> perturbed_coeffs = w_coeffs - perturb

# Use NumPy to compute the roots of the perturbed polynomial.
>>> perturbed_roots = np.roots(np.poly1d(perturbed_coeffs))
```

Below we plot the polynomials $w(x)$ and $\tilde{w}(x)$ and compare their roots in the complex plane.



(a) The original and perturbed Wilkinson polynomials. They match for only about half of the domain.



(b) Roots of the original and pertubed Wilkinson polynomials. About half of the perturbed roots are imaginary.

From the figure, it's clear that a perturbation drastically changes the nature of the polynomial and its root. To quantify the difference, we estimate the condition numbers in the L^∞ norm.

```
# Sort the roots to ensure that they are in the same order.
>>> w_roots = np.sort(w_roots)
>>> perturbed_roots = np.sort(perturbed_roots)

# Estimate the absolute condition number in the infinity norm.
>>> k = la.norm(perturbed_roots - w_roots, np.inf) / la.norm(perturb, np.inf)
>>> print(k)
28262391.3304

# Estimate the relative condition number in the infinity norm.
>>> k*la.norm(w_coeffs, np.inf) / la.norm(w_roots, np.inf)
1.95063629993970+25                    # This is huge!!
```

There are some caveats to this example. First, when we compute the quotients in (11.1) and (11.2) for a fixed $\mathbf{h}$, we are only *approximating* the condition number. The actual condition number is the limit of such quotients. We hope that when $||\mathbf{h}||$ is small, a random quotient is at least the same order of magnitude as the limit, but we have no way to be sure.

Second, this example assumes that NumPy's root-finding algorithm is *stable*, so that the difference between the roots of `w_coeffs` and `perturbed_coeffs` is due to the difference in coefficients, and not the difference in roots. We will return to this issue in the next section.

Problem 2. Write a function that carries out the following experiment 100 times.

1. Randomly perturb the true coefficients by replacing each coefficient a_i with $a_i * r_i$, where r_i is drawn from a normal distribution centered at 1 with standard deviation 10^{-10} (use `np.random.normal()`).
2. Plot the perturbed roots as small points in the complex plane. That is, plot the real part of the coefficients on the x-axis and the imaginary part on the y-axis. Plot on the same figure in each experiment.
3. Compute the absolute and relative condition numbers with the L^∞ norm.

Plot the roots of the unperturbed Wilkinson polynomial with the perturbed roots. Your final plot should resemble Figure 11.2. Finally, return the average computed absolute and relative condition numbers.

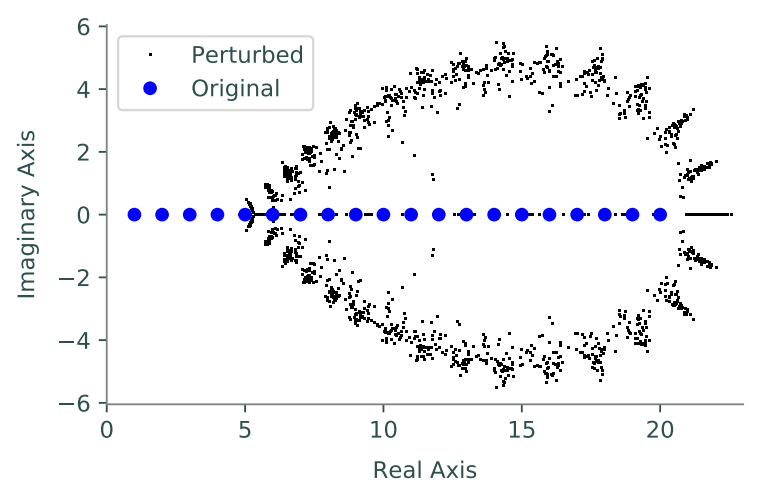


Figure 11.2: This figure replicates Figure 12.1 on p. 93 of *Numerical Linear Algebra* by Lloyd N. Trefethen and David Bau III.

Example: Calculating Eigenvalues

Let $f : \mathbb{C}^{n^2} \to \mathbb{C}^n$ be the function that maps an $n \times n$ matrix to its n eigenvalues. This problem is well-conditioned for symmetric matrices, but can be extremely ill-conditioned for non-symmetric matrices. Let A be an $n \times n$ matrix and let $\boldsymbol{\lambda}$ be the vector of the n eigenvalues of A. If $\tilde{A} = A + H$ and $\tilde{\boldsymbol{\lambda}}$ are a perturbation of A and its eigenvalues, then the condition numbers of f are

$$\hat{\kappa}(A) = \frac{\|\boldsymbol{\lambda} - \tilde{\boldsymbol{\lambda}}\|}{\|H\|}, \qquad \kappa(A) = \frac{\|A\|}{\|\boldsymbol{\lambda}\|}\hat{\kappa}(A). \tag{11.4}$$

Problem 3. Write a function that accepts a matrix A and estimates the condition number of the eigenvalue problem using (11.4). For the perturbation H, use arandom complex matrices with entries drawn from a normal distribution.

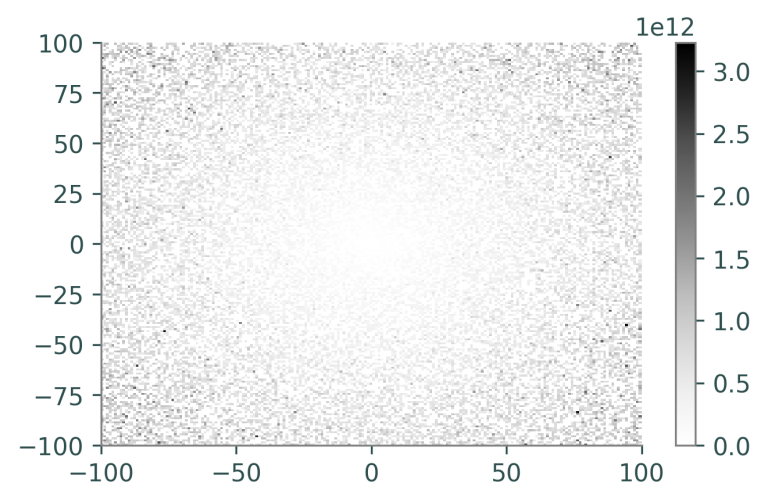
```
H = np.random.normal(0, 1e-10, A.shape) + np.random.normal(
                                                0, 1e-10, A.shape)*1j
```

Use the 2-norm for both the vector and matrix norms. Return the absolute and relative condition numbers.

Problem 4. Write a function that accepts minimal and maximal values for x and y as well as a resolution parameter `res`. Use your function from Problem 3 to compute the relative condition number of the eigenvalue for the 2x2 matrix

$$\begin{bmatrix} 1 & x \\ y & 1 \end{bmatrix}$$

at every point in the domain $[x_{min}\ x_{max}] \times [y_{min}\ y_{max}]$, where each axis is partitioned into `res` points. Plots these estimated relative condition numbers using `plt.pcolormesh()`. With `res`=200, your plot should similar to the following figure.



Stability of an Algorithm

The stability of an algorithm is measured by the error in its output. Suppose we have some algorithm to compute $f : \mathbb{R}^m \to \mathbb{R}^n$. Let $\tilde{f}(\mathbf{x})$ represent the value computed by the algorithm given an input $\mathbf{x}$. Then the *forward error* of f at $\mathbf{x}$ is $||f(\mathbf{x}) - \tilde{f}(\mathbf{x})||$, and the *relative forward error* of f at $\mathbf{x}$ is

$$\frac{||f(\mathbf{x}) - \tilde{f}(\mathbf{x})||}{||f(\mathbf{x})||}.$$

An algorithm is *stable* if its relative forward error is small.

As an example, let us examine the stability of NumPy's root finding algorithm that we used to investigate the Wilkinson polynomial. We know the exact roots of $w(x)$, and we can also compute these roots using NumPy's `np.roots()` function.

```
>>> roots = np.arange(1,21)
 # w_coeffs is an array with the coefficients of the Wilkinson polynomial.
>>> computed_roots = np.roots(np.poly1d(w_coeffs))

# Sort the roots for comparison.
>>> roots = np.sort(roots)
>>> computed_roots = np.sort(computed_roots)
```

```
# Compute the forward error.
>>> forward_error = la.norm(roots-computed_roots)
>>> print(forward_error)
0.020612653126379665

# Compute the relative forward error.
>>> forward_error / la.norm(roots)
0.00038476268486104599                              # Nice and small.
```

This analysis suggests that questions of stability did not interfere too much with our experiments in Problem 2.

Example: Least Squares

The least squares problem is to find the $\mathbf{x}$ that minimizes $\|A\mathbf{x}-\mathbf{b}\|_2$ for fixed A and $\mathbf{b}$. It can be shown that an equivalent problem is finding the solution of $A^\mathsf{T}A\mathbf{x} = A^\mathsf{T}\mathbf{b}$, called the *normal equations*. We will consider two different algorithms that solve this problem.

1. Invert the matrix $A^\mathsf{T}A$ and then right multiply by $A^\mathsf{T}\mathbf{b}$ to solve the normal equations. Although this approach seems intuitive, it is actually highly unstable and can return an answer with a very large forward error.
2. Use the QR-decomposition, factoring the $m\times n$ matrix A of rank $n \geq m$, where Q has orthonormal columns and R is upper triangular. It can also be shown that the solution of $R\mathbf{x} = Q\mathbf{b}$ is equivalent to solving the least squares problem. This algorithm has the advantage of being stable.

A common application of least squares is polynomial approximation. Given a set of data points $\{(x_k, y_k)\}_{k=1}^m$ we would like to find the set of coefficients $\{c_k\}_{k=1}^n$ such that

$$y_k = c_n x_k^n + c_{n-1}x_k^{n-1} + \cdots + c_2 x_k^2 + c_1 x_k + c_0$$

for all k. Since this system will typically be over-determined, there will not be a set of coefficients that exactly satisfies this equation for all k. A common approach is to use least squares to pick the set of coefficients that minimizes the L^2 error of the system of equations.

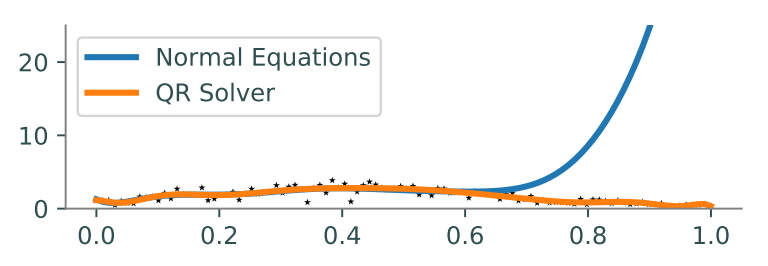
```
>>> from scipy import linalg as la

# Use least squares to approximate sin(x) with a five-degree polynomial.
>>> x = np.linspace(0, 6, 10)           # The x-values of the data.
>>> b = np.sin(x) + .2*np.random.randn(10) # The y-values of the data (noisy).
>>> A = np.vander(x, 6)                 # Set up the matrix of data values.
>>> coeffs = la.lstsq(A, b)[0]          # Get the polynomial coefficients.

>>> domain = np.linspace(0, 6, 100)     # Define a finer domain for plotting.
>>> plt.plot(x, b, 'k*')
>>> plt.plot(domain, np.sin(domain))
>>> plt.plot(domain, np.poly1d(coeffs)(domain))
```

Problem 5. Write two functions that solve the least squares problem using the normal equation. One of your functions should solve the problem directly using `np.linalg.inv()` while the other should use a more stable algorithm, such as the QR-decomposition. The functions `la.qr()` and `la.solve_triangular()` may be helpful when implementing the QR-decomposition. Both of your functions should accept a matrix A and a vector $\mathbf{b}$.

Approximate the data from `stability_data.npy` on the interval $[0,\ 1]$ with a degree-fourteen polynomial using two approaches to get the least squares solution:

1. Use `la.inv()` and the normal equations: $\mathbf{x} = (A^\mathsf{T}A)^{-1}A^\mathsf{T}\mathbf{b}$.
2. Use `la.qr()` and `la.solve_triangular()` to solve the system $R\mathbf{x} = Q\mathbf{b}$.

Plot both of your solutions with the data points for comparision. Return the error $\|A\mathbf{x} - \mathbf{b}\|_2$ of both approximations. Your plot should look similar to the following figure.



Catastrophic Cancellation

A common cause of instability in algorithms is catastrophic cancellation. *Catastrophic cancellation* is the term for when a computer takes the difference of two very similar numbers, and the result is stored with a small number of significant digits. Because of the way computers store and perform arithmetic on numbers, future computations can amplify a catastrophic cancellation into a large error.

You are at risk for catastrophic cancellation whenever you subtract floats or large integers that are very close to each other. You can avoid this problem by either rewriting your program to not use subtraction, or by increasing the number of significant digits that your computer tracks.

Here is an example of catastrophic cancellation. Suppose we wish to compute $\sqrt{a} - \sqrt{b}$. We can either do this subtraction directly or perform the equivalent division

$$\sqrt{a} - \sqrt{b} = (\sqrt{a} - \sqrt{b})\frac{\sqrt{a} + \sqrt{b}}{\sqrt{a} + \sqrt{b}} = \frac{a - b}{\sqrt{a} + \sqrt{b}}.$$

We will perform this computation both ways in NumPy with $a = 10^{20} + 1$ and $b = 10^{20}$.

```
>>> from math import sqrt           # np.sqrt() fails for very large numbers

>>> a = 10**20+1
>>> b = 10**20
>>> sqrt(a)- sqrt(b)
0.0
```

```
>>> (a-b) / (np.sqrt(a)+np.sqrt(b))
5e-11
```

Since $a \neq b$, $\sqrt{a} - \sqrt{b}$ should clearly be nonzero.

Problem 6. Let $I(n) = \int_0^1 x^n e^{x-1} dx$.

1. Prove that $0 \leq I(n) \leq 1$ for all n.

2. It can be shown that for $n > 1$,

$$I(n) = (-1)^n !n + (-1)^{n+1} \frac{n!}{e}$$

   where $!n$ is the *subfactorial* of n. Use this formula to write a function that computes the integral.
   (Hint: Use SymPy's `subfactorial()` function.)

3. The actual values of $I(n)$ for many values of n are listed in the table below. Use your function `integral()` to compute $I(n)$ for these same values of n, and create a table comparing the data. How can you explain what is happening?

n	Actual value of $I(n)$
1	0.367879441171
5	0.145532940573
10	0.0838770701034
15	0.0590175408793
20	0.0455448840758
25	0.0370862144237
30	0.0312796739322
35	0.0270462894091
40	0.023822728669
45	0.0212860390856
50	0.0192377544343

12 Monte Carlo Integration

Lab Objective: *Implement Monte Carlo integration to estimate integrals. Use Monte Carlo Integration to calculate the integral of the joint normal distribution.*

Some multivariable integrals which are critical in applications are impossible to evaluate symbolically. For example, the integral of the joint normal distribution

$$\int_\Omega \frac{1}{\sqrt{(2\pi)^k}} e^{-\frac{\mathbf{x}^T\mathbf{x}}{2}}$$

is ubiquitous in statistics. However, the integrand does not have a symbolic antiderivative. This means we must use numerical methods to evaluate this integral. The standard technique for numerically evaluating multivariable integrals is *Monte Carlo Integration*. In the next lab, we will approximate this integral using a modified version of Monte Carlo Integration. In this lab, we address the basics of Monte Carlo Integration.

Monte Carlo integration is radically different from techniques like Simpson's rule. Whereas Simpson's rule is purely computational and deterministic, Monte Carlo integration uses randomly chosen points in the domain to calculate the integral. Although it converges slowly, Monte Carlo integration is frequently used to evaluate multivariable integrals because the higher-dimensional analogs of methods like Simpson's rule are extremely inefficient.

A Motivating Example

Suppose we want to numerically compute the area of a circle of radius 1. From analytic methods, we know the answer is π. Empirically, we can estimate the area by randomly choosing points in a 2×2 square. The percentage of points that land in the inscribed circle, times the area of the square, should approximately equal the area of the circle (see Figure 12.1).

We do this in NumPy as follows. First generate 500 random points in the square $[0, 1] \times [0, 1]$.

```
>>> N = 500 # Number of sample points
>>> points = np.random.rand(2, N)
```

We rescale and shift these points to be uniformly distributed in $[-1, 1] \times [-1, 1]$.

```
>>> points = points*2-1
```

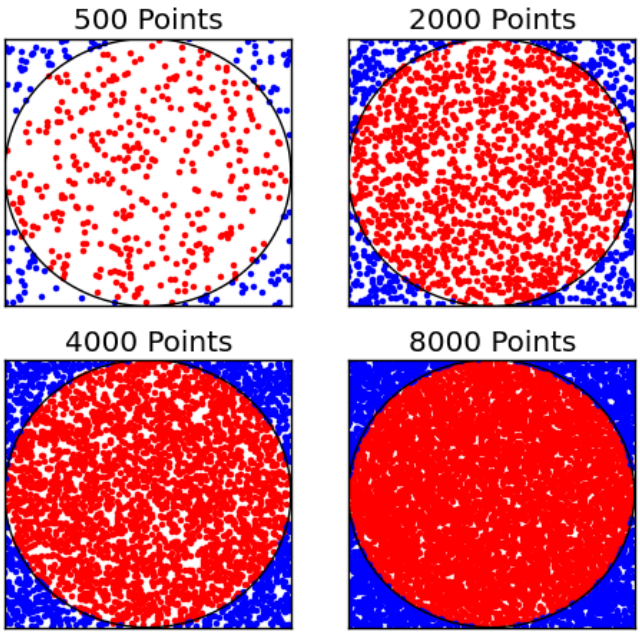


Figure 12.1: Finding the area of a circle using random points

Next we determine the number of points in the unit circle. We compute the Euclidean distance from the origin for each point, then count the points that are within a distance of 1 from the origin.

```
>>> # Compute the distance from the origin for each point
>>> pointsDistances = np.linalg.norm(points,axis=0)
>>> # Count how many are less than 1
>>> numInCircle = np.count_nonzero(pointsDistances < 1)
```

The fraction of points inside the circle is `numInCircle` divided by `N`. By multiplying this fraction by the square's area, we can estimate the area of the circle.

```
>>> circleArea = 4.*(numInCircle/N)
>>> circleArea
3.024
```

This differs from π by about 0.117.

Problem 1. Write a function that estimates the volume of the unit sphere. Your function should have a keyword argument `N` that defaults to 10^5. Your function should draw `N` points uniformly from $[-1,1]\times[-1,1]\times[-1,1]$ to make your estimate. The true volume is $\frac{4}{3}\pi \approx 4.189$.

Monte Carlo Integration

In the examples above, we drew a bounding box around a volume, then used random points drawn from the box to estimate that volume. This is easy and intuitive when the volume is a circle or sphere. But it's hard to generalize this to any arbitrary integral - in order to draw the box, we have to already know something about the volume we are estimating. Instead, given an arbitrary function $f(x) : \mathbb{R}^n \mapsto \mathbb{R}$ and a region $\Omega \subset \mathbb{R}^n$ in the domain of f, we would like to use random points drawn from Ω to estimate the integral $\int_\Omega f(x)\, dV$, *without* having to specify a bounding box around the volume of integration.

We can estimate this integral using the approximation.

$$\int_\Omega f(x)\, dV \approx V(\Omega)\frac{1}{N}\sum_{i=1}^{N} f(x_i) \tag{12.1}$$

where x_i are uniformly distributed random points in Ω and $V(\Omega)$ is the volume of Ω. This is the generalized formula for Monte Carlo integration.

The intuition behind (12.1) is that $\frac{1}{N}\sum_{i=1}^{N} f(x_i)$ approximates the average value of f on Ω. We multiply this (approximate) average value by the volume of Ω to get the (approximate) integral of f on Ω.

For further intuition, compare (12.1) to the Average Value Theorem from single-variable calculus. By the Average Value Theorem, the average value of $f(x) : \mathbb{R} \mapsto \mathbb{R}$ on $[a, b]$ is given by

$$f_{avg} = \frac{1}{b-a}\int_a^b f(x)\, dx. \tag{12.2}$$

If we let $\Omega = [a, b]$ in (12.2) (noting that $V(\Omega) = b-a$) and replace f_{avg} with the approximation $\frac{1}{N}\sum_{i=1}^{N} f(x_i)$, then we get precisely the Monte Carlo integration formula in Equation (12.1)!

As it turns out, we can refactor the circle-area problem slightly so that it uses Equation (12.1). Let f be defined by

$$f(x, y) = \begin{cases} 1 & \text{if } (x,y) \text{ is in the unit circle} \\ 0 & \text{otherwise} \end{cases}$$

and let $\Omega = [-1, 1] \times [-1, 1]$. The area of the circle is given by $\int_\Omega f(x)\, dV$, which we can estimate with the Monte Carlo integration formula:

$$\text{Area of unit circle } \approx V(\Omega)\frac{1}{N}\sum_{i=1}^{N} f(x_i) = \frac{4}{N}\sum_{i=1}^{N} f(x_i).$$

To summarize, we have the following steps to estimate the integral of any function f over a region Ω in the domain of f:

1. Draw N random points uniformly distributed in Ω.
2. Find the image of each point under f, and take the average of these images.
3. Multiply by the volume of Ω.

Problem 2. Write a function that performs 1-dimensional Monte Carlo integration. Given a function $f : \mathbb{R} \mapsto \mathbb{R}$, an interval $[a, b]$, and the number of random points to use, your function should return an approximation of the integral $\int_a^b f(x)\,dx$. Let the number of sample points default to 10^5. Test your function by estimating integrals that you can calculate by hand.

Problem 3. Generalize Problem 2 to multiple dimensions. Write a function that accepts a function handle f to integrate, the bounds of the interval to integrate over, and the number of points to use. Let the number of sample points default to 10^5. Your implementation should be robust enough to integrate any function $f : \mathbb{R}^n \mapsto \mathbb{R}$ over any interval in $\mathbb{R}^n$.

Hints:

1. To draw a random array of points from the given interval, first create a random array of points in $[0, 1] \times \ldots \times [0, 1]$. Multiply this array by the dimensions of the interval to rescale it, then add the lower bounds of integration to shift it. Think about using array broadcasting.

2. You can use `np.apply_along_axis()` to apply a function to each column of an array. Here is an example of applying a function to points in $\mathbb{R}^2$:

```
>>> points = np.random.rand(2,4)
>>> points
array([[ 0.33144631,  0.52558001,  0.67766158,  0.45570083],
       [ 0.70935864,  0.20985475,  0.25917177,  0.19431292]])
# Apply the norm function to each point
>>> np.apply_along_axis(np.linalg.norm,0,points)
array([ 0.78297275,  0.565927  ,  0.72553099,  0.49539959])
```

   This is especially useful for functions that don't work nicely with array inputs. For example, the code below uses a simple thresholding function `f`; calling `f(points)` would throw an error, but using `np.apply_along_axis` gives the expected result. (Note that `points` must have at least 2 dimensions for this to work.) Refer to the NumPy docs for more information.

```
# Simple function that returns a 0 if x is less than 0.5
>>> f = lambda x: x if x > 0.5 else 0.
# Get 4 random points. The 1 forces the array to be 2-D.
>>> points = np.random.rand(1,4)
>>> points
array([[ 0.2144746 ,  0.02490517,  0.86593995,  0.86401139]])
# Evaluate f at each element of points
>>> np.apply_along_axis(f,0,points)
array([ 0.        ,  0.        ,  0.86593995,  0.86401139])
```

One application of Monte Carlo integration is integrating probability density functions that do not have closed form solutions.

Problem 4. The joint normal distribution of N independent random variables with mean 0 and variance 1 is

$$f(\mathbf{x}) = \frac{1}{\sqrt{2\pi}^N} e^{-\frac{\mathbf{x}^T\mathbf{x}}{2}}.$$

The integral of $f(\mathbf{x})$ over a box is the probability that a draw from the distribution will be in the box. This is an important distribution in statistics. However, $f(\mathbf{x})$ does not have a symbolic antiderivative.

1. Let $\Omega = [-1.5, 0.75] \times [0, 1] \times [0, 0.5] \times [0, 1] \subset \mathbb{R}^4$. Use the function you wrote in Problem 1 to integrate $f(\mathbf{x})$ on Ω. Use 50000 sample points.

2. SciPy has a built in function specifically for integrating the joint normal distribution. The integral of $f(\mathbf{x})$ on $B = [-1, 1] \times [-1, 1] \times [-1, 1] \subset \mathbb{R}^3$ can be computed in SciPy with the following code.

```
>>> from scipy import stats

# Define the bounds of the box to integrate over
>>> mins = np.array([-1, -1, -1])
>>> maxs = np.array([1, 1, 1])

# Each variable has mean 0
>>> means = np.zeros(3)

# The covariance matrix of N independent random variables
#    is the NxN identity matrix.
>>> covs = np.eye(3)

# Compute the integral
>>> value, inform = stats.mvn.mvnun(mins, maxs, means, covs)
```

   Then `value` is the integral of $f(\mathbf{x})$ on B.

   Use SciPy to integrate $f(\mathbf{x})$ on Ω.

3. Return your Monte Carlo estimate, SciPy's answer, and (assuming SciPy is correct) the relative error of your Monte Carlo estimate.

Convergence

The error of the Monte Carlo method is proportional to $1/\sqrt{N}$, where N is the number of points used in the estimation. This means that to divide the error by 10, we must sample *100 times* more points.

This is a slow convergence rate, but it is independent of the number of dimensions of the problem. The error converges at the same rate whether integrating a 2-dimensional or a 20-dimensional function. This gives Monte Carlo integration an advantage over other methods, and makes it especially useful for estimating integrals in high dimensions.

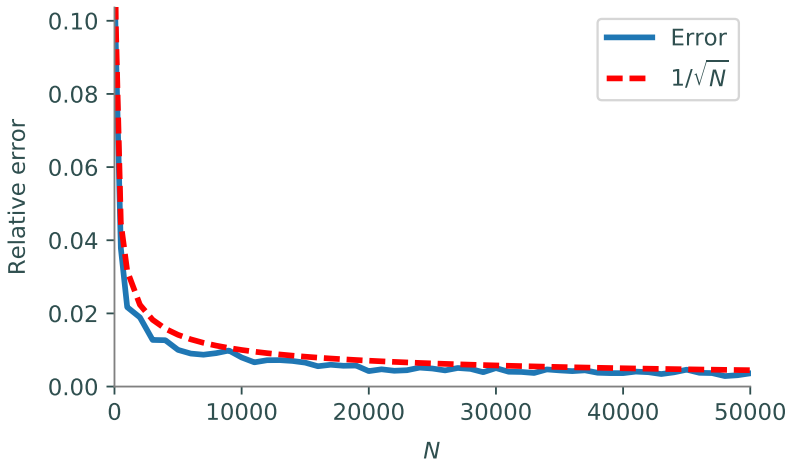


Figure 12.2: The Monte Carlo integration method was used to compute the volume of the unit sphere. The blue line plots the average error in 50 runs of the Monte Carlo method on N sample points. The red line is a plot of $1/\sqrt{N}$.

Problem 5. In this problem we will visualize how the error in Monte Carlo integration depends on the number of sample points.

Run Problem 1 with `N` equal to 50, 100 and 500, as well as 1000, 2000, 3000, ..., 50000; having some additional small values of `N` will help make the visualization better.

For each value of `N`:

1. Estimate the volume of the unit sphere using Problem 1, and use the true volume to calculate the relative error of the estimate.
2. Repeat this multiple times to get an average estimate of the relative error. Your function should accept a keyword argument `numEstimates` that defaults to 50.
3. Calculate and store the mean of the errors.

Plot the mean relative error as a function of `N`. For comparison, plot the function $1/\sqrt{N}$ on the same graph. Your plot should resemble Figure 12.2).

A Caution

You can run into trouble if you try to use Monte Carlo integration on an integral that does not converge. For example, we may attempt to evaluate

$$\int_0^1 \frac{1}{x}\,dx$$

with Monte Carlo integragtion using the following code.

```
>>> k = 5000
```

```
>>> np.mean(1/np.random.rand(k,1))
21.237332864358656
```

Since this code returns a finite value, we could assume that this integral has a finite value. In fact, the integral is infinite. We could discover this empirically by using larger and larger values of k, and noting that Monte Carlo integration fails to converge.

13 Importance Sampling

Lab Objective: *Use importance sampling to reduce the error and variance of Monte Carlo Simulations.*

Introduction

The traditional methods of Monte Carlo integration as discussed in the previous lab are not always the most efficient means to estimate an integral. For example, assume we were trying to find the probability that a randomly chosen variable X from the standard normal distribution is greater than 3. We know that one way to solve this is by solving the following integral:

$$P(X > 3) = \int_3^\infty f_X(t)\,dt = \frac{1}{\sqrt{2\pi}} \int_3^\infty e^{-t^2/2}\,dt \tag{13.1}$$

If we define the function $h : \mathbb{R} \to \mathbb{R}$ as

$$h(t) = \begin{cases} 1 & \text{if } t > 3 \\ 0 & \text{if } t \leq 3 \end{cases},$$

we can rewrite this integral as

$$\int_3^\infty f_X(t)\,dt = \int_{-\infty}^\infty h(t) f_X(t)\,dt.$$

By the Law of the Unconscious Statistician (see Volume 2 §3.5), we can restate the integral above as

$$\int_{-\infty}^\infty h(t) f_X(t)\,dt = E[h(X)].$$

Being able to write integrals as expected values is an essential tool in this lab.

Monte Carlo Simulation

In the last section, we expressed the probability of drawing a number greater than 3 from the normal distribution as an expected value problem. We can now easily estimate this same probabilty using Monte Carlo simulation. Given a random i.i.d. sample $x_1, x_2, \cdots, x_N$ generated by f_X, we can estimate $E[h(X)]$ using

$$\widehat{E}_n[h(X)] = \frac{1}{N}\sum_{i=1}^{N} h(x_i) \tag{13.2}$$

Now that we have defined the estimator, it is now quite manageable to approximate Equation 13.1. By the Weak Law of Large Numbers (see Volume 2 §3.6), the estimate will get closer and closer to the actual value as we use more and more sample points.

Problem 1. Write a function in Python that estimates the probability that a random draw from the standard normal distribution is greater than 3 using Equation 13.2. Your function should accept a parameter `n` for the number of samples to use in your approximation. Your answer should approach 0.0013499 for sufficiently large samples.

Though this approach gets the job done, it turns out that this isn't very efficient. Since the probability of drawing a number greater than 3 from the standard normal distribution is so unlikely, it turns out we need many sample points to get a good approximation.

Importance Sampling

Importance sampling is one way to make Monte Carlo simulations converge much faster. We choose a different distribution to sample our points to generate more *important* points. With our example, we want to choose a distribution that would generate more numbers around 3 to get a more reliable estimate. The theory behind importance sampling boils down to the following result. In these equations, the random variable X is generated by f_X and the random variable Y is generated by g_Y. We will refer to X and Y in this way for the remainder of the lab.

$$\begin{aligned} E[h(X)] &= \int_{-\infty}^{\infty} h(t) f_X(t)\, dt \\ &= \int_{-\infty}^{\infty} h(t) f_X(t) \left(\frac{g_Y(t)}{g_Y(t)}\right) dt \\ &= \int_{-\infty}^{\infty} \left(\frac{h(t) f_X(t)}{g_Y(t)}\right) g_Y(t)\, dt \\ &= E\left[\frac{h(Y) f_X(Y)}{g_Y(Y)}\right] \end{aligned} \tag{13.3}$$

The corresponding estimator is

$$\begin{aligned} \widehat{E}[h(X)] &= \widehat{E}\left[\frac{h(Y) f_X(Y)}{g_Y(Y)}\right] \\ &= \frac{1}{N}\sum_{i=1}^{N} \frac{h(y_i) f_X(y_i)}{g_Y(y_i)} \end{aligned} \tag{13.4}$$

The function f_X is the p.d.f. of the *target distribution*. The function g_Y is the p.d.f. of the *importance distribution*. The fraction $\frac{f_X(X)}{g_Y(X)}$ is called the *importance weight*. This allows us to draw a sample from any distribution with p.d.f. g_Y as long as we multiply $h(X)$ by the importance weight.

Choosing the Importance Distribution

There is no correct choice for the importance distribution. It may be possible to find the distribution that allows the simulation to converge the fastest, but oftentimes, we don't need a perfect answer. Close to perfect is good enough.

We will solve the same problem as in Problem 1 using importance sampling. We will choose g_Y to be the normal distribution with $\mu = 4$ and $\sigma = 1$. We have chosen this distribution for g_Y because it will give us more points closer to and greater than 3. Note that it is not necessary to choose an importance distribution of the same type.

Figure 13.1: In our problem, we choose an importance distribution that will generate more samples that are greater than 3. Though not a perfect choice, choosing a normal distribution with $\mu = 4$ and $\sigma = 1$ will suffice.

```
>>> from scipy import stats
>>> h = lambda x : x > 3
>>> f = lambda x : stats.norm().pdf(x)
>>> g = lambda x : stats.norm(loc=4,scale=1).pdf(x)

# Sample from the N(4,1).
>>> N = 10**7
>>> X = np.random.normal(4,scale=1,size=N)

# Calculate estimate.
>>> 1./N * np.sum(h(X)*f(X)/g(X))
0.00134921134631
```

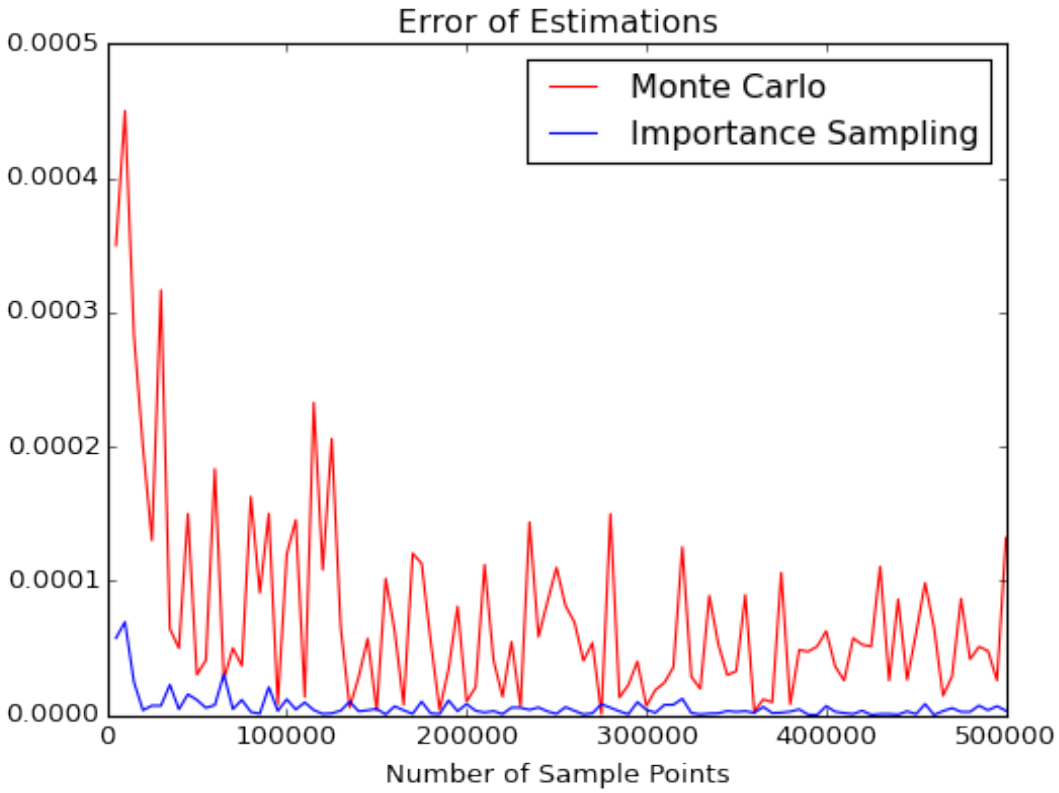


Figure 13.2: Comparison of error between standard method Monte Carlo and Importance Sampling method of Monte Carlo.

Problem 2. A tech support hotline receives an average of 2 calls per minute. What is the probability that they will have to wait at least 10 minutes to receive 9 calls? Implement your estimator using importance sampling. Calculate estimates using 5000, 10000, 15000, $\cdots$, 500000 sample points. Return an array of estimates. Your answers should approach 0.00208726.

Hint: In Volume 2 §3.5, the gamma distribution is defined as,

$$f_X(x) = \frac{b^a x^{a-1} e^{-xb}}{\Gamma(a)}.$$

The version of the gamma distribution in `scipy.stats` is determined by the shape (a) and the scale (θ) of the distribution.

$$f_X(x) = \frac{x^{a-1} e^{-x/\theta}}{\Gamma(a)\theta^a}$$

You can switch between these representations this with the fact that $\theta = 1/b$.

Problem 3. In this problem, we will visualize the benefits of importance sampling. Create a plot of the error of the traditional methods of Monte Carlo integration and the importance sampling methods of Monte Carlo for Problem 2. What do you observe? Your plot should resemble Figure 13.2.

Hint: The following code solves Problem 2 using traditional methods of Monte Carlo integration:

```
h = lambda x : x > 10
MC_estimates = []
for N in xrange(5000,505000,5000):
    X = np.random.gamma(9,scale=0.5,size=N)
    MC = 1./N*np.sum(h(X))
    MC_estimates.append(MC)
MC_estimates = np.array(MC_estimates)
```

Hint: To determine the error of your approximations, the following code returns the actual value of the probability:

```
1 - stats.gamma(a=9,scale=0.5).cdf(10)
```

Now that we have visualized the benefits of importance sampling, note that we can achieve the same results as traditional Monte Carlo with a fraction of the samples.

Generalizing the Principles of Importance Sampling

The examples we have explored to this point in the lab were merely educational. Since we have a simple means of calculating the correct answer to Problem 2, it doesn't make much sense to use methods of Monte Carlo in this situation. However, as discussed in the previous lab, there are not always closed-form solutions to the integrals we want to compute.

We can extend the same principles we have discussed thus far to solve many types of problems. For a more general problem, we can implement importance sampling by doing the following:

1. Define a function h where, $h(t) = \begin{cases} 1 & \text{if condition is met} \\ 0 & \text{otherwise} \end{cases}$.
2. Define a function f_X which is the p.d.f. of the target distribution.
3. Define a function g_Y which is the p.d.f. of the importance distribution.
4. Use these functions in conjunction with Equation (13.4).

Problem 4. The joint normal distribution of N independent random variables with mean 0 and variance 1 is

$$f_X(\mathbf{x}) = \frac{1}{\sqrt{(2\pi)^N}} e^{-(\mathbf{x}^T\mathbf{x})/2}.$$

The integral of $f_X(\mathbf{x})$ over a box is the probability that a draw from the distribution will be in the box. However, $f_X(\mathbf{x})$ does not have a symbolic antiderivative.

Use what you have learned about importance sampling to estimate the probability that a given random variable in $\mathbb{R}^2$ generated by f_X will be less than -1 in the x-direction and greater than 1 in the y-direction.

Treat f_X as the p.d.f. of your target distribution. Use the function `stats.multivariate_normal` to create a multivariate normal distribution to serve as your importance distribution. For more information on how to use this function, consult the documentation for `stats.multivariate_normal`.

Unnormalized Target Densities

The methods discussed so far are only applicable if the target density is normalized, or in other words, has an integral of 1. If the target density is not normalized, Equation 13.3 becomes

$$\begin{aligned} E[h(X)] &= \frac{\int h(t)f(t)\,dt}{\int f(t)\,dt} \\ &= \frac{\int h(t)f(t)\left(\frac{g_Y(t)}{g_Y(t)}\right)\,dt}{\int f(t)\left(\frac{g_Y(t)}{g_Y(t)}\right)\,dt} \\ &= \frac{\int \left(\frac{h(t)f(t)}{g_Y(t)}\right) g_Y(t)\,dt}{\int \left(\frac{f(t)}{g_Y(t)}\right) g_Y(t)\,dt} \\ &= \frac{E\left[\frac{h(Y)f(Y)}{g_Y(Y)}\right]}{E\left[\frac{f(Y)}{g_Y(Y)}\right]} \end{aligned}$$

The corresponding estimator becomes

$$\begin{aligned} \widehat{E}_n[h(X)] &= \frac{\widehat{E}\left[\frac{h(Y)f(Y)}{g_Y(Y)}\right]}{\widehat{E}\left[\frac{f(Y)}{g_Y(Y)}\right]} \\ &= \frac{\frac{1}{N}\sum_{i=1}^{N}\frac{h(y_i)f(y_i)}{g_Y(y_i)}}{\frac{1}{N}\sum_{i=1}^{N}\frac{f(y_i)}{g_Y(y_i)}} \end{aligned}$$

14 Visualizing Complex-valued Functions

Lab Objective: *Create visualizations of complex functions. Visually estimate their zeros and poles, and gain intuition about their behavior in the complex plane.*

Representations of Complex Numbers

A complex number $z = x + iy$ can be written in *polar coordinates* as $re^{i\theta}$ where

- $r = \sqrt{x^2 + y^2}$ is the magnitude of z, and
- $\theta = \arctan(y/x)$ is the angle between z and 0, as in Figure 14.1.

Conversely, Euler's formula implies $re^{i\theta} = r\cos(\theta) + ir\sin(\theta)$. Then if we set $re^{i\theta} = x + iy$ and equate real and imaginary parts, we find $x = r\cos(\theta)$ and $y = r\sin(\theta)$.

NumPy makes it easy to work with complex numbers and convert between coordinate systems. The function `np.angle()` returns the angle of a complex number (between $-\pi$ and π) and the function `np.absolute()` returns the magnitude. Use these to compute θ and r, respectively. These functions also operate elementwise on NumPy arrays.

Note that in Python, `1j` is used for the complex number $i = \sqrt{-1}$. See the code below for an example.

```
>>> import numpy as np
>>> from matplotlib import pyplot as plt
# Set z = 2 - 2i
>>> z = 2 - 2*1j
>>> theta = np.angle(z)
>>> r = np.absolute(z)
# np.angle() returns a value between -pi and pi.
>>> print r, theta
(2.8284271247461903, -0.78539816339744828)
# Check that z=re^(i*theta)
>>> np.allclose(z, r*np.exp(1j*theta))
True
```

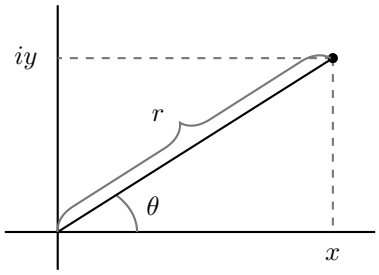


Figure 14.1: The complex number represented by the black dot equals both $x + iy$ and $re^{i\theta}$, when θ is written in radians.

Complex Functions

Suppose we wish to graph a function $f(z) : \mathbb{C} \to \mathbb{C}$. The difficulty is that $\mathbb{C}$ has 2 real dimensions, so the graph of f should use 4 real dimensions. Since we already have ways to visualize 3 dimensions, we should choose one dimension to ignore. We will ignore the magnitude $r = |f(z)|$ of the output.

To visualize f, we will assign a color to each point $z \in \mathbb{C}$. The color will correspond to the angle θ of the output $f(z)$. As an example, we have plotted the identity function $f(z) = z$ in Figure 14.2. As θ goes from 0 to 2π, the colors cycle smoothly counterclockwise from red to green to purple and back to red.

This kind of plot uses rectangular coordinates in the domain and polar coordinates (or rather, just the θ-coordinate) in the codomain. Note that this kind of plot tells us nothing about $|f(z)|$.

You can create the plot in Figure 14.2 as follows. Begin by creating a grid of complex numbers. We create the real and imaginary parts separately, and then use `np.meshgrid()` to turn them into a single array of complex numbers.

```
>>> x = np.linspace(-1, 1, 401)
>>> y = np.linspace(-1, 1, 401)
>>> X, Y = np.meshgrid(x, y)
>>> Z = X + 1j*Y
```

Now we compute the angles of the points in `Z` and plot them using `plt.pcolormesh()`. We use the colormap `'hsv'`, which is red at both ends, so that 0 and 2π will map to the same color.

```
>>> plt.pcolormesh(X, Y, np.angle(Z), cmap='hsv')
>>> plt.show()
```

Problem 1. Write the following function to plot any function from $\mathbb{C}$ to $\mathbb{C}$. Plot the angle only, as above, ignoring the magnitude.

```
def plot_complex(f, xbounds, ybounds, res=401):
    '''Plot the complex function f.

    INPUTS:
    f        - A function handle. Should represent a function
```

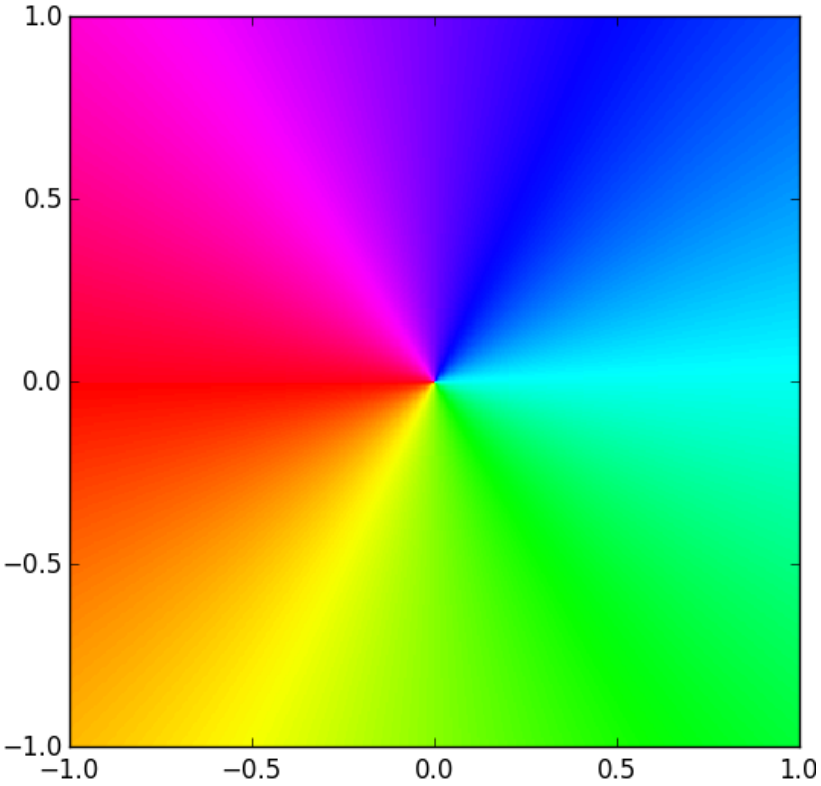


Figure 14.2: Plot of $f : \mathbb{C} \to \mathbb{C}$ defined by $f(z) = z$. The color at each point z represents the argument of $f(z)$.

```
            from C to C.
xbounds  - A tuple (xmin, xmax) describing the bounds on the real part
            of the domain.
ybounds  - A tuple (ymin, ymax) describing the bounds on the imaginary
            part of the domain.
res      - A scalar that determines the resolution of the plot.
            Defaults to 401.
'''
```

Check your function on $f(z) = z$ (graphed in Figure 14.2) and on the function $f(z) = \sqrt{z^2 + 1}$, which is graphed in Figure 14.3.

Hint: When you call `plt.pcolormesh()`, specify the keyword arguments `vmin` and `vmax`. These define which values should map to each end of the color scale. We want $-\pi$ to map to the low end of the color scale, and π to map to the high end. If not specified, matplotlib will scale the colormap to fit your data exactly.

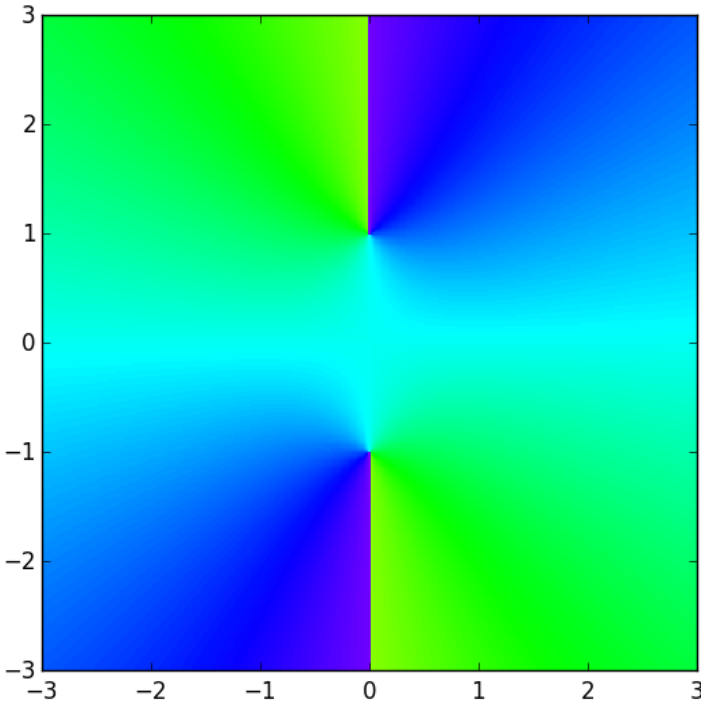


Figure 14.3: Plot of the angle of $\sqrt{z^2+1}$ on the domain $\{x+iy \mid x \in [-3,3],\ y \in [-3,3]\}$ created by `plot_complex()`.

The choice to ignore the magnitude may seem arbitrary. We can also write a complex plotting function to ignore the angle and only plot the magnitude. This will give us some different intuition about the function, while losing some information that we would get from the angle plot.

Problem 2. Write a new complex plotting function called `plot_complex_magnitude` which ignores the angle and plots only the magnitude. This should resemble your answer to Problem 1, with small modifications. Leave `vmin` and `vmax` unspecified when plotting.

Check your function on $f(z) = \sqrt{z^2+1}$. Your plot should look like the right subplot in Figure 14.4. Note the difference between this plot and the one from the previous problem.

Hint: A wraparound colormap like `'hsv'` doesn't work well here. Use any sequential colormap that makes it easy to distinguish between high and low values. See the matplotlib documentation for a list of colormaps.

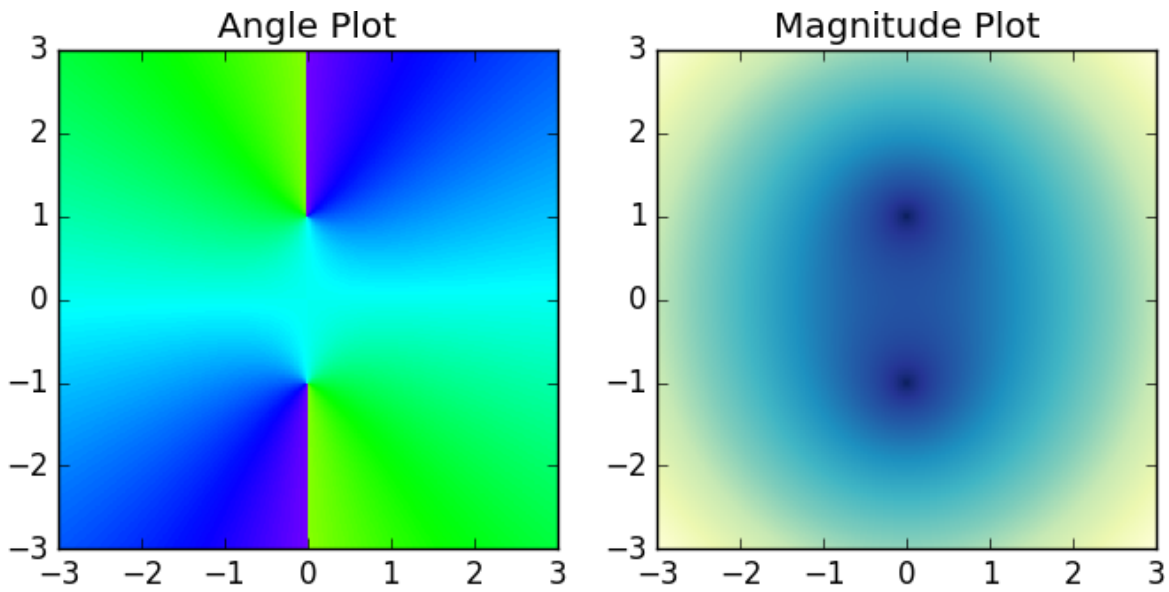


Figure 14.4: Plots of $\sqrt{z^2+1}$ on $\{x+iy \mid x \in [-3,3],\ y \in [-3,3]\}$, visualizing the angle and the magnitude of the function. Notice how a discontinuity is clearly visible on the left, but disappears from the plot on the right.

Analyzing Complex Plots

The angle plot is generally more useful than the magnitude plot for visualizing function behavior, zeros, and poles. Throughout the rest of the lab, use `plot_complex` to plot only the angle, and ignore the magnitude.

Zeros

Complex plots can be surprisingly informative. From an angle plot we can estimate not only a function's zeros, but also their multiplicities.

Problem 3.

1. Use `plot_complex()` to plot the functions z^2, z^3, and z^4.
2. Plot $z^3 - iz^4 - 3z^6$ on the domain $\{x+iy \mid x \in [-1,1],\ y \in [-1,1]\}$ (this plot is Figure 14.5). Compare it to your plot of z^3, especially near the origin. Based on these plots, what can you learn about the zeros of a function from its graph?

In Problem 3 you should have noticed that in a plot z^n, the colors cycle n times counterclockwise around 0. (Note: For the remainder of this lab we will define red $\to$ yellow $\to$ green $\to$ blue $\to$ red to be the "forward" direction, such that the colors are circling counterclockwise in Figure 14.2.)

This is explained by looking at z^n in polar coordinates:

$$z^n = (re^{i\theta})^n = r^n e^{i(n\theta)}.$$

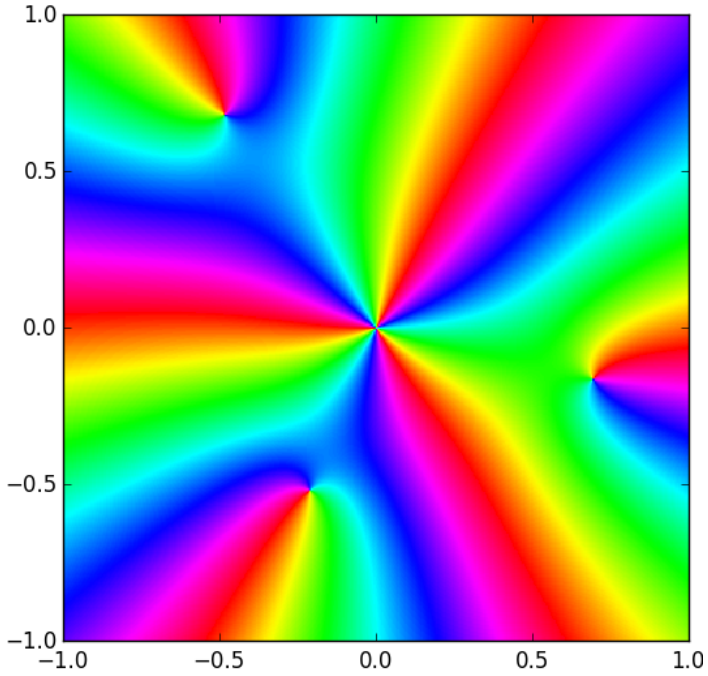


Figure 14.5: Plot of $f(z) = z^3 - iz^4 - 3z^6$ on the domain $\{x + iy \mid x \in [-1, 1],\ y \in [-1, 1]\}$. From this plot we see that $f(z)$ has a zero of order 3 at the origin, and 3 zeros of order 1 scattered around it. This accounts for the 6 roots of $f(z)$ that are guaranteed to exist by the Fundamental Theorem of Algebra.

Multiplying θ by a number greater than 1 compresses the graph along the "θ-axis" by a factor of n. In other words, the output angle repeats itself n times in one cycle of θ. Compare this to replacing $f(x)$ with $f(nx)$ when f is a function from $\mathbb{R}$ to $\mathbb{R}$.

From Problem 3 you should also have noticed that the plot of $z^3 - iz^4 - 3z^6$ looks a lot like the plot of z^3 near the origin. This is because when z is very small, z^4 and z^6 are much smaller than z^3, and so the behavior of z^3 dominates the function.

In general, $f(z)$ has a *zero of order n at z_0* if the Taylor series of $f(z)$ centered at z_0 can be written as

$$f(z) = \sum_{k=n}^{\infty} a_k (z - z_0)^k \qquad \text{with } a_n \neq 0.$$

In other words, $f(z) = a_n(z - z_0)^n + a_{n+1}(z - z_0)^{n+1} + \ldots$. In a small neighborhood of z_0, the quantity $|z - z_0|^{n+k}$ is much smaller than $|z - z_0|^n$, and so the function behaves like $a_n(z - z_0)^n$. This explains why we can estimate the order of a zero by counting the number of times the colors circle a point (see Figure 14.5).

Poles

The plots created by `plot_complex()` also contain information about the poles of the function plotted.

Problem 4.

1. Use `plot_complex()` to plot the function $f(z) = 1/z$. Compare this to the plot of $f(z) = z$ in Figure 14.2.
2. Plot z^{-2}, z^{-3}, and $z^2 + iz^{-1} + z^{-3}$ on the domain $\{x + iy \mid x \in [-1, 1],\ y \in [-1, 1]\}$. Compare the plots of the last two functions near the origin. Based on these plots, what can you learn about the poles of a function from its graph?

In Problem 4 you should have noticed that in the graph of $1/z^n$, the colors cycle n times *clockwise* around 0. Again this can be explained by looking at the polar representation:

$$z^{-n} = (re^{i\theta})^{-n} = r^{-n}e^{i(-n\theta)}.$$

The minus-sign on the θ reverses the direction of the colors, and the n makes them cycle n times.

In general, a function has a *pole of order* n at z_0 if its Laurent series on a punctured neighborhood of z_0 is

$$f(z) = \sum_{k=-n}^{\infty} a_k(z - z_0)^k \qquad \text{with } a_{-n} \neq 0.$$

In other words, $f(z) = a_{-n}(z - z_0)^{-n} + a_{-n+1}(z - z_0)^{-n+1} + \ldots$. Since $|z - z_0|^{-n+k}$ is much smaller than $|z - z_0|^{-n}$ when $|z - z_0|$ is small, near z_0 the function behaves like $a_{-n}(z - z_0)^{-n}$. This explains why we can estimate the order of a pole by counting the number of times the colors circle a point in the clockwise direction.

Finally, a function has an *essential pole* at z_0 if its Laurent series in a punctured neighborhood of z_0 requires infinitely many terms with negative exponents. For example,

$$e^{1/z} = \sum_{k=0}^{\infty} \frac{1}{n!z^n} = 1 + \frac{1}{z} + \frac{1}{2}\frac{1}{z^2} + \frac{1}{6}\frac{1}{z^3} + \ldots.$$

The plot of $f(z) = e^{1/z}$ is in Figure 14.6. The colors cycle infinitely many times around an essential singularity.

Using Plots to Estimate Poles and Zeros

To summarize, poles and zeros can be estimated from a complex plot with the following rules.

- Colors circle counterclockwise around zeros.
- Colors circle clockwise around poles.
- The number of times the colors cycle equals the order of the zero or pole.

Problem 5. Plot these functions on the domains given. Estimate the number and order of their poles and zeros.

- $f(z) = e^z$ on $\{x + iy \mid x \in [-8, 8],\ y \in [-8, 8]\}$
- $f(z) = \tan(z)$ on $\{x + iy \mid x \in [-8, 8],\ y \in [-8, 8]\}$

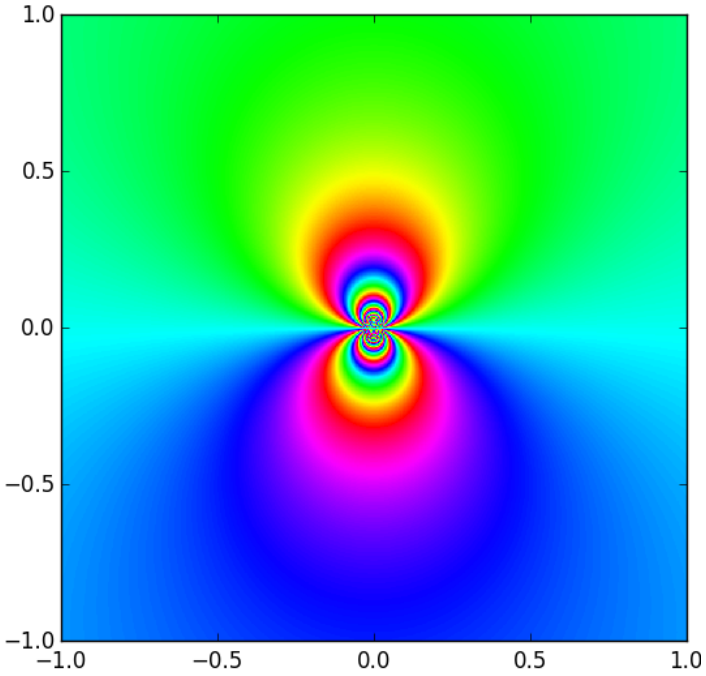


Figure 14.6: Plot of $e^{1/z}$ on the domain $\{x+iy \mid x \in [-1,1],\ y \in [-1,1]\}$. The colors circle clockwise around the origin because it is a singularity, not a zero. Because the singularity is essential, the colors repeat infinitely many times.

- $f(z) = \frac{16z^4+32z^3+32z^2+16z+4}{16z^4-16z^3+5z^2}$ on $\{x+iy \mid x \in [-1,1],\ y \in [-1,1]\}$

One useful application of complex plots is to estimate the zeros of polynomials and their multiplicity.

Problem 6. Use complex plots to determine the multiplicity of the zeros of each of the following polynomials. Use the Fundamental Theorem of Algebra to ensure that you have found them all.

1. $-4z^5 + 2z^4 - 2z^3 - 4z^2 + 4z - 4$
2. $z^7 + 6z^6 - 131z^5 - 419z^4 + 4906z^3 - 131z^2 - 420z + 4900$

Plotting functions is not a substitute for rigorous mathematics. Often, plots can be deceptive.

Problem 7.

1. This example shows that sometimes you have to "zoom in" to see all the information about a pole.
   (a) Plot the function $f(z) = \sin(\frac{1}{100z})$ on the domain $\{x+iy \mid x \in [-1,1],\ y \in [-1,1]\}$. What might you conclude about this function?

(b) Now plot $f(z)$ on $\{x+iy \mid x \in [-.01,.01],\ y \in [-.01,.01]\}$. Now what do you conclude about the function?

2. This example shows that from far away, two distinct zeros (or poles) can appear to be a single zero (or pole) of higher order.

   (a) Plot the function $f(z) = z + 1000z^2$ on the domain $\{x+iy \mid x \in [-1,1],\ y \in [-1,1]\}$. What does this plot imply about the zeros of this function?

   (b) Calculate the true zeros of $f(z)$.

   (c) Plot $f(z)$ on a domain that allows you to see the true nature of its zeros.

Multi-Valued Functions

Every complex number has two complex square roots, since if $w^2 = z$, then also $(-w)^2 = z$. If z is not zero, these roots are distinct.

Over the nonnegative real numbers, it is possible to define a continuous square root function. However, it is not possible to define a continuous square root function over any open set of the complex numbers that contains 0. This is intuitive after graphing $\sqrt{z}$ on the complex plane.

Problem 8. 1. Use `plot_complex` to graph $f(z) = \sqrt{z}$. Use `np.sqrt()` to take the square root.

2. Now plot $f(z) = -\sqrt{z}$ to see the "other square root" of z. Describe why these two plots look the way they do.

Just as raising z to a positive integer "compresses the θ-axis", making the color wheel repeat itself n times around 0, raising z to a negative power *stretches* the θ-axis, so that only one n^{th} of the color wheel appears around 0. The colors at the ends of this n^{th}-slice are not the same, but they appear next to each other in the plot of z^{-n}. This discontinuity will appear in every neighborhood of the origin.

If your domain does not contain the origin, it is possible to define a continuous root function by picking one of the roots.

Appendix

It is possible to visualize the argument and the modulus of the output of a complex function $f(z)$. One way to do so is to assign the modulus to a *lightness* of color. For example, suppose we have a complex number with argument 0, so it will map to red in the color plots described above. If its modulus is very small, then we can map it to a blackish red, and if its modulus is large, we can map it to a whitish red. With this extra rule, our complex plots will still be very much the same, except that zeros will look like black dots and poles will look like white dots (see Figure 14.7 for an example).

The code below implements the map we just described. Be warned that this implementation does not scale well. For example, if you try to plot a complex function whose outputs are all very small in modulus, the entire plot will appear black.

```
import numpy as np
import matplotlib.pyplot as plt
from colorsys import hls_to_rgb

def colorize(z):
    '''
    Map a complex number to a color (or hue) and lightness.

    INPUT:
    z - an array of complex numbers in rectangular coordinates

    OUTPUT:
    If z is an n x m array, return an n x m x 3 array whose third axis encodes
    (hue, lightness, saturation) tuples for each entry in z. This new array can
    be plotted by plt.imshow().
    '''

    zy=np.flipud(z)
    r = np.abs(zy)
    arg = np.angle(zy)

    # Define hue (h), lightness (l), and saturation (s)
    # Saturation is constant in our visualizations
    h = (arg + np.pi)  / (2 * np.pi) + 0.5
    l = 1.0 - 1.0/(1.0 + r**0.3)
    s = 0.8

    # Convert the HLS values to RGB values.
    # This operation returns a tuple of shape (3,n,m).
    c = np.vectorize(hls_to_rgb) (h,l,s)

    # Convert c to an array and change the shape to (n,m,3)
    c = np.array(c)
    c = c.swapaxes(0,2)
    c = c.swapaxes(0,1)
    return c
```

The following code uses the `colorize()` function to plot $\frac{z^2-1}{z}$. The output is Figure 14.7.

```
>>> f = lambda z :  (z**2-1)/z
>>> x = np.linspace(-.5, 1.5, 401)
>>> y = np.linspace(-1, 1, 401)
>>> X,Y = np.meshgrid(x,y)
>>> Z=f(X+Y*1j)
>>> Zc=colorize(Z)
>>> plt.imshow(Zc, extent=(-.5, 1.5, -1, 1))
>>> plt.show()
```

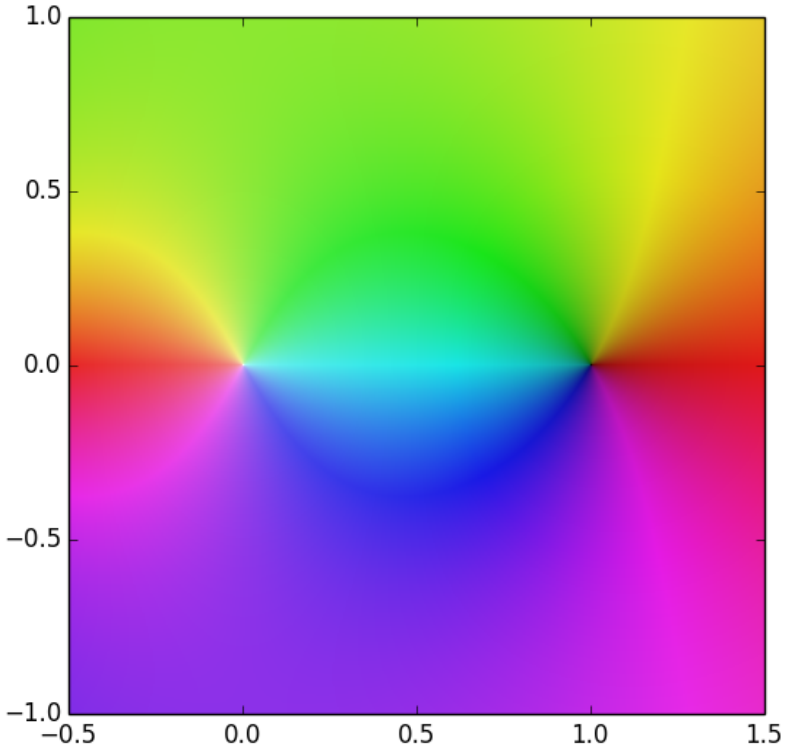


Figure 14.7: Plot of the function $\frac{z^2-1}{z}$ created with `colorize()`. Notice that the zero at 1 is a black dot and the pole at 0 is a white dot.

15 The PageRank Algorithm

Lab Objective: *Model a network as a graph and implement the PageRank algorithm based on this model. Use PageRank to predict the rankings of sports teams.*

As of 2013, the PageRank algorithm is one of over 200 algorithms that Google uses to determine the *rank*, or relative importance, of a webpage. Named for Larry Page, cofounder of Google, this algorithm ranks pages based on how many other pages link to them.

The Internet as a Graph

The PageRank algorithm models the internet with a directed graph. Each webpage is a node, and there is an edge from node i to node j if page i links to page j. Let $\text{In}(i)$ be the websites linking to page i and let $\text{Out}(i)$ be the websites that page i links to. That is, $\text{In}(i)$ is the set of nodes with an arrow to node i, and $\text{Out}(i)$ is the set of nodes with an arrow from node i. An example is illustrated in Figure 15.1.

The PageRank algorithm ranks pages by how many others link to them. A link from a more important page counts more than one from a less important page. For example, in Figure 15.1 we would expect node 0 to have a very high rank because every other node links to it. Consequently, we would expect node 7 to have a fairly high rank because node 0 links to it, even though node 0 is the only node to do so.

The PageRank Algorithm

The PageRank algorithm assumes that a surfer chooses a starting webpage randomly. Then, if the surfer is at page i, they randomly select a page from $\text{Out}(i)$ to visit next. This means that the surfer's chance of being on page i at time t is determined by where they were at time $t-1$.

Suppose the internet has N webpages, and let $p_i(t)$ be the likelihood that the surfer is on page i at time t. Then the probabilities $p_i(t)$ are given by

$$p_i(0) = \frac{1}{N} \qquad p_i(t+1) = \sum_{j \in \text{In}(i)} \frac{p_j(t)}{|\text{Out}(j)|}. \tag{15.1}$$

For example, in Figure 15.1 we have $N = 8$, and

$$p_6(t+1) = \frac{p_3(t)}{3} + \frac{p_4(t)}{3} + \frac{p_5(t)}{2}.$$

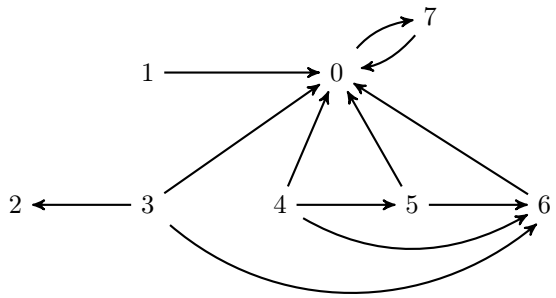


Figure 15.1: This directed graph describes the links between 8 webpages. In this example, $\text{In}(0) = \{1, 3, 4, 5, 6, 7\}$ and $\text{Out}(0) = \{7\}$.

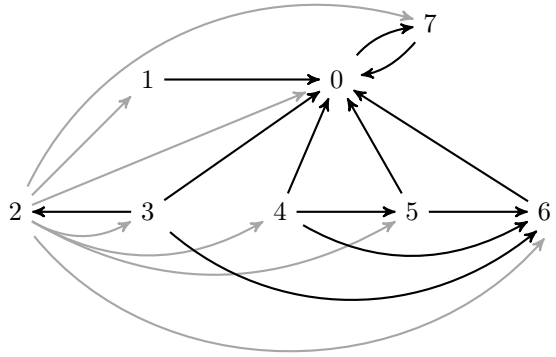


Figure 15.2: Here Figure 15.1 has been modified to guarantee that page 2 is no longer a sink. A new link has been added from page 2 to every other page (the added links are grey).

Refining the Model: Pages with No Outbound Links

A node with no outbound links, such as node 2 in Figure 15.1, is called a *sink*. According to our model, if the surfer ever visits a sink, they will stay there forever.

This is not very realistic; in this situation, a person would likely select another webpage at random and begin surfing again. Hence, in our model we replace sinks with nodes linking to every other page. This means we modify Figure 15.1 (where node 2 is a sink) to look like Figure 15.2.

Refining the Model: Adding Boredom

The equations in (15.1) assume that the current page must link to the next page. However, the model is more realistic if we assume that the surfer sometimes gets bored and randomly picks a new starting page. We will denote the probability that a surfer stays interested at step t by a constant d, called the *damping factor*. Then the probability that the surfer gets bored at time t is $1 - d$. The formulas in (15.1) then become

$$p_i(0) = \frac{1}{N} \qquad p_i(t+1) = d \sum_{j \in \text{In}(i)} \frac{p_j(t)}{|\text{Out}(j)|} + \frac{1-d}{N}. \tag{15.2}$$

Matrix Form of the PageRank Algorithm

We can rewrite (15.2) as the matrix equation

$$\mathbf{p}(0) = \frac{1}{N}\mathbf{1} \qquad \mathbf{p}(t+1) = dK\mathbf{p}(t) + \frac{1-d}{N}\mathbf{1} \tag{15.3}$$

where $\mathbf{p}(t) = (p_1(t), p_2(t), \ldots, p_N(t))^T$, $\mathbf{1}$ is a vector of N ones, and K is defined by

$$K_{ij} = \begin{cases} \frac{1}{|\mathrm{Out}(j)|} & \text{if j links to i} \\ 0 & \text{otherwise.} \end{cases}$$

Defining Page Rank

As given by the PageRank algorithm, the *rank* of page i is

$$p_i = \lim_{t\to\infty} p_i(t).$$

For those familiar with Markov Chains, Equation 15.3 defines a Markov chain. Page ranks are simply the steady state of this Markov chain.

Implementation in Python

The adjacency matrix A of a directed graph has $A_{ij} = 1$ if there is an edge from node i to node j, and $A_{ij} = 0$ otherwise. The adjacency matrix of the graph in Figure 15.1 is defined below. We use a code environment to describe A so you can easily use this example to debug the problems in this lab.

```
A = np.array([[ 0,  0,  0,  0,  0,  0,  0,  1],
              [ 1,  0,  0,  0,  0,  0,  0,  0],
              [ 0,  0,  0,  0,  0,  0,  0,  0],
              [ 1,  0,  1,  0,  0,  0,  1,  0],
              [ 1,  0,  0,  0,  0,  1,  1,  0],
              [ 1,  0,  0,  0,  0,  0,  1,  0],
              [ 1,  0,  0,  0,  0,  0,  0,  0],
              [ 1,  0,  0,  0,  0,  0,  0,  0]])
```

Problem 1. Write a function that creates an adjacency matrix from a file. The function should accept a filename, and an integer N that represents the number of nodes in the graph described by the datafile. Return the adjacency matrix as a `SciPy` sparse `dok_matrix`.
Hints:

1. The file `matrix.txt` included with this lab describes the matrix in Figure 15.1 and has the adjacency matrix `A` given above. You may use it to test your function.
2. You can open a file in Python using the `with` syntax. Then, you can iterate through the lines using a `for` loop. Here is an example.

```
# Open `matrix.txt' for read-only
with open('./matrix.txt', 'r') as myfile:
```

```
    for line in myfile:
        print line
```

3. Here is an example of how to process a line of the form in `datafile`.

```
>>> line = '0\t4\n'
# strip() removes trailing whitespace from a line.
# split() returns a list of the space-separated pieces of the line.
>>> line.strip().split()
['0', '4']
```

4. Rather than testing for lines of `matrix.txt` that contain comments, put all your string operations in a `try` block with an `except` block following.

Note

It makes sense to initialize A as a sparse matrix, since A is mostly zeros. To make the coding easier, throughout the rest of the lab the algorithms will be coded using non-sparse matrices. This means when using an adjacency matrix created in Problem 1, cast it `toarray()` when inputing it to test the other functions. In other words, you may say `test_calculateK(A.toarray(), N)`. Don't forget, however, that in a real-world sparse adjacency matrices are generally much more time-efficient than dense matrices.

The next step is to compute K from (15.3). A good strategy for computing K comes from writing

$$K = (D^{-1}A)^T$$

where A is the adjacency matrix of the directed graph representing the internet and D is a diagonal matrix with $D_{jj} = |\text{Out}(j)|$. Modify A so that rows corresponding to sinks have all ones instead of all zeros. For Figure 15.2, the modified adjacency matrix is defined below.

```
Am = np.array([[ 0,  0,  0,  0,  0,  0,  0,  1],
               [ 1,  0,  0,  0,  0,  0,  0,  0],
               [ 1,  1,  1,  1,  1,  1,  1,  1],
               [ 1,  0,  1,  0,  0,  0,  1,  0],
               [ 1,  0,  0,  0,  0,  1,  1,  0],
               [ 1,  0,  0,  0,  0,  0,  1,  0],
               [ 1,  0,  0,  0,  0,  0,  0,  0],
               [ 1,  0,  0,  0,  0,  0,  0,  0]])
```

The matrix D is easily obtained by summing the rows of A. Although $K = (D^{-1}A)^T$, it is better practice to only store the diagonal entries of D as a vector, and then use array broadcasting to divide A by D.

Notice that we need to transpose $D^{-1}A$ to get K. This is because $D^{-1}A$ is *row stochastic* (meaning that the rows sum to 1), but we need to multiply *column stochastic* matrices (where the columns sum to 1) To make K be column stochastic, we have to take a transpose.

For Figure 15.2, the matrix K is as follows.

```
K = np.array([[ 0   ,  1   ,  1./8,  1./3,  1./3,  1./2,  1   ,  1   ],
              [ 0   ,  0   ,  1./8,  0   ,  0   ,  0   ,  0   ,  0   ],
              [ 0   ,  0   ,  1./8,  1./3,  0   ,  0   ,  0   ,  0   ],
              [ 0   ,  0   ,  1./8,  0   ,  0   ,  0   ,  0   ,  0   ],
              [ 0   ,  0   ,  1./8,  0   ,  0   ,  0   ,  0   ,  0   ],
              [ 0   ,  0   ,  1./8,  0   ,  1./3,  0   ,  0   ,  0   ],
              [ 0   ,  0   ,  1./8,  1./3,  1./3,  1./2,  0   ,  0   ],
              [ 1   ,  0   ,  1./8,  0   ,  0   ,  0   ,  0   ,  0   ]])
```

Problem 2. Write a function that computes and returns the K matrix given an adjacency matrix.

1. Compute the diagonal matrix D.
2. Compute the modified adjacency matrix where the rows corresponding to sinks all have ones instead of zeros.
3. Compute K using array broadcasting.

Solving for the Page Ranks

There are several ways to solve for $\lim_{t\to\infty}\mathbf{p}(t)$.

Algebraic Method

Again, for those familiar with Markov chains, one possibility is to assume the modified Markov chain has a steady state $\mathbf{p}$ and solve for it algebraically:

$$(I - dK)\mathbf{p} = \frac{1-d}{N}\mathbf{1}. \tag{15.4}$$

We can use SciPy's solver to find the page ranks of the network in Figure 15.2.

```
>>> from scipy import linalg as la
>>> I = np.eye(8)
>>> d = .85
>>> la.solve(I-d*K, ((1-d)/8)*np.ones(8))
array([ 0.43869288,  0.02171029,  0.02786154,  0.02171029,  0.02171029,
        0.02786154,  0.04585394,  0.39459924])
```

As expected, node 0 has the highest rank, approximately equal to .44. Node 7 has a higher rank than node 6, even though $\text{In}(7) = 1$ and $\text{In}(6) = 3$. This is because node 7's single in-edge comes from a node that has a very high rank (node 0).

Iterative Method

Solving the system in (15.4) is feasible for our small working example, but this is not an efficient strategy for very large systems.

One option for large systems is an iterative method. Starting with a guess for $\mathbf{p}(0)$, we iterate on Equation (15.3) until $\|\mathbf{p}(t) - \mathbf{p}(t-1)\|$ is sufficiently small. At this point we assume we have reached the steady state.

Problem 3. Implement a function that uses the iterative method to find the steady state of the PageRank algorithm. You function should accept an adjacency matrix `A`, an integer `N` that defaults to `None`, the damping factor `d` that defaults to `0.85`, and a tolerance `tol` that defaults to `1E-5`. Return the approximation to the steady state as a float. When the argument `N` is not `None`, work with only the upper $N \times N$ portion of the array `adj`. Test your function against the example datafile that accompanies this lab.
Hints:

1. Try making your initial guess for $\mathbf{p}(0)$ a random vector.
2. NumPy can do unexpected things with the dimensions when performing matrix-vector multiplication. When debugging, check at each iteration that all arrays have the dimensions you expect.

Eigenvalue Method

Another way to solve this problem is to make it into an eigenvalue problem. Let E be an $N \times N$ matrix of ones; then $E\mathbf{p}(t) = \mathbf{1}$. Hence, the matrix equation (15.3) for $\mathbf{p}(t+1)$ becomes

$$\mathbf{p}(t+1) = \left(dK + \frac{1-d}{N}E\right)\mathbf{p}(t).$$

If we write $B = dK + \frac{1-d}{N}E$, this simplifies to $\mathbf{p}(t+1) = B\mathbf{p}(t)$. Thus, the steady state $\mathbf{p}(t)$ is an eigenvector of B corresponding to the eigenvalue 1.

The columns of B sum to 1, and the entries of B are strictly positive (because the entries of E are all positive). With these hypotheses, the Perron-Frobenius theorem says that 1 is the unique eigenvalue of B of largest magnitude, and the corresponding eigenvector is unique. In this case, the "iterative method" described above is just the power method for finding the eigenvector corresponding to a dominant eigenvalue, introduced in the lab on eigensolvers.

We can also compute $\mathbf{p}$ using eigenvalue solvers in SciPy.

Problem 4. Implement a function that uses the eigenvalue method to find the steady state of the PageRank algorithm. Your function should accept an adjacency matrix `A`, an integer `N` that defaults to `None`, and the damping factor `d` that defaults to `0.85`. Return the approximation to the steady state as a float.

Application: Ranking Sports Teams

This ranking algorithm can be applied not only to webpages, but to any problem with a directed graph structure. One such application is ranking sports teams.

Suppose we have data about a collection of sports teams, including which teams played each other and who won each match. We can model this as a directed graph. Each node in the graph represents a team. An edge between two nodes points from the losing team to the winning team. If two teams never played each other, there is no edge between them. Wins and losses do not cancel out; if BYU and Boise played twice, and each team won once, then there is an edge from BYU to Boise and another edge from Boise to BYU.

To simplify our model, edges are not weighted. So if Duke ever beat Harvard, no matter whether they beat them once or 5 times, there is only one edge pointing from Harvard to Duke.

The key here is that edges tend to lead from worse teams to better teams. So by starting with some team and randomly following edges, we should end up visiting better teams more often. This is reminiscent of the PageRank algorithm! Given an appropriate dataset, we can use PageRank to estimate team rankings.

Note that in this scenario, the parameter d no longer represents boredom. It allows us to jump randomly from one team to another, so it could represent a surprise upset, or the random outcome of a game between two teams who have never played each other.

Problem 5. By applying the PageRank algorithm to win-loss data from the 2013 NCAA basketball season, produce a comparative ranking of the teams.

1. The file `ncaa2013.csv` contains data on over 5000 basketball games. The first line is a header. After the header, each line represents a game and has the winning team followed by the losing team (there are no ties in basketball).

   Load this file and use it to create the adjacency matrix A, where $A_{ij} = 1$ if team j beat team i. Make sure to ignore the header line. You will need some way of mapping from team names to the integers and vice versa.

2. Use the iterative method from Problem 3 with $d = 0.7$ to find the steady state. The steady-state solution is your vector of ranks.

3. Return the ranks sorted from largest to smallest, and the corresponding list of teams sorted from "best" to "worst".

Hints:

1. The code below may be helpful for processing the .csv file:

```
>>> with open('./ncaa2013.csv', 'r') as ncaafile:
>>>     ncaafile.readline() #reads and ignores the header line
>>>     for line in ncaafile:
>>>         teams = line.strip().split(',') #split on commas
>>>         print teams
>>> ['Middle Tenn St', 'Alabama St']
>>> ...
>>> ['Mississippi', 'Florida']
```

2. Before creating the adjacency matrix, you can get all the unique teams by running through all the matches once and adding every team to a set. Next, count the number of unique teams and initialize A to be the right size. Try using dictionaries, lists, or both to map numbers to teams and teams to numbers and fill in A. There is more than one right way to do this.
3. The function `np.argsort()` will be useful for sorting the ranks and teams.
4. There should be 347 teams. PageRank should predict that the top five ranked teams are Duke, Butler, Louisville, Illinois, and Indiana (in that order). Use this to check your results.

NetworkX: Python package for networks

The purpose of this section is not to give an introduction to NetworkX, but rather, to introduce you to just enough to be able to analyze the basic properties of a network and apply NetworkX's implementation of PageRank. NetworkX takes advantage of the sparse nature of these networks. Therefore, they are more efficient than the ones we have coded in this lab.

We will first run through the simple steps to initialize the graph defined in Figure 15.1. We will initialize this graph using the edges defined in `matrix.txt`. If we create an $n \times 2$ matrix of the edges of this graph, we would get,

```
>>> edges = array([[ 0,  7],
...                [ 1,  0],
...                [ 3,  0],
...                [ 3,  6],
...                [ 4,  0],
...                [ 4,  5],
...                [ 4,  6],
...                [ 5,  0],
...                [ 5,  6],
...                [ 6,  0],
...                [ 7,  0]])
```

.

We can now initialize a NetworkX graph using this array of edges.

```
>>> import networkx as nx
>>> G = nx.from_edgelist(edges, create_using=nx.DiGraph())
```

Now that we have initialized the `DiGraph` object, we can use all the analysis tools that come with NetworkX to gain further insight into the structure of the graph. Verify the following characteristics match the graph in Figure 15.1.

```
>>> G.in_degree()
{0: 6, 1: 0, 3: 0, 4: 0, 5: 1, 6: 3, 7: 1}

>>> G.out_degree()
{0: 1, 1: 1, 3: 2, 4: 3, 5: 2, 6: 1, 7: 1}
```

```
>>> G.in_edges(0)
[(1, 0), (3, 0), (4, 0), (5, 0), (6, 0), (7, 0)]

>>> G.out_edges(0)
[(0, 7)]
```

NetworkX also comes with a `pagerank()` function that can be used simply by passing the function your `DiGraph` object. Compare the results to the values calculated using our methods.

```
>>> nx.pagerank(G, alpha=0.85) # alpha is the dampening factor.
{0: 0.45323691210120065,
 1: 0.021428571428571432,
 3: 0.021428571428571432,
 4: 0.021428571428571432,
 5: 0.027500000000000004,
 6: 0.04829464285714287,
 7: 0.406682730755942}
```

Application: Twitter Datasets

The SNAP graph library, located at `http://snap.stanford.edu/data/index.html`, provides a variety of medium sized data sets for public use. These datasets have to do with networks, including road systems, social networks, and online communities. There are some interesting resources here for those wanting to experiment further with the PageRank algorithm on different datasets.

Problem 6 (Optional). The `twitter_combined.txt` file contains a list of edges that represent a Twitter network. To protect the privacy of users, the data has been anonymized. Each number is an ID for a user. The users in the first column represent Twitter users that follow the users in the second column.

Using these edges,

1. Create a `DiGraph` object using all the edges described in `twitter_combined.txt`.
2. Calcualte the page ranks for this graph. The page ranks create a ranking of which users are the most “influential". Even though the results will just be numbers, remember that they represent actual Twitter users.
3. Analyze the in-degree and out-degree of the top 10 ranked users. What do you notice about the second-highest ranked user? Why would this user be ranked so high? HINT: Use `G.in_edges()` and `G.out_edges()` to gain further insight into this result.
4. Return the top 10 most influential users and their scores

16 The Drazin Inverse

Lab Objective: *The Drazin inverse of a matrix is a pseudoinverse which preserves certain spectral properties of the matrix. In this lab, we compute the Drazin inverse using the Schur decomposition, then use it to compute the effective resistance of a graph and perform link prediction.*

Definition of the Drazin Inverse

The *index* of an $n \times n$ matrix A is the smallest nonnegative integer k for which $\mathscr{N}(A^k) = \mathscr{N}(A^{k+1})$. The *Drazin inverse* A^D of A is the unique $n \times n$ matrix satisfying the following properties.

- $AA^D = A^DA$
- $A^{k+1}A^D = A^k$
- $A^DAA^D = A^D$

Note that if A is *invertible*, in which case $k = 0$, then $A^D = A^{-1}$. On the other hand, if A is *nilpotent*, meaning $A^j = \mathbf{0}$ for some nonnegative integer j, then A^D is the zero matrix.

Problem 1. Write a function that accepts an $n \times n$ matrix A, the index k of A, and an $n \times n$ matrix A^D. Use the criteria described above to determine whether or not A^D is the Drazin inverse of A. Return `True` if A^D satisfies all three conditions; otherwise, return `False`.

Use the following matrices as test cases for your function.

$$A = \begin{bmatrix} 1 & 3 & 0 & 0 \\ 0 & 1 & 3 & 0 \\ 0 & 0 & 1 & 3 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \quad A^D = \begin{bmatrix} 1 & -3 & 9 & 81 \\ 0 & 1 & -3 & -18 \\ 0 & 0 & 1 & 3 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \quad k = 1$$

$$B = \begin{bmatrix} 1 & 1 & 3 \\ 5 & 2 & 6 \\ -2 & -1 & -3 \end{bmatrix}, \quad B^D = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad k = 3$$

(Hint: `np.allclose()` and `np.linalg.matrix_power()` may be useful).

Computing the Drazin Inverse

The Drazin inverse is often defined theoretically in terms of the eigenprojections of a matrix. However, eigenprojections are often costly or unstable to calculate, so we resort to a different method to calculate the Drazin inverse.

To begin, suppose that the $n \times n$ matrix A can be written in the form

$$A = S^{-1} \begin{bmatrix} M & \mathbf{0} \\ \mathbf{0} & N \end{bmatrix} S, \tag{16.1}$$

where S is a change of basis matrix, N is nilpotent, and M is the restriction of A onto the range of $I - P_0$, where P_0 is the 0-eigenprojection in the spectral decomposition. Then the Drazin inverse can be calculated as

$$A^D = S^{-1} \begin{bmatrix} M^{-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} S. \tag{16.2}$$

Next, the *Schur decomposition* of A is given by

$$A = QTQ^{-1}, \tag{16.3}$$

where Q is orthonormal and T is upper triangular. Since T is similar to A, the eigenvalues of A are listed along the diagonal of T. Then if A is singular, at least one diagonal entry of T must be 0. The columns that contain the 0 eigenvalues of A form the nilpotent matrix N in (16.1). To compute M and N, we sort the Schur decomposition so that the 0 eigenvalues are listed last along the diagonal of T, and then we can use (16.2) to compute A^D.

SciPy's `la.schur()` is a routine for computing the Schur decomposition of a matrix, but it does not automatically sort it by eigenvalue. However, sorting can be accomplished by specifying the `sort` keyword argument.

```
>>> from scipy import linalg as la

# The standard Schur decomposition.
>>> A = np.array([[0,0,2],[-3,2,6],[0,0,1]])
>>> T,Z = la.schur(A)
>>> T                        # The eigenvalues (2, 0, and 1) are not sorted.
array([[ 2., -3.,  6.],
       [ 0.,  0.,  2.],
       [ 0.,  0.,  1.]])

# Specify a sorting function to get the desired result.
>>> f = lambda x: abs(x) > 0
>>> T1,Z1,k = la.schur(A, sort=f)
>>> T1
array([[ 2.        ,  0.        ,  6.70820393],
       [ 0.        ,  1.        ,  2.        ],
       [ 0.        ,  0.        ,  0.        ]])
>>> k                         # k is the number of columns satisfying the sort,
2                            # which is the number of nonzero eigenvalues.
```

The procedure for finding the Drazin inverse using the Schur decomposition and (16.1) is given in Algorithm 16.1. Due to possible floating point arithmetic errors, consider all eigenvalues smaller than a certain tolerance to be 0.

Algorithm 16.1

procedure DRAZIN(A, tol)
  $(n, n) \leftarrow \text{shape}(A)$
  $Q_1, S, k_1 \leftarrow \text{schur}(A, |x| > \text{tol})$ ▷ Sort the Schur decomposition.
  $Q_2, T, k_2 \leftarrow \text{schur}(A, |x| \leq \text{tol})$
  $U \leftarrow [S_{:,:k_1} \mid T_{:,:n-k_1}]$ ▷ Concatenate part of S and T column-wise.
  $U^{-1} \leftarrow \text{inverse(U)}$
  $V \leftarrow U^{-1}AU$
  $Z \leftarrow \mathbf{0}_{n\times n}$ ▷ The $n \times n$ zero matrix **as floats**, not ints.
  if $k_1 \neq 0$ **then**
    $M^{-1} \leftarrow \text{inverse}(V_{:k_1,:k_1})$
    $Z_{:k_1,:k_1} \leftarrow M^{-1}$
  return UZU^{-1}

Problem 2. Write a function that accepts an $n \times n$ matrix A and a tolerance for rounding eigenvalues to zero. Use Algorithm 16.1 to compute the Drazin inverse A^D. Use your function from Problem 1 to verify your implementation.

ACHTUNG!

Because the algorithm for the Drazin inverse requires calculation of the inverse of a matrix, it is unstable when that matrix has a high condition number. If the algorithm does not find the correct Drazin inverse, check the condition number of V from Algorithm 16.1

NOTE

The Drazin inverse is called a *pseudoinverse* because $A^D = A^{-1}$ for invertible A, and for noninvertible A, A^D always exists and acts similarly to an inverse. There are other matrix pseudoinverses that preserve different qualities of A, including the *Moore-Penrose pseudoinverse* $A^\dagger$, which can be thought of as the least squares approximation to A^{-1}.

Applications of the Drazin Inverse

Effective Resistance

The *effective resistance* between two nodes in a undirected graph is a measure of how connected those nodes are. The concept originates from the study of circuits to measure the resistance between two points on the circuit. A *resistor* is a device in a circuit which limits or regulates the flow of electricity. Two points that have more resistors between them have more resistance, while those with fewer resistors between them have less resistance. The entire circuit can be represented by a graph where the nodes are the points of interest and the number of edges connecting two nodes indicates the number of resistors between the corresponding points. See Figure 16.1 for an example.

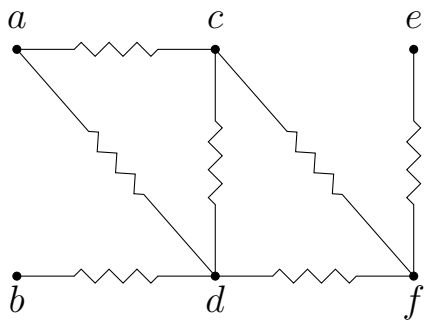


Figure 16.1: A graph with a resistor on each edge.

In electromagnetism, there are rules for manually calculating the effective resistance between two nodes for relatively simple graphs. However, this is infeasible for large or complicated graphs. Instead, we can use the Drazin inverse to calculate effective resistance for any graph.

First, create the *adjacency matrix*[1] of the graph, the matrix where the (ij)th entry is the number of connections from node i to node j. Next, calculate the Laplacian L of the adjacency matrix. Then if R_{ij} be the effective resistance from node i to node j,

$$R_{ij} = \begin{cases} (\widetilde{L}^j)^D_{ii} & \text{if } i \neq j \\ 0 & \text{if } i = j \end{cases}, \tag{16.4}$$

where $\widetilde{L}^j$ is the Laplacian with the jth row of the Laplacian replaced by the jth row of the identity matrix, and $(\widetilde{L}^j)^D$ is its Drazin inverse.

Problem 3. Write a function that accepts the $n \times n$ adjacency matrix of an undirected graph. Use (16.4) to compute the effective resistance from each node to every other node. Return an $n \times n$ matrix where the (ij)th entry is the effective resistance from node i to node j. Keep the following in mind:

- The resulting matrix should be symmetric.
- The effective resistance from a node to itself is 0.
- Consider creating the matrix column by column instead of entry by entry. Every time you compute the Drazin inverse, the whole diagonal of the matrix can be used.

Test your function using the graphs and values from Figure 16.2.

[1]See Problem 1 of Image Segmentation for a refresher on adjacency matrices and the Laplacian.

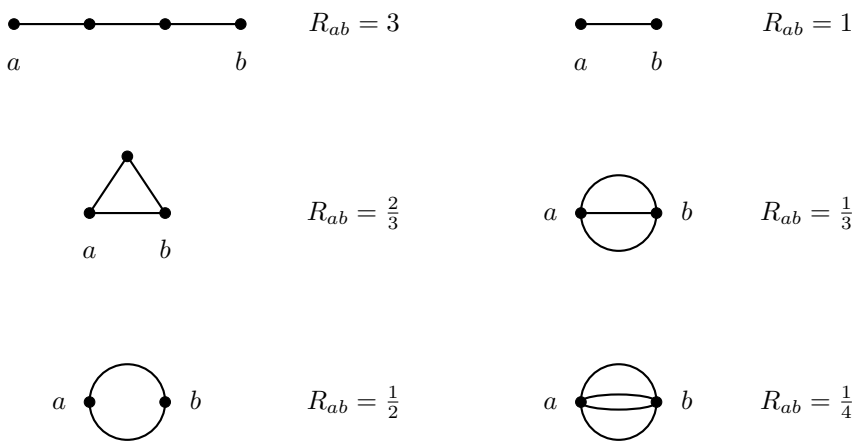


Figure 16.2: The effective resistance between two points for several simple graphs. Nodes that are farther apart have a larger effective resistance, while nodes that are nearer or better connected have a smaller effective resistance.

Link Prediction

Link prediction is the problem of predicting the likelihood of a future association between two unconnected nodes in a graph. Link prediction has application in many fields, but the canonical example is friend suggestions on Facebook. The Facebook network can be represented by a large graph where each user is a node, and two nodes have an edge connecting them if they are "friends." Facebook aims to predict who you would like to become friends with in the future, based on who you are friends with now, as well as discover which friends you may have in real life that you have not yet connected with online. To do this, Facebook must have some way to measure how closely two users are connected.

We will compute link prediction using effective resistance as a metric. Effective resistance measures how closely two nodes are connected, and nodes that are closely connected at present are more likely to be connected in the future. Given an undirected graph, the next link should connect the two unconnected nodes with the least effective resistance between them.

Problem 4. Write a class called `LinkPredictor` for performing link prediction. Implement the `__init__()` method so that it accepts the name of a `csv` file containing information about a social network. Each row of the file should contain the names of two nodes which are connected by an (undirected) edge.

Store each of the names of the nodes of the graph as an ordered list. Next, create the adjacency matrix for the network where the ith row and column of the matrix correspond to the ith member of the list of node names. Finally, use your function from Problem 3 to compute the effective resistance matrix. Save the list of names, the adjacency matrix, and the effective resistance matrix as attributes.

Problem 5. Implement the following methods in the `LinkPredictor` class:

1. `predict_link()`: Accept a parameter `node` which is either `None` or a string representing a node in the network. If `node` is `None`, return a tuple with the names of the nodes between which the next link should occur. However, if `node` is a string, return the name of the node which should be connected to `node` next out of all other nodes in the network. If `node` is not in the network, raise a `ValueError`. Take the following into consideration:

   (a) You want to find the two nodes which have the smallest effective resistance between them which are not yet connected. Use information from the adjacency matrix to zero out all entries of the effective resistance matrix that represent connected nodes. The "`*`" operator multiplies arrays component-wise, which may be helpful.

   (b) Find the next link by finding the minimum value of the array that is nonzero. Your array may be the whole matrix or just a column if you are only considering links for a certain node. This can be accomplished by passing `np.min()` a masked version of your matrix to exclude entries that are 0.

   (c) NumPy's `np.where()` is useful for finding the minimum value in an array:

```
>>> A = np.random.randint(-9,9,(3,3))
>>> A
array([[ 6, -8, -9],
       [-2,  1, -1],
       [ 4,  0, -3]])

# Find the minimum value in the array.
>>> minval = np.min(A)
>>> minval
-9

# Find the location of the minimum value.
>>> loc = np.where(A==minval)
>>> loc
(array([0], dtype=int64), array([2], dtype=int64))
```

2. `add_link()`: Take as input two names of nodes, and add a link between them. If either name is not in the network, raise a `ValueError`. Add the link by updating the adjacency matrix and the effective resistance matrix.

Figure 16.3 visualizes the data in `social_network.csv`. Use this graph to verify that your class is suggesting plausible new links. You should observe the following:

- In the entire network, Emily and Oliver are most likely to become friends next.
- Melanie is predicted to become friends with Carol next.
- Alan is expected to become friends with Sonia, then with Piers, and then with Abigail.

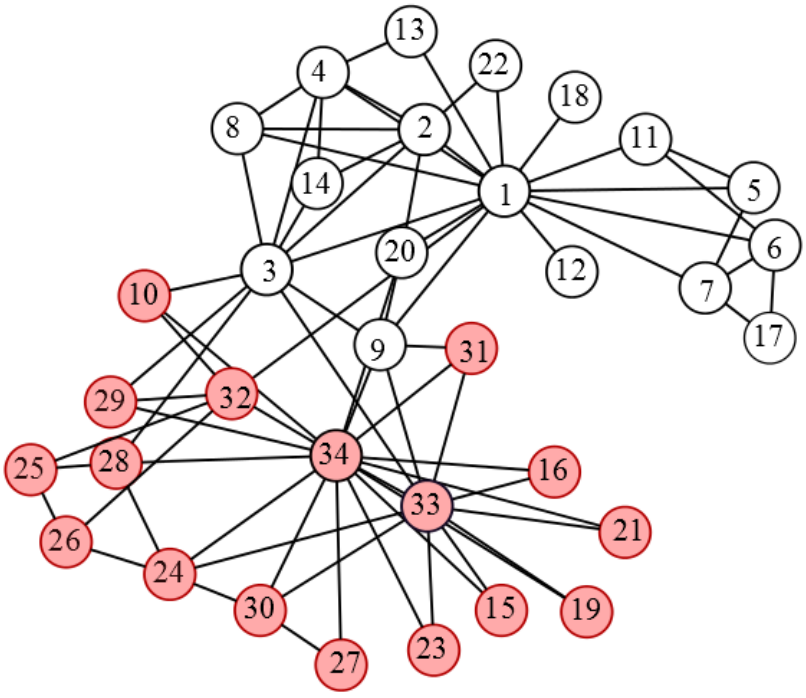


Figure 16.3: The social network contained in `social_network.csv`. Adapted from data by Wayne. W Zachary (see `https://en.wikipedia.org/wiki/Zachary%27s_karate_club`).

1. Piers
2. Abigail
3. Oliver
4. Stephanie
5. Carol
6. Melanie
7. Stephen
8. Sally
9. Penelope
10. Alan
11. Trevor
12. Jake
13. Mary
14. Anna
15. Ruth
16. Evan
17. Connor
18. John
19. Max
20. Eric
21. Theresa
22. Paul
23. Alexander
24. Colin
25. Jake
26. Jane
27. Brandon
28. Thomas
29. Christopher
30. Charles
31. Madeleine
32. Tracey
33. Sonia
34. Emily

17 Iterative Solvers

Lab Objective: *Many real-world problems of the form $A\mathbf{x} = \mathbf{b}$ have tens of thousands of parameters. Solving such systems with Gaussian elimination or matrix factorizations could require trillions of floating point operations (FLOPs), which is of course infeasible. Solutions of large systems must therefore be approximated iteratively. In this lab, we implement three popular iterative methods for solving large systems: Jacobi, Gauss-Seidel, and Successive Over-Relaxation.*

Iterative methods are often useful to solve large systems of equations. In this lab, let $\mathbf{x}^{(k)}$ denote the k-th iteration of the iterative method for solving the problem $A\mathbf{x} = \mathbf{b}$ for $\mathbf{x}$. Furthermore, let x_i be the i-th component of $\mathbf{x}$ so that $x_i^{(k)}$ is the i-th component of $\mathbf{x}$ in the k-th iteration. Choose a very small $\epsilon > 0$ and an integer $N \in \mathbb{N}$, and continue iterating until either

$$\|\mathbf{x}^{(k-1)} - \mathbf{x}^{(k)}\| < \epsilon \qquad \text{or} \qquad k > N. \tag{17.1}$$

The Jacobi Method

The *Jacobi Method* is a simple but powerful method used for solving certain kinds of large linear systems. The main idea is simple: solve for each variable in terms of the others, then use the previous values to update each approximation. As a (very small) example, consider the following 3×3 system.

$$\begin{array}{rcrcrcr} 2x_1 & & & - & x_3 & = & 3 \\ -x_1 & + & 3x_2 & + & 2x_3 & = & 3 \\ & + & x_2 & + & 3x_3 & = & -1 \end{array}$$

Solving the first equation for x_1, the second for x_2, and the third for x_3 yields the following.

$$\begin{aligned} x_1 &= \tfrac{1}{2}(3 + x_3) \\ x_2 &= \tfrac{1}{3}(3 + x_1 - 2x_3) \\ x_3 &= \tfrac{1}{3}(-1 - x_2) \end{aligned}$$

Now begin with an initial guess $\mathbf{x}^{(0)} = [x_1^{(0)}, x_2^{(0)}, x_3^{(0)}]^\mathsf{T} = [0, 0, 0]^\mathsf{T}$. To compute the first approximation $\mathbf{x}^{(1)}$, use the entries of $\mathbf{x}^{(0)}$ as the variables on the right side of the previous equation.

$$\begin{array}{rcccccc} x_1^{(1)} &=& \tfrac{1}{2}(3 + x_3^{(0)}) &=& \tfrac{1}{2}(3 + 0) &=& \tfrac{3}{2} \\ x_2^{(1)} &=& \tfrac{1}{3}(3 + x_1^{(0)} - 2x_3^{(0)}) &=& \tfrac{1}{3}(3 + 0 - 0) &=& 1 \\ x_3^{(1)} &=& \tfrac{1}{3}(-1 - x_2^{(0)}) &=& \tfrac{1}{3}(-1 - 0) &=& -\tfrac{1}{3} \end{array}$$

So $\mathbf{x}^{(1)} = [\frac{3}{2}, 1, -\frac{1}{3}]^\mathsf{T}$. Computing $\mathbf{x}^{(2)}$ is similar.

$$\begin{array}{rclcrcl} x_1^{(2)} & = & \frac{1}{2}(3 + x_3^{(1)}) & = & \frac{1}{2}(3 - \frac{1}{3}) & = & \frac{4}{3} \\ x_2^{(2)} & = & \frac{1}{3}(3 + x_1^{(1)} - 2x_3^{(1)}) & = & \frac{1}{3}(3 + \frac{3}{2} + \frac{2}{3}) & = & \frac{31}{18} \\ x_3^{(2)} & = & \frac{1}{3}(-1 - x_2^{(1)}) & = & \frac{1}{3}(-1 - 1) & = & -\frac{2}{3} \end{array}$$

The process is repeated until at least one of the two stopping criteria in (17.1) is met. For this particular problem, convergence to 8 decimal places ($\epsilon = 10^{-8}$) is reached in 29 iterations.

	$x_1^{(k)}$	$x_2^{(k)}$	$x_3^{(k)}$
$\mathbf{x}^{(0)}$	0	0	0
$\mathbf{x}^{(1)}$	1.5	1	-0.33333
$\mathbf{x}^{(2)}$	1.33333333	1.72222222	-0.66666667
$\mathbf{x}^{(3)}$	1.16666667	1.88888889	-0.90740741
$\mathbf{x}^{(4)}$	1.04629630	1.99382716	-0.96296296
$\vdots$	$\vdots$	$\vdots$	$\vdots$
$\mathbf{x}^{(28)}$	0.99999999	2.00000001	-0.99999999
$\mathbf{x}^{(29)}$	1	2	-1

Matrix Representation

The iterative steps performed above can be expressed in matrix form. First, decompose A into its diagonal entries, its entries below the diagonal, and its entries above the diagonal, as $A = D + L + U$.

$$\underset{D}{\begin{bmatrix} a_{11} & 0 & \dots & 0 \\ 0 & a_{22} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & a_{nn} \end{bmatrix}} \quad \underset{L}{\begin{bmatrix} 0 & 0 & \dots & 0 \\ a_{21} & 0 & \dots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ a_{n1} & \dots & a_{n,n-1} & 0 \end{bmatrix}} \quad \underset{U}{\begin{bmatrix} 0 & a_{12} & \dots & a_{1n} \\ 0 & 0 & \ddots & \vdots \\ \vdots & \vdots & \ddots & a_{n-1,n} \\ 0 & 0 & \dots & 0 \end{bmatrix}}$$

With this decomposition, we solve for $\mathbf{x}$ in the following way.

$$\begin{aligned} A\mathbf{x} &= \mathbf{b} \\ (D + L + U)\mathbf{x} &= \mathbf{b} \\ D\mathbf{x} &= -(L + U)\mathbf{x} + \mathbf{b} \\ \mathbf{x} &= D^{-1}(-(L + U)\mathbf{x} + \mathbf{b}) \end{aligned}$$

Now using $\mathbf{x}^{(k)}$ as the variables on the right side of the equation to produce $\mathbf{x}^{(k+1)}$ on the left, and noting that $L + U = A - D$, we have the following.

$$\begin{aligned} \mathbf{x}^{(k+1)} &= D^{-1}(-(A - D)\mathbf{x}^{(k)} + \mathbf{b}) \\ &= D^{-1}(D\mathbf{x}^{(k)} - A\mathbf{x}^{(k)} + \mathbf{b}) \\ &= \mathbf{x}^{(k)} + D^{-1}(\mathbf{b} - A\mathbf{x}^{(k)}) \end{aligned} \tag{17.2}$$

There is a potential problem with (17.2): calculating a matrix inverse is the cardinal sin of numerical linear algebra, yet the equation contains D^{-1}. However, since D is a diagonal matrix, D^{-1} is also diagonal, and is easy to compute.

$$D^{-1} = \begin{bmatrix} \frac{1}{a_{11}} & 0 & \dots & 0 \\ 0 & \frac{1}{a_{22}} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \frac{1}{a_{nn}} \end{bmatrix}$$

Because of this, the Jacobi method requires that A have nonzero diagonal entries.

The diagonal D can be represented by the 1-dimensional array $\mathbf{d}$ of the diagonal entries. Then the matrix multiplication $D\mathbf{x}$ is equivalent to the component-wise vector multiplication $\mathbf{d} * \mathbf{x} = \mathbf{x} * \mathbf{d}$. Likewise, the matrix multiplication $D^{-1}\mathbf{x}$ is equivalent to the component-wise "vector division" $\mathbf{x}/\mathbf{d}$.

Problem 1. Write a function that accepts a matrix A, a vector $\mathbf{b}$, a convergence tolerance ϵ, and a maximum number of iterations N. Implement the Jacobi method using (17.2), returning the approximate solution to the equation $A\mathbf{x} = \mathbf{b}$.

Run the iteration until $\|\mathbf{x}^{(k-1)} - \mathbf{x}^{(k)}\|_\infty < \epsilon$, and only iterate at most N times. Avoid using `la.inv()` to calculate D^{-1}, but use `la.norm()` to calculate the vector ∞-norm $\|\mathbf{x}\|_\infty = \sup |x_i|$.

```
>>> from scipy import linalg as la

>>> x = np.random.random(10)
>>> la.norm(x, ord=np.inf)          # Use la.norm() for ||x||.
0.74623726404168045
>>> np.max(np.abs(x))               # Use pure NumPy for ||x||.
0.74623726404168045
```

Your function should be robust enough to accept systems of any size. To test your function, use the following function to generate an $n \times n$ matrix A for which the Jacobi method is guaranteed to converge.

```
def diag_dom(n, num_entries=None):
    """Generate a strictly diagonally dominant nxn matrix.
    Inputs:
        n (int): The dimension of the system.
        num_entries (int): The number of nonzero values.
            Defaults to n^(3/2)-n.
    Returns:
        A ((n,n) ndarray): An nxn strictly diagonally dominant matrix.
    """
    if num_entries is None:
        num_entries = int(n**1.5) - n
    A = np.zeros((n,n))
    rows = np.random.choice(np.arange(0,n), size=num_entries)
    cols = np.random.choice(np.arange(0,n), size=num_entries)
    data = np.random.randint(-4, 4, size=num_entries)
```

```
    for i in range(num_entries):
        A[rows[i], cols[i]] = data[i]
    for i in range(n):
        A[i,i] = np.sum(np.abs(A[i])) + 1
    return A
```

Generate a random $\mathbf{b}$ with `np.random.random()`. Run the iteration, then check that $A\mathbf{x}^{(k)}$ and $\mathbf{b}$ are close using `np.allclose()`.

Also test your function on random $n \times n$ matrices. If the iteration is non-convergent, the successive approximations will have increasingly large entries.

Convergence

Most iterative methods only converge under certain conditions. For the Jacobi method, convergence mostly depends on the nature of the matrix A. If the entries a_{ij} of A satisfy the property

$$|a_{ii}| > \sum_{j \neq i} |a_{ij}| \text{ for all } i = 1, 2, \ldots, n$$

then A is called *strictly diagonally dominant* (for example, `diag_dom()` in Problem 1 generates a strictly diagonally dominant $n \times n$ matrix). If this is the case, then the Jacobi method always converges, regardless of the initial guess $\mathbf{x}_0$.[1] Other iterative methods, such as Newton's method, depend mostly on the initial guess.

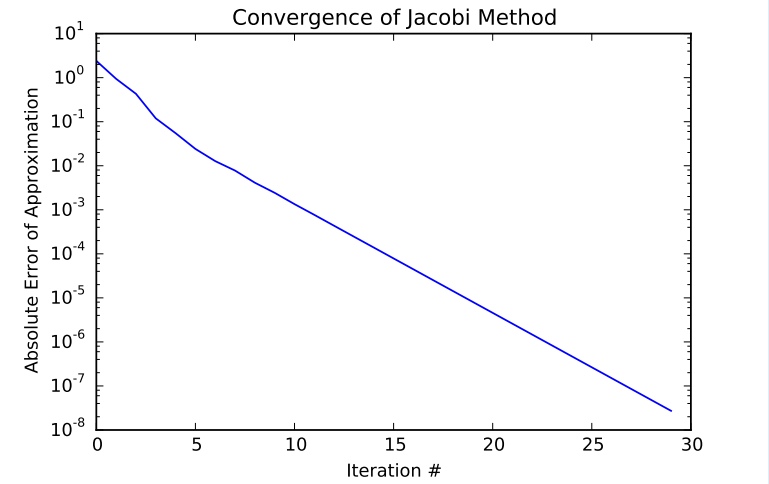
There are a few ways to determine whether or not an iterative method is converging. For example, since the approximation $\mathbf{x}^{(k)}$ should satisfy $A\mathbf{x}^{(k)} \approx \mathbf{b}$, the normed difference $\|A\mathbf{x}^{(k)} - \mathbf{b}\|_\infty$ should be small. This value is called the *absolute error* of the approximation. If the iterative method converges, the absolute error should decrease to ϵ.

Problem 2. Modify your Jacobi method function in the following ways:

1. Add a keyword argument called `plot`, defaulting to `False`.
2. Keep track of the absolute error $\|A\mathbf{x}^{(k)} - \mathbf{b}\|_\infty$ of the approximation for each value of k.
3. If `plot` is `True`, produce a lin-log plot of the error against iteration count (use `plt.semilogy()` instead of `plt.plot()`). Return the approximate solution $\mathbf{x}$ even if `plot` is `True`.

If the iteration converges, your plot should resemble the following figure.

[1] Although this seems like a strong requirement, most real-world linear systems can be represented by strictly diagonally dominant matrices.



The Gauss-Seidel Method

The Gauss-Seidel method is essentially a slight modification of the Jacobi method. The main difference is that in Gauss-Seidel, new information is used immediately. Consider the same system as in the previous section.

$$\begin{array}{rcrcrcr} 2x_1 & & & - & x_3 & = & 3 \\ -x_1 & + & 3x_2 & + & 2x_3 & = & 3 \\ & + & x_2 & + & 3x_3 & = & -1 \end{array}$$

As with the Jacobi method, solve for x_1 in the first equation, x_2 in the second equation, and x_3 in the third equation.

$$\begin{array}{rcl} x_1 & = & \frac{1}{2}(3 + x_3) \\ x_2 & = & \frac{1}{3}(3 + x_1 - 2x_3) \\ x_3 & = & \frac{1}{3}(-1 - x_2) \end{array}$$

Use $\mathbf{x}^{(0)}$ to compute $x_1^{(1)}$ in the first equation.

$$x_1^{(1)} = \frac{1}{2}(3 + x_3^{(0)}) = \frac{1}{2}(3 + 0) = \frac{3}{2}$$

Now, however, use the updated value of $x_1^{(1)}$ in the calculation of $x_2^{(1)}$.

$$x_2^{(1)} = \frac{1}{3}(3 + x_1^{(1)} - 2x_3^{(0)}) = \frac{1}{3}(3 + \frac{3}{2} - 0) = \frac{3}{2}$$

Likewise, use the updated values of $x_1^{(1)}$ and $x_2^{(1)}$ to calculate $x_3^{(1)}$.

$$x_3^{(1)} = \frac{1}{3}(-1 - x_2^{(1)}) = \frac{1}{3}(-1 - \frac{3}{2}) = -\frac{5}{6}$$

This process of using calculated information immediately is called *forward substitution*, and causes the algorithm to (generally) converge much faster.

	$x_1^{(k)}$	$x_2^{(k)}$	$x_3^{(k)}$
$x^{(0)}$	0	0	0
$x^{(1)}$	1.5	1.5	-0.833333
$x^{(2)}$	1.08333333	1.91666667	-0.97222222
$x^{(3)}$	1.01388889	1.98611111	-0.99537037
$x^{(4)}$	1.00231481	1.99768519	-0.9992284
$\vdots$	$\vdots$	$\vdots$	$\vdots$
$x^{(11)}$	1.00000001	1.99999999	-1
$x^{(12)}$	1	2	-1

Notice that Gauss-Seidel converged in less than half as many iterations.

Implementation

Because Gauss-Seidel updates only one element of the solution vector at a time, the iteration cannot be summarized by a single matrix equation. Instead, the process is most generally described by the following equation.

$$x_i^{(k+1)} = \frac{1}{a_{ii}}\left(b_i - \sum_{j<i} a_{ij}x_j^{(k)} - \sum_{j>i} a_{ij}x_j^{(k)}\right) \tag{17.3}$$

Let A_i be the ith row of A. The two sums closely resemble the regular vector product of A_i and $\mathbf{x}^{(k)}$ without the i^{th} term $a_{ii}x_i^{(k)}$. This gives a simplification.

$$\begin{aligned} x_i^{(k+1)} &= \frac{1}{a_{ii}}\left(b_i - A_i^\mathsf{T}\mathbf{x}^{(k)} + a_{ii}x_i^{(k)}\right) \\ &= x_i^{(k)} + \frac{1}{a_{ii}}\left(b_i - A_i^\mathsf{T}\mathbf{x}^{(k)}\right) \end{aligned} \tag{17.4}$$

One sweep through all the entries of $\mathbf{x}$ completes one iteration.

Problem 3. Write a function that accepts a matrix A, a vector $\mathbf{b}$, a convergence tolerance ϵ, a maximum number of iterations N, and a keyword argument `plot` that defaults to `False`. Implement the Gauss-Seidel method using (17.4), returning the approximate solution to the equation $A\mathbf{x} = \mathbf{b}$.

Use the same stopping criterion as in Problem 1. Also keep track of the absolute errors of the iteration, as in Problem 2. If `plot` is `True`, plot the error against iteration count. Use `diag_dom()` to generate test cases.

ACHTUNG!

Since the Gauss-Seidel algorithm operates on the approximation vector in place (modifying it one entry at a time), the previous approximation $\mathbf{x}^{(k-1)}$ must be stored at the beginning of the kth iteration in order to calculate $\|\mathbf{x}^{(k-1)} - \mathbf{x}^{(k)}\|_\infty$. Additionally, since NumPy arrays are mutable, the past iteration must be stored as a **copy**.

```
>>> x0 = np.random.random(5)        # Generate a random vector.
>>> x1 = x0                         # Attempt to make a copy.
>>> x1[3] = 1000                    # Modify the "copy" in place.
>>> np.allclose(x0, x1)             # But x0 was also changed!
True

# Instead, make a copy of x0 when creating x1.
>>> x0 = np.copy(x1)                # Make a copy.
>>> x1[3] = -1000
>>> np.allclose(x0, x1)
False
```

Convergence

Whether or not the Gauss-Seidel method converges depends on the nature of A. If all of the eigenvalues of A are positive, A is called *positive definite*. If A is positive definite *or* if it is strictly diagonally dominant, then the Gauss-Seidel method converges regardless of the initial guess $\mathbf{x}^{(0)}$.

Problem 4. The Gauss-Seidel method is faster than the standard system solver used by `la.solve()` if the system is sufficiently large and sufficiently sparse. For each value of $n = 5, 6, \ldots, 11$, generate a random $2^n \times 2^n$ matrix A using `diag_dom()` and a random 2^n vector $\mathbf{b}$. Time how long it takes to solve $A\mathbf{x} = \mathbf{b}$ using your Gauss-Seidel function from Problem 3, and how long it takes to solve using `la.solve()`.

Plot the times against the system size. Use log scales if appropriate.

Solving Sparse Systems Iteratively

Iterative solvers are best suited for solving very large sparse systems. However, using the Gauss-Seidel method on sparse matrices requires translating code from NumPy to `scipy.sparse`. The algorithm is the same, but there are some functions that are named differently between these two packages.

Problem 5. Write a new function that accepts a sparse matrix A, a vector $\mathbf{b}$, a convergence tolerance ϵ, and a maximum number of iterations N (plotting the convergence is not required for this problem). Implement the Gauss-Seidel method using (17.4), returning the approximate solution to the equation $A\mathbf{x} = \mathbf{b}$. Use the usual stopping criterion.

The Gauss-Seidel method requires extracting the rows A_i from the matrix A and computing $A_i^\mathsf{T}\mathbf{x}$. There are many ways to do this that cause some fairly serious runtime issues, so we provide the code for this specific portion of the algorithm.

```
# Get the indices of where the i-th row of A starts and ends if the
# nonzero entries of A were flattened.
rowstart = A.indptr[i]
rowend = A.indptr[i+1]

# Dot only the nonzero elements of the i-th row of A with the
# corresponding elements of x.
Aix = np.dot(A.data[rowstart:rowend], x[A.indices[rowstart:rowend]])
```

To test your function, cast the result of `diag_dom()` as a sparse matrix.

```
from scipy import sparse

>>> A = sparse.csr_matrix(diag_dom(50000))
>>> b = np.random.random(50000)
```

Successive Over-Relaxation (SOR)

Some systems meet the requirements for convergence with the Gauss-Seidel method, but do not converge very quickly. A slightly altered version of the Gauss-Seidel method, called *Successive Over-Relaxation*, can result in faster convergence. This is achieved by introducing a *relaxation factor*, ω. The iterative equation for Gauss-Seidel, (17.3) becomes the following.

$$x_i^{(k+1)} = (1-\omega)x_i^{(k)} + \frac{\omega}{a_{ii}}\left(b_i - \sum_{j<i} a_{ij}x_j^{(k)} - \sum_{j>i} a_{ij}x_j^{(k)}\right)$$

Simplifying the equation results in the following.

$$x_i^{(k+1)} = x_i^{(k)} + \frac{\omega}{a_{ii}}\left(b_i - A_i^\mathsf{T}\mathbf{x}^{(k)}\right) \tag{17.5}$$

Note that when $\omega = 1$, Successive Over-Relaxation reduces to Gauss-Seidel.

Problem 6. Write a function that accepts a sparse matrix A, a vector $\mathbf{b}$, a relaxation factor ω, a convergence tolerance ϵ, and a maximum number of iterations N. Implement Successive Over-Relaxation using (17.5), returning the approximate solution to the equation $A\mathbf{x} = \mathbf{b}$. Use the usual stopping criterion.
(Hint: this requires changing only one line of code from the sparse Gauss-Seidel function.)

A Finite Difference Method

Laplace's equation is an important partial differential equation that arises often in both pure and applied mathematics. In two dimensions, the equation has the following form.

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \tag{17.6}$$

Laplace's equation can be used to model heat flow. Consider a square metal plate where the top and bottom borders are fixed at 0° Celsius and the left and right sides are fixed at 100° Celsius. Given these boundary conditions, we want to describe how heat diffuses through the rest of the plate. The solution to Laplace's equation describes the plate when it is in a *steady state*, meaning that the heat at a given part of the plate no longer changes with time.

It is possible to solve (17.6) analytically. However, the problem can also be solved numerically using a *finite difference method*. To begin, we impose a discrete, square grid on the plate with uniform spacing. Denote the points on the grid by (x_i, y_j) and the value of u at these points (the heat) as $u(x_i, y_j) = U_{i,j}$. Using the centered difference quotient for second derivatives,

$$\begin{aligned} 0 &= \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \\ &\approx \frac{U_{i+1,j} - 2U_{i,j} + U_{i-1,j}}{h^2} + \frac{U_{i,j+1} - 2U_{i,j} + U_{i,j-1}}{h^2} \\ &= \frac{1}{h^2}\left(-4U_{i,j} + U_{i+1,j} + U_{i-1,j} + U_{i,j+1} + U_{i,j-1}\right), \end{aligned} \tag{17.7}$$

where $h = x_{i+1} - x_i = y_{j+1} - y_j$ is the distance between the grid points in either direction.

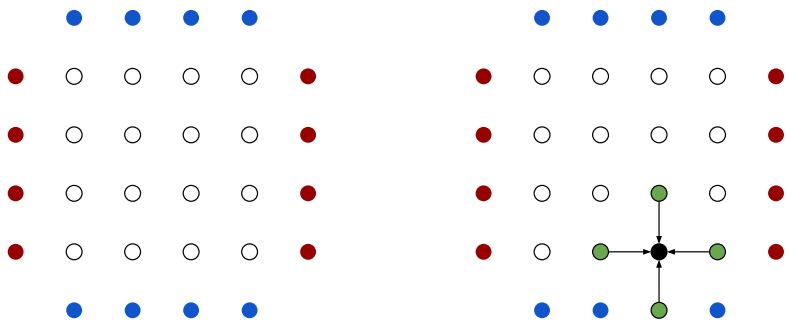


Figure 17.1: On the left, an example of a 6×6 grid ($n = 4$) where the red dots are hot boundary zones and the blue dots are cold boundary zones. On the right, the green dots are the neighbors of the interior black dot that are used to approximate the heat at the black dot.

This problem can be formulated as a linear system. Suppose the grid has exactly $(n+2)\times(n+2)$ entries. Then the interior of the grid (where $u(x, y)$ is unknown) is $n \times n$, and can be flattened into an $n^2 \times 1$ vector $\mathbf{u}$. The entire first row goes first, then the second row, proceeding to the n^{th} row.

$$\mathbf{u} = [U_{1,1},\ U_{1,2},\ \cdots,\ U_{1,n},\ U_{2,1},\ U_{2,2},\ \cdots,\ U_{2,n}\ \ldots,\ U_{n,n}]^\mathsf{T}$$

From (17.7), we have the following for an interior point $U_{i,j}$.

$$-4U_{i,j} + U_{i+1,j} + U_{i-1,j} + U_{i,j+1} + U_{i,j-1} = 0 \tag{17.8}$$

If any of the neighbors to $U_{i,j}$ is a boundary point on the grid, its value is already determined by the boundary conditions. For example, for $U_{3,1}$, the neighbor $U_{3,0} = 100$, so

$$-4U_{3,1} + U_{2,1} + U_{3,2} + U_{4,1} = -100.$$

The constants on the right side of (17.8) become the $n^2 \times 1$ vector $\mathbf{b}$. All nonzero entries of $\mathbf{b}$ correspond to interior points that touch the left or right boundaries.

For example, writing (17.8) for the 16 interior points of the grid in Figure 17.1 results in the following 16×16 system $A\mathbf{u} = \mathbf{b}$. Note the block structure (empty blocks are all zeros).

$$\left[\begin{array}{cccc|cccc|cccc|cccc}
-4 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & & & & & & & & \\
1 & -4 & 1 & 0 & 0 & 1 & 0 & 0 & & & & & & & & \\
0 & 1 & -4 & 0 & 0 & 0 & 1 & 0 & & & & & & & & \\
0 & 0 & 1 & -4 & 0 & 0 & 0 & 1 & & & & & & & & \\
\hline
1 & 0 & 0 & 0 & -4 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & & & & \\
0 & 1 & 0 & 0 & 1 & -4 & 1 & 0 & 0 & 1 & 0 & 0 & & & & \\
0 & 0 & 1 & 0 & 0 & 1 & -4 & 1 & 0 & 0 & 1 & 0 & & & & \\
0 & 0 & 0 & 1 & 0 & 0 & 1 & -4 & 0 & 0 & 0 & 1 & & & & \\
\hline
 & & & & 1 & 0 & 0 & 0 & -4 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\
 & & & & 0 & 1 & 0 & 0 & 1 & -4 & 1 & 0 & 0 & 1 & 0 & 0 \\
 & & & & 0 & 0 & 1 & 0 & 0 & 1 & -4 & 1 & 0 & 0 & 1 & 0 \\
 & & & & 0 & 0 & 0 & 1 & 0 & 0 & 1 & -4 & 0 & 0 & 0 & 1 \\
\hline
 & & & & & & & & 1 & 0 & 0 & 0 & -4 & 1 & 0 & 0 \\
 & & & & & & & & 0 & 1 & 0 & 0 & 1 & -4 & 1 & 0 \\
 & & & & & & & & 0 & 0 & 1 & 0 & 0 & 1 & -4 & 1 \\
 & & & & & & & & 0 & 0 & 0 & 1 & 0 & 0 & 1 & -4
\end{array}\right]
\left[\begin{array}{c} U_{1,1} \\ U_{1,2} \\ U_{1,3} \\ U_{1,4} \\ U_{2,1} \\ U_{2,2} \\ U_{2,3} \\ U_{2,4} \\ U_{3,1} \\ U_{3,2} \\ U_{3,3} \\ U_{3,4} \\ U_{4,1} \\ U_{4,2} \\ U_{4,3} \\ U_{4,4} \end{array}\right]
=
\left[\begin{array}{c} -100 \\ 0 \\ 0 \\ -100 \\ -100 \\ 0 \\ 0 \\ -100 \\ -100 \\ 0 \\ 0 \\ -100 \\ -100 \\ 0 \\ 0 \\ -100 \end{array}\right]$$

More concisely, for any positive integer n, the matrix A can be written as

$$A = \begin{bmatrix} B & I & & & \\ I & B & I & & \\ & I & \ddots & \ddots & \\ & & \ddots & \ddots & I \\ & & & I & B \end{bmatrix}, \quad \text{where } B = \begin{bmatrix} -4 & 1 & & & \\ 1 & -4 & 1 & & \\ & 1 & \ddots & \ddots & \\ & & \ddots & \ddots & 1 \\ & & & 1 & -4 \end{bmatrix} \text{ is } n \times n.$$

Problem 7. Write a function that accepts an integer n, a relaxation factor ω, a convergence tolerance ϵ that defaults to 10^{-8}, a maximum number of iterations N that defaults to 100, and a bool `plot` that defaults to `False`. Generate and solve the corresponding system $A\mathbf{u} = \mathbf{b}$ using Problem 6.
(Hint: see Problem 5 of Linear Systems. Also, `np.tile()` may be useful for constructing $\mathbf{b}$.)

If `plot=True`, visualize the solution $\mathbf{u}$ with a heatmap using `plt.pcolormesh()` (the colormap `"seismic"` is a good choice in this case). This shows the distribution of heat over the hot plate after it has reached its steady state. Note that the $\mathbf{u}$ must be reshaped as an $n \times n$ array to properly visualize the result.

Problem 8. To demonstrate how convergence is affected by the value of the relaxation factor ω in SOR, time your function from Problem 7 with $\omega = 1,\ 1.05,\ 1.1,\ \ldots, 1.9, 1.95$ and $n = 20$. Plot the times as a function of ω.

Note that the matrix A is not strictly diagonally dominant. However, A is positive definite, so the algorithm will converge. Unfortunately, convergence for these kinds of systems usually requires more iterations than for strictly diagonally dominant systems. Therefore, set `tol=1e-2` and `N = 1000`.

Recall that $\omega = 1$ corresponds to the Gauss-Seidel method. Choosing a more optimal relaxation factor saves a large number of iterations. This could translate to saving days or weeks of computation time while solving extremely large linear systems on a supercomputer.

18 GMRES

Lab Objective: *In this lab we will learn how to use the GMRES algorithm.*

The GMRES ("Generalized Minimal Residuals") algorithm is an efficient way to solve large linear systems. It is an iterative method that uses Krylov subspaces to reduce a high-dimensional problem to a sequence of smaller dimensional problems.

The GMRES Algorithm

Let A be an invertible $m \times m$ matrix and let $\mathbf{b}$ be an m-vector. Let $\mathcal{K}_n(A, \mathbf{b})$ be the order-n Krylov subspace generated by A and $\mathbf{b}$. The idea of the GMRES algorithm is that instead of solving $A\mathbf{x} = \mathbf{b}$ directly, we use least squares to find $\mathbf{x}_n \in \mathcal{K}_n$ that minimizes the residual $r_n = \|\mathbf{b} - A\mathbf{x}_n\|_2$. The algorithm returns when this residual is sufficiently small. In good circumstances, this will happen when n is still much less than m.

The GMRES algorithm is implemented with the Arnoldi iteration for numerical stability. The Arnoldi iteration produces H_n, an $(n+1)\times n$ upper Hessenberg matrix, and Q_n, the matrix containing the basis vectors of $\mathcal{K}_n(A, \mathbf{b})$, such that $AQ_n = Q_{n+1}H_n$. We are looking for $\mathbf{x}_n = Q_n\mathbf{y}_n + \mathbf{x}_0$ for some $\mathbf{y}_n \in \mathbb{R}^n$ which minimizes the norm of $\mathbf{b} - A\mathbf{x}_n$. Since the columns of Q are orthonormal, we can compute the residual equivalently as

$$\|\mathbf{b} - A\mathbf{x}_n\|_2 = \|Q_{n+1}(\beta e_1 - H_n\mathbf{y}_n)\|_2 = \|H_n\mathbf{y}_n - \beta e_1\|_2. \tag{18.1}$$

Here $\mathbf{e}_1$ is the vector $(1, 0, \dots, 0)$ of length $n + 1$. β is the Euclidean norm of $\mathbf{b} - A\mathbf{x}_0$, where $\mathbf{x}_0$ is an initial arbitrary guess of the solution. (Ordinarily this guess is zero, and then the $A\mathbf{x}_0$ could be left out; however, a modified version of the algorithm will be discussed at the end of the lab, in which other nonzero guesses will be made.) Thus to minimize the left side of 18.1, we can minimize the right, and $\mathbf{x}_n$ can be computed as $Q_n\mathbf{y}_n + \mathbf{x}_0$.

This algorithm is outlined in Algorithm 18.1. For a complete derivation see [TODO: ref textbook].

Problem 1. Use Algorithm 18.1 to complete the following Python function implementing the GMRES algorithm.

```
def gmres(A, b, x0, k=100, tol=1e-8):
```

Algorithm 18.1 The GMRES algorithm. This algorithm operates on a vector $\mathbf{b}$ and matrix A. It iterates k times or until the residual is less than tol, returning an approximate solution to $A\mathbf{x} = \mathbf{b}$ and the error in this approximation.

procedure GMRES($A, \mathbf{b}, \mathbf{x}_0, k, tol$)
  $Q \leftarrow \text{empty}(\text{size}(\mathbf{b}), k+1)$ ▷ Initialize
  $H \leftarrow \text{zeros}(k+1, k)$
  $r_0 \leftarrow \mathbf{b} - A\mathbf{x}_0$
  $Q[:, 0] = r_0 / \|r_0\|_2$
  for $n = 1 \dots k$ **do**
    Set entries of Q and H as in Arnoldi iteration.
    Compute the residual res and the least squares solution $\mathbf{y}_n$ for the part of H so far created (equation 18.1).
    if $res < tol$ **then**
      return $Q[:, :n+1]\mathbf{y} + \mathbf{x}_0,\ res$
  return $Q[:, :n+1]\mathbf{y} + \mathbf{x}_0,\ res$

```
'''Calculate approximate solution of Ax=b using GMRES algorithm.

INPUTS:
A    - Callable function that calculates Ax for any input vector x.
b    - A NumPy array of length m.
x0   - An arbitrary initial guess.
k    - Maximum number of iterations of the GMRES algorithm. Defaults
       to 100.
tol  - Stop iterating if the residual is less than 'tol'. Defaults to
       1e-8.

RETURN:
Return (y, res) where 'y' is an approximate solution to Ax=b and 'res'
is the residual.

Examples:
>>> a = np.array([[1,0,0],[0,2,0],[0,0,3]])
>>> A = lambda x: a.dot(x)
>>> b = np.array([1, 4, 6])
>>> x0 = np.zeros(b.size)
>>> gmres(A, b, x0)
(array([ 1.,  2.,  2.]), 1.09808907533e-16)
'''
```

You may assume that the input `b` is a real array and the function `A()` always outputs real arrays.

Hint: Use `numpy.linalg.lstsq()` to solve the least squares problem. Be sure to read the documentation so you know what the function returns to you.

Convergence of GMRES

At the n-th iteration, GMRES computes the best approximate solution $\mathbf{x} \in \mathcal{K}_n$ to $A\mathbf{x} = \mathbf{b}$. If A is full rank, then $\mathcal{K}_m = \mathbb{F}^m$, so the m^{th} iteration will always return an exact answer. However, we say the algorithm converges after n steps if the n^{th} residual is sufficiently small.

The rate of convergence of GMRES depends on the eigenvalues of A.

Problem 2. Implement the following Python function by modifying your solution to Problem 1.

```
def plot_gmres(A, b, x0, tol=1e-8):
    '''Use the GMRES algorithm to approximate the solution to Ax=b. Plot ↩
        the eigenvalues of A and the convergence of the algorithm.

    INPUTS:
    A   - A 2-D NumPy array of shape mxm.
    b   - A 1-D NumPy array of length m.
    x0  - An arbitrary initial guess.
    tol - Stop iterating and create the desired plots when the residual is
          less than 'tol'. Defaults to 1e-8.

    OUTPUT:
    Follow the GMRES algorithm until the residual is less than tol, for a
    maximum of m iterations. Then create the two following plots (subplots
    of a single figure):

    1. Plot the eigenvalues of A in the complex plane.

    2. Plot the convergence of the GMRES algorithm by plotting the
    iteration number on the x-axis and the residual on the y-axis.
    Use a log scale on the y-axis.
    '''
```

Use this function to investigate the convergence of GMRES as follows. Define an $m \times m$ matrix

$$A_n = nI + P,$$

where I is the $m \times m$ identity matrix and P is a $m \times m$ matrix of numbers from a random normal distribution with mean 0 and standard deviation $1/(2\sqrt{m})$. Write a function that calls `plot_gmres` on A_n for $n = -4, -2, 0, 2, 4$. Use $m = 200$, let `b` be an array of ones, and let `x0` be the zero vector or anything else that suits you. How does the convergence of the GMRES algorithm relate to the eigenvalues?

Hints:

1. Create a plot with a log scale on the y-axis with `plt.yscale('log')`.
2. Create a matrix with entries from a random normal distribution with `np.random.normal()`. Read the documentation for more information.

3. Note that the parameter A required here is not a callable function but a matrix; this is to allow the finding of the eigenvalues.

4. Output for $n = 2$, $m = 200$ is in Figure 18.1 below.

Ideas for this problem were taken from Example 35.1 on p. 271 of [**Trefethen1997**].

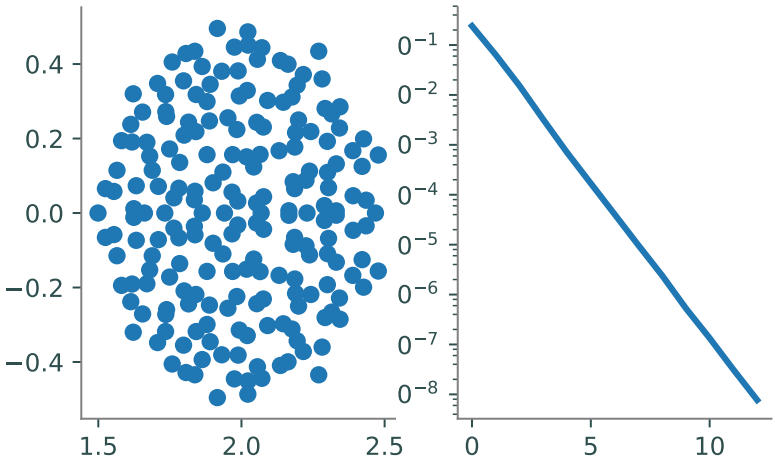


Figure 18.1: The left plot is the eigenvalues of the matrix A_2, which is defined in Problem 2. The right plot is the convergence of the GMRES algorithm on A_2 with starting vector $\mathbf{b} = (1, 1, \ldots, 1)$. This figure is one possible output of the function `plot_gmres()`.

Improving GMRES

There are many ways to make the GMRES algorithm more robust and efficient.

Breakdowns in GMRES

One of the selling points of GMRES is that it can't break down unless it reaches an exact solution. In other words, the only way GMRES could break down is if a vector found by the Arnoldi iteration is 0. That is, suppose, we have already computed

$$\mathcal{K}_n(A, \mathbf{b}) = \text{span}\{\mathbf{b}, A\mathbf{b}, \ldots, A^{n-1}\mathbf{b}\} = \text{span}\{\mathbf{q}_1, \ldots, \mathbf{q}_n\}.$$

We next compute $A^n\mathbf{b}$ and orthogonalize it against $\mathcal{K}_n(A, \mathbf{b})$, yielding $\mathbf{q}_{n+1}$. But if $A^n\mathbf{b} \in \mathcal{K}_n(A, \mathbf{b})$ then $\mathbf{q}_{n+1}$ will be 0, and our algorithm will break when we try to normalize $\mathbf{q}_{n+1}$.

In this situation, the least squares solution to (18.1) is an *exact* solution to $A\mathbf{x} = \mathbf{b}$. In other words, $\mathbf{b}$ is in the $\text{span}\{\mathbf{q}_1, \ldots, \mathbf{q}_n\}$. Fortunately, precautions against this have been taken in our implementation of the Arnoldi algorithm.

GMRES with Restarts

The first few iterations of GMRES have low spatial and temporal complexity. However, as k increases, the k^{th} iteration of GMRES becomes more expensive in both time and memory. In fact, computing the k^{th} iteration of GMRES for very large k can be prohibitively complex.

This issue is addressed by using GMRES(k), or GMRES with restarts. When k becomes large, this algorithm restarts GMRES but with an improved initial guess. GMRES with restarts is outlined in Algorithm 18.2.

Algorithm 18.2 The GMRES(k) algorithm. This algorithm performs GMRES on a vector $\mathbf{b}$ and matrix A. It iterates k times before restarting. It terminates after *restarts* restarts or when the residual is less than *tol*, returning an approximate solution to $A\mathbf{x} = \mathbf{b}$ and the error in this approximation.

procedure GMRES(K)$(A, \mathbf{b}, \mathbf{x}_0, k, tol, restarts)$
  $n \leftarrow 0$ ▷ Initialize
  while $n \leq restarts$ **do**
    Perform the GMRES algorithm, obtaining a least squares solution $\mathbf{y}$.
    If the desired tolerance was reached, return. Otherwise, continue.
    $\mathbf{x}_0 \leftarrow \mathbf{y}$
    $n \leftarrow n + 1$
  return $\mathbf{y}$, res ▷ Return the approximate solution and the residual

The algorithm GMRES(k) will always have manageable spatial and temporal complexity, but it is less reliable than GMRES. If the true solution $\mathbf{x}$ to $A\mathbf{x} = \mathbf{b}$ is nearly orthogonal to the Krylov subspaces $\mathcal{K}_n(A, \mathbf{b})$ for $n \leq k$, then GMRES(k) could converge very slowly or not at all.

Problem 3. Implement Algorithm 18.2 with the following function.

```
def gmres_k(A, b, x0, k=5, tol=1E-8, restarts=50):
    '''Use the GMRES(k) algorithm to approximate the solution to Ax=b.

    INPUTS:
    A        - A callable function that calculates Ax for any vector x.
    b        - A NumPy array.
    x0       - An arbitrary initial guess.
    k        - Maximum number of iterations of the GMRES algorithm before
               restarting. Defaults to 5.
    tol      - Stop iterating if the residual is less than 'tol'. Defaults
               to 1E-8.
    restarts - Maximum number of restarts. Defaults to 50.

    RETURN:
    Return (y, res) where 'y' is an approximate solution to Ax=b and 'res'
    is the residual.
    '''
```

Compare the speed of `gmres()` from Problem 1 and `gmres_k()` on the matrices in Problem 2.

GMRES in SciPy

The GMRES algorithm is implemented in SciPy as the function `scipy.sparse.linalg.gmres()`. Here we use this function to solve $A\mathbf{x} = \mathbf{b}$ where A is a random 300×300 matrix and $\mathbf{b}$ is a random vector.

```
>>> import numpy as np
>>> from scipy import sparse as spar
>>> from scipy import linalg as la
>>>
>>> A = np.random.rand(300, 300)
>>> b = np.random(300)
>>> x, info = spar.linalg.gmres(A, b)
>>> info
3000
```

The function outputs two objects: the approximate solution `x` and a constant `info` telling if the function converged. If `info=0` then convergence occured; if `info` is positive then it equals the number of iterations performed. In this case, the function performed 3000 iterations of GMRES before returning the approximate solution `x`. We can check how close the solution is.

```
>>> la.norm(A.dot(x)-b)
4.744196381683801
```

We can get a better approximation using GMRES with restarts.

```
>>> # Restart after 1000 iterations
>>> x, info = spar.linalg.gmres(A, b, restart=1000)
>>> info
0
>>> la.norm(A.dot(x)-b)
1.0280404494143551e-12
```

This time, the returned approximation `x` is about as close to a true solution as we could hope for.

19 The Arnoldi Iteration

Lab Objective: *Use Krylov subspaces to find eigenvalues of extremely large matrices.*

One of the biggest difficulties in computational linear algebra is the amount of memory needed to store a large matrix and the amount of time needed to read its entries. Methods using Krylov subspaces avoid this difficulty by studying how a matrix acts on vectors, making it unnecessary in many cases to create the matrix itself.

The *Arnoldi iteration* is an algorithm for finding an orthonormal basis of a Krylov subspace. One of its strengths is it can run on any linear operator without knowing the operator's underlying matrix representation. The outputs of the Arnoldi algorithm can be used to approximate the eigenvalues of the matrix of the linear operator.

Krylov Subspaces

The order-N Krylov subspace of A generated by $\mathbf{x}$ is

$$\mathcal{K}_n(A, \mathbf{x}) = \text{span}\{\mathbf{x}, A\mathbf{x}, A^2\mathbf{x}, \dots, A^{n-1}\mathbf{x}\}.$$

If the vectors $\{\mathbf{x}, A\mathbf{x}, A^2\mathbf{x}, \dots, A^{n-1}\mathbf{x}\}$ are linearly independent, then they form a basis for $\mathcal{K}_n(A, \mathbf{x})$. However, this basis is usually far from orthogonal, and hence computations using this basis will likely be ill-conditioned.

The Arnoldi Iteration Algorithm

One way to find an orthonormal basis for $\mathcal{K}_n(A, \mathbf{x})$ is to use the modified Gram-Schmidt algorithm from Lab 3 on the set $\{\mathbf{x}, A\mathbf{x}, A^2\mathbf{x}, \dots, A^{n-1}\mathbf{x}\}$. The Arnold iteration does this more efficiently by integrating the creation of $\{\mathbf{x}, A\mathbf{x}, A^2\mathbf{x}, \dots, A^{n-1}\mathbf{x}\}$ with the modified Gram-Schmidt algorithm. It returns an orthonormal basis for $\mathcal{K}_n(A, \mathbf{x})$. This algorithm is described in Algorithm 19.1.

In Algorithm 19.1, k is the number of times we multiply by A. This will result in an order-$k+1$ Krylov subspace.

Something perhaps unexpected happens in the Arnoldi iteration if the starting vector $\mathbf{x}$ is an eigenvector of A. If the corresponding eigenvalue is λ, then by definition $\mathcal{K}_k(A, \mathbf{x}) = \text{span}\{\mathbf{x}, \lambda\mathbf{x}, \lambda^2\mathbf{x}, \dots, \lambda^k\mathbf{x}\}$, which is equal to the span of $\mathbf{x}$. Let us trace through Algorithm 19.1 in this case. We will use $\mathbf{q}_i$ to denote the i^{th} column of Q.

Algorithm 19.1 The Arnoldi Iteration. This algorithm accepts a square matrix A and starting vector $\mathbf{b}$. It iterates k times or until the norm of the next vector in the iteration is less than tol. The algorithm returns upper Hessenberg H and orthonormal Q such that $H = Q^{\mathsf{H}}AQ$.

```
1:  procedure ARNOLDI(b, A, k, tol)
2:      Q ← empty(size(b), k + 1)                    ▷ Some initialization steps
3:      H ← zeros(k + 1, k)
4:      Q[:, 0] ← b/‖b‖_2
5:      for j = 0 ... k − 1 do                       ▷ Perform the actual iteration.
6:          Q[:, j + 1] ← AQ[:, j]
7:          for i = 0 ... j do                       ▷ Modified Gram-Schmidt.
8:              H[i, j] ← Q[:, i]^T Q[:, j + 1]
9:              Q[:, j + 1] ← Q[:, j + 1] − H[i, j]Q[:, i]
10:         H[j + 1, j] ← ‖Q[:, j + 1]‖_2            ▷ Set subdiagonal element of H.
11:         if |H[j + 1, j]| < tol then              ▷ Stop if ‖Q[:, j + 1]‖_2 is too small.
12:             return H[: j + 1, : j + 1], Q[:, : j + 1]
13:         Q[:, j + 1] ← Q[:, j + 1]/H[j + 1, j]    ▷ Normalize q_{j+1}.
14:     return H[: −1, :], Q                         ▷ Return H_k.
```

In line 4 we normalize $\mathbf{x}$, setting $\mathbf{q}_1 = \mathbf{x}/\|\mathbf{x}\|$. In line 6 we set $\mathbf{q}_2 = A\mathbf{q}_1 = \lambda\mathbf{q}_1$. Then in line 8

$$H_{1,1} = \langle \mathbf{q}_1, \mathbf{q}_2 \rangle = \langle \mathbf{q}_1, \lambda\mathbf{q}_1 \rangle = \lambda \langle \mathbf{q}_1, \mathbf{q}_1 \rangle = \lambda,$$

so in line 9 we subtract $\lambda\mathbf{q}_1$ from $\mathbf{q}_2$, ending with $\mathbf{q}_2 = 0$.

The vector $\mathbf{q}_2$ is supposed to be the next vector in the orthonormal basis for $\mathcal{K}_k(A, \mathbf{x})$, but since it is 0, it is not linearly independent of $\mathbf{q}_1$. In fact, $\mathbf{q}_1$ already spans $\mathcal{K}_k(A, \mathbf{x})$. Hence, when in line 11 we find that the norm of $\mathbf{q}_2$ is zero (or close to it, allowing for numerical error), we terminate the algorithm early, returning the 1×1 matrix $H = H_{1,1} = \lambda$ and the $n \times 1$ matrix $Q = \mathbf{q}_1$.

A similar phenomenon may occur if the starting vector $\mathbf{x}$ is contained in a proper invariant subspace of A.

Arnoldi Iteration on Linear Operators

A major strength of the Arnoldi Iteration is that it can run on a linear operator, even without knowing the matrix representation of the operator. If A_{mul} is some linear function, then we can modify the pseudocode above by replacing $AQ[:, j]$ with $A_{mul}(Q[:, j])$. This will make it possible to find the eigenvalues of an arbitrary linear transformation. We will use this method in the problem below.

Problem 1. Using Algorithm 19.1, complete the following Python function that performs the Arnoldi iteration. Write this function so that it can run on complex arrays.

```
def arnoldi(b, Amul, k, tol=1e-8):
    """Perform `k' steps of the Arnoldi iteration on the linear operator
    defined by `Amul', starting with the vector 'b'.

    Inputs:
```

```
        b (ndarray): The starting vector for the iteration.
        Amul (function): A function handle that describes a linear ↩
            operator.
        k (int): The number of times to perform the iteration.
        tol (float): Stop iterating if the next vector in the iteration ↩
            has
            norm less than `tol'. Defaults to 1e-8.

    Returns:
        H_n (ndarray)
        Q_n (ndarray)
            The number n will equal k, unless the algorithm terminated ↩
                early,
            in which case n will be less than k.

    Examples:
        >>> A = np.array([[1,0,0],[0,2,0],[0,0,3]])
        >>> Amul = lambda x: A.dot(x)
        >>> H, Q = arnoldi(np.array([1,1,1]), Amul, 3)
        >>> np.allclose(H, np.conjugate(Q.T).dot(A).dot(Q) )
        True

        >>> H, Q = arnoldi(np.array([1,0,0]), Amul, 3)
        >>> H
        array([[ 1.+0.j]])
        >>> np.conjugate(Q.T).dot(A).dot(Q)
        array([[ 1.+0.j]])
    """
```

Hints:

1. Since `H` and `Q` will eventually hold complex numbers, initialize them as complex arrays (e.g., `A = np.empty((3,3), dtype=np.complex128)`).
2. Remember to use complex inner products.
3. This function can be tested on a matrix A by passing in `A.dot` for `Amul`.

Finding Eigenvalues Using Arnoldi Iteration

Let A be an $n \times n$ matrix. Let Q_k be the matrix whose columns $\mathbf{q}_1, \ldots, \mathbf{q}_k$ are the orthonormal basis for $\mathcal{K}_m(A, \mathbf{x})$ generated by the Arnoldi algorithm, and let H_k be the $k \times k$ upper Hessenburg matrix defined at the k^{th} stage of the algorithm. Then these matrices satisfy

$$H_k = Q_k^{\mathsf{H}} A Q_k. \tag{19.1}$$

If $k < n$, then H_k is a low-rank approximation to A. We may use its eigenvalues as approximations to the eigenvalues of A. The eigenvalues of H_k are called *Ritz values*, and in fact they converge quickly to the largest eigenvalues of A.

Problem 2. Finish the following function that computes the Ritz values of a matrix.

```
def ritz(Amul, dim, k, iters):
    """Find `k' Ritz values of the linear operator defined by `Amul'.

    Inputs:
        Amul (function): A function describing a linear operator on R^(dim↩
            ).
        dim (int): The dimension of the space on which `Amul' acts.
        k (int): The number of Ritz values to return.
        iters (int): The number of times to perform the Arnoldi iteration.
            Must be between `k' and `dim'.

    Returns:
        ((k,) ndarray): `k' Ritz values of the operator defined by `Amul.'
    """
```

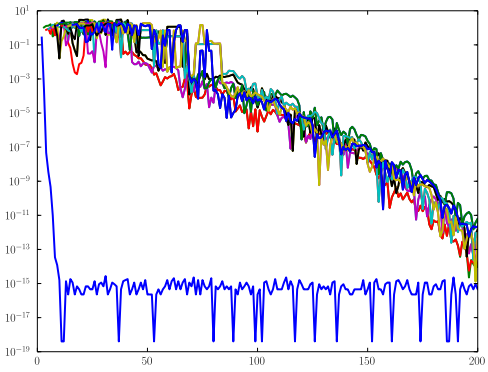
One application of the Arnoldi iteration is to find the eigenvalues of linear operators that are too large to store in memory. For example, if an operator acts on $\mathbb{C}^{2^{20}}$, then its matrix representation contains 2^{40} complex values. Storing such a matrix would require 64 terabytes of memory!

An example of such an operator is the Fast Fourier Transform, cited by SIAM as one of the top algorithms of the century [**Cipra2000**]. The Fast Fourier Transform is used ubiquitously in the field of signal processing.

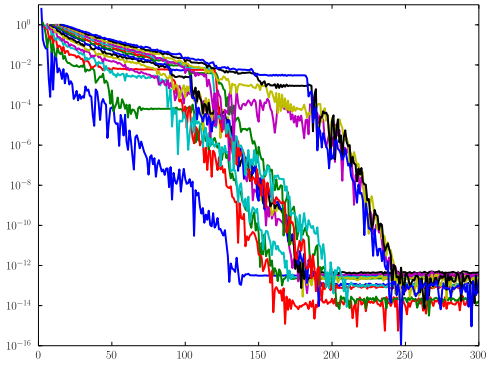
Problem 3. The four largest eigenvalues of the Fast Fourier Transform are known to be $\{-\sqrt{N}, \sqrt{N}, -i\sqrt{N}, i\sqrt{N}\}$ where N is the dimension of the space on which the transform acts. Use your function `ritz()` from Problem 2 to approximate the eigenvalues of the Fast Fourier Transform. Set `k` to be 10 and set `dim` to be 2^{20}. For the argument `Amul`, use the `fft` function from `scipy.fftpack`.

The Arnoldi iteration for finding eigenvalues is implemented in a Fortran library called ARPACK. SciPy interfaces with the Arnoldi iteration in this library via the function `scipy.sparse.linalg.eigs()`. This function has many more options than the implementation we wrote in Problem 2. In this example, the keyword argument `k=5` specifies that we want five Ritz values. Note that even though this function comes from the `sparse` library in SciPy, we can still call it on regular NumPy arrays.

```
>>> B = np.random.rand(10000).reshape(100, 100)
>>> sp.sparse.linalg.eigs(B, k=5, return_eigenvectors=False)
array([ -1.15577072-2.59438308j,  -2.63675878-1.09571889j,
        -2.63675878+1.09571889j,  -3.00915592+0.j        ,  50.14472893+0.j ])
```



(a) The blue line plots the error of the Ritz value of largest magnitude. This eigenvalue converges after fewer than 20 iterations



(b) All Ritz values have roughly equivalent magnitude. They take from 150 to 250 iterations to converge.

Figure 19.1: These plots show the relative error of the Ritz values as approximations to the eigenvalues of a matrix. The figure at left plots the largest 15 Ritz values for a 500×500 matrix with random entries. The figure at right plots the largest 15 Ritz values for a 500×500 matrix with uniformly distributed eigenvalues.

Convergence

The Arnoldi method for finding eigenvalues quickly converges to eigenvalues whose magnitude is distinctly larger than the rest. For example, matrices with random entries tend to have one eigenvalue of distinctly greatest magnitude. Convergence of the Ritz values for such a matrix is plotted in Figure 19.1a.

However, Ritz values converge more slowly for matrices with random eigenvalues. Figure 19.1b plots convergence of the Ritz values for a matrix with eigenvalues uniformly distributed in $[0, 1)$.

Problem 4. Finish the following function to visualize the convergence of the Ritz values.

```
def plot_ritz(A, n, iters):
    """Plot the relative error of the Ritz values of `A'. Use the number ↩
       of
    iterations as the x-axis and the relative error of the Ritz values of ↩
       H_k
    a approximations to the eigenvalues of A as the y-axis.

    Inputs:
        A (ndarray)
        n (int): The number of Ritz values to plot.
        iters (int): The number of times to perform the Arnoldi iteration.
    """
```

If $\tilde{\mathbf{x}}$ is an an approximation to $\mathbf{x}$, then the *absolute error* in the approximation is

$$\frac{\|\mathbf{x} - \tilde{\mathbf{x}}\|}{\|\mathbf{x}\|}.$$

Hint: The most difficult part of this problem is to identify which Ritz values correspond to which eigenvalues. After finding the Ritz values (or eigenvalues) of largest magnitude, use `np.sort()` to put them in order. Make sure that this order is preserved throughout your program.

It may help to use the following algorithm.

1. Find n eigenvalues of A of largest magnitude. Store these in order.
2. Create an empty array to store the relative errors. For every $k \in$`[1, iters)`,
   (a) Compute H_k with the Arnoldi iteration.
   (b) Find n eigenvalues of A of largest magnitude. Note that for small k, the matrix H_k may not have this many eigenvalues.
   (c) Store the absolute error. Make sure that the errors are stored in the correct order. For small k, some entries in the row or column may not be used.
3. Use array broadcasting to compute the absolute error.
4. Iteratively plot the errors. Lines for distinct eigenvalues should start at different places on the x-axis.

Run your function on these examples. The plots should be fairly similar to Figures 19.1b and 19.1a.

```
>>> # A matrix with random entries
>>> A = np.random.rand(300, 300)
>>> plot_ritz(A, 10, 175)
>>>
>>> # A matrix with uniformly distributed eigenvalues
>>> D = np.diag(np.random.rand(300))
>>> B = A.dot( D.dot(la.inv(A)) )
>>> plot_ritz(B, 10, 175)
```

If your code takes too long to run, consider integrating your solutions to Problems 1 and 2 with the body of this function.

Lanczos Iteration (Optional)

The Lanczos iteration is a version of the Arnoldi iteration that is optimized to operate on symmetric matrices. If A is symmetric, then (19.1) shows that H_k is symmetric and hence tridiagonal. This leads to two simplifications of the Arnoldi algorithm.

First, we have $0 = H_{k,n} = \langle \mathbf{q}_k, A\mathbf{q}_n \rangle$ for $k \leq n-2$; i.e., $A\mathbf{q}_n$ is orthogonal to $\mathbf{q}_1, \ldots, \mathbf{q}_{n-2}$. Thus, if the goal is only to compute H_k (say to find the Ritz values), then we only need to store the two most recently computed columns of Q. Second, the data of H_k can also be stored in two vectors, one containing the main diagonal and one containing the first subdiagonal of H_k. (By symmetry, the first superdiagonal equals the first subdiagonal of H_k.)

The Lanczos iteration is found in Algorithm 19.2.

Algorithm 19.2 The Lanczos Iteration. This algorithm operates on a vector $\mathbf{b}$ of length n and an $n \times n$ symmetric matrix A. It iterates k times or until the norm of the next vector in the iteration is less than *tol*. It returns two vectors $\mathbf{x}$ and $\mathbf{y}$ that respectively contain the main diagonal and first subdiagonal of the current Hessenberg approximation.

procedure LANCZOS($\mathbf{b}, A, k, tol$)
  $\mathbf{q}_0 \leftarrow$ zeros(size($\mathbf{b}$)) ▷ Some initialization
  $\mathbf{q}_1 \leftarrow \mathbf{b}/\|\mathbf{b}\|_2$
  $\mathbf{x} \leftarrow$ empty(k)
  $\mathbf{y} \leftarrow$ empty(k)
  for $i = 0 \ldots k-1$ **do** ▷ Perform the iteration.
    $\mathbf{z} \leftarrow A\mathbf{q}_1$ ▷ $\mathbf{z}$ is a temporary vector to store $\mathbf{q}_{i+1}$.
    $\mathbf{x}[i] \leftarrow \mathbf{q}_1^\mathsf{T}\mathbf{z}$ ▷ $\mathbf{q}_1$ is used to store the previous $\mathbf{q}_i$.
    $\mathbf{z} \leftarrow \mathbf{z} - \mathbf{x}[i]\mathbf{q}_1 + \mathbf{y}[i-1]\mathbf{q}_0$ ▷ $\mathbf{q}_0$ is used to store $\mathbf{q}_{i-1}$.
    $\mathbf{y}[i] = \|\mathbf{z}\|_2$ ▷ Initialize $\mathbf{y}[i]$.
    if $\mathbf{y}[i] < tol$ **then** ▷ Stop if $\|\mathbf{q}_{i+1}\|_2$ is too small.
      return $\mathbf{x}[:i+1]$, $\mathbf{y}[:i]$
    $\mathbf{z} = \mathbf{z}/\mathbf{y}[i]$
    $\mathbf{q}_0, \mathbf{q}_1 = \mathbf{q}_1, \mathbf{z}$ ▷ Store new $\mathbf{q}_{i+1}$ and $\mathbf{q}_i$ on top of $\mathbf{q}_1$ and $\mathbf{q}_0$.
  return $\mathbf{x}$, $\mathbf{y}[:-1]$

Problem 5. Implement Algorithm 19.2 by completing the following function. Write it so that it can operate on complex arrays.

```
def lanczos(b, Amul, k, tol=1E-8):
    '''Perform `k' steps of the Lanczos iteration on the symmetric linear
    operator defined by `Amul', starting with the vector 'b'.

    INPUTS:
    b    - A NumPy array. The starting vector for the Lanczos iteration.
    Amul - A function handle. Should describe a symmetric linear operator.
    k    - Number of times to perform the Lanczos iteration.
    tol  - Stop iterating if the next vector in the Lanczos iteration has
           norm less than `tol'. Defaults to 1E-8.

    RETURN:
    Return (alpha, beta) where alpha and beta are the main diagonal and
    first subdiagonal of the tridiagonal matrix computed by the Lanczos
    iteration.
    '''
```

As it is described in Algorithm 19.2, the Lanczos iteration is not stable. Roundoff error may cause the $\mathbf{q}_i$ to be far from orthogonal. In fact, it is possible for the $\mathbf{q}_i$ to be so adulterated by roundoff error that they are no longer linearly independent.

Problem 6. The following code performs multiplication by a tridiagonal symmetric matrix.

```
def tri_mul(a, b, u):
    ''' Return Au where A is the tridiagonal symmetric matrix with main
    diagonal a and subdiagonal b.
    '''
     v = a * u
     v[:-1] += b * u[1:]
     v[1:] += b * u[:-1]
     return v
```

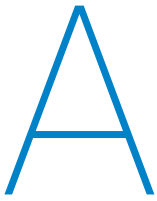
Let A be a 1000×1000 symmetric tridiagonal matrix with random values in its nonzero diagonals. Use the function `lanczos()` from Problem 5 with 100 iterations to estimate the 5 eigenvalues of A of largest norm. Compare these to the 5 largest true eigenvalues of A

If you do this problem for different vectors a and b, you may notice that occasionally the largest Ritz value is repeated. This happens because the vectors used in the Lanczos iteration may not be orthogonal. These erroneous eigenvalues are called “ghost eigenvalues."

There are modified versions of the Lanczos iteration that are numerically stable. One of these, the Implicitly Restarted Lanczos Method, is found in SciPy as the function `scipy.sparse.linalg.eigsh()`.

Part II

Appendices



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.

$$A[0] = \begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \end{bmatrix} \qquad A[2,1] = \begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \end{bmatrix}$$

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.

$$A = \begin{bmatrix} \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \end{bmatrix} \qquad B = \begin{bmatrix} * & * & * \\ * & * & * \\ * & * & * \end{bmatrix}$$

$$\texttt{np.hstack((A,B,A))} = \begin{bmatrix} \times & \times & \times & * & * & * & \times & \times & \times \\ \times & \times & \times & * & * & * & \times & \times & \times \\ \times & \times & \times & * & * & * & \times & \times & \times \end{bmatrix}$$

$$\texttt{np.vstack((A,B,A))} = \begin{bmatrix} \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \\ * & * & * \\ * & * & * \\ * & * & * \\ \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \end{bmatrix}$$

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()`.

$$x = \begin{bmatrix} \times & \times & \times & \times \end{bmatrix} \qquad y = \begin{bmatrix} * & * & * & * \end{bmatrix}$$

$$\texttt{np.hstack((x,y,x))} = \begin{bmatrix} \times & \times & \times & \times & * & * & * & * & \times & \times & \times & \times \end{bmatrix}$$

$$\texttt{np.vstack((x,y,x))} = \begin{bmatrix} \times & \times & \times & \times \\ * & * & * & * \\ \times & \times & \times & \times \end{bmatrix} \qquad \texttt{np.column\_stack((x,y,x))} = \begin{bmatrix} \times & * & \times \\ \times & * & \times \\ \times & * & \times \\ \times & * & \times \end{bmatrix}$$

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.

$$A = \begin{bmatrix} 1 & 2 & 3 \\ 1 & 2 & 3 \\ 1 & 2 & 3 \end{bmatrix} \qquad x = \begin{bmatrix} 10 & 20 & 30 \end{bmatrix}$$

$$\texttt{A + x} = \begin{bmatrix} 1 & 2 & 3 \\ 1 & 2 & 3 \\ 1 & 2 & 3 \end{bmatrix} + \begin{bmatrix} 10 & 20 & 30 \end{bmatrix} = \begin{bmatrix} 11 & 22 & 33 \\ 11 & 22 & 33 \\ 11 & 22 & 33 \end{bmatrix}$$

$$\texttt{A + x.reshape((1,-1))} = \begin{bmatrix} 1 & 2 & 3 \\ 1 & 2 & 3 \\ 1 & 2 & 3 \end{bmatrix} + \begin{bmatrix} 10 \\ 20 \\ 30 \end{bmatrix} = \begin{bmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{bmatrix}$$

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`.

$$A = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \end{bmatrix}$$

$$\texttt{A.sum(axis=0)} = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \end{bmatrix} = \begin{bmatrix} 4 & 8 & 12 & 16 \end{bmatrix}$$

$$\texttt{A.sum(axis=1)} = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \end{bmatrix} = \begin{bmatrix} 10 & 10 & 10 & 10 \end{bmatrix}$$