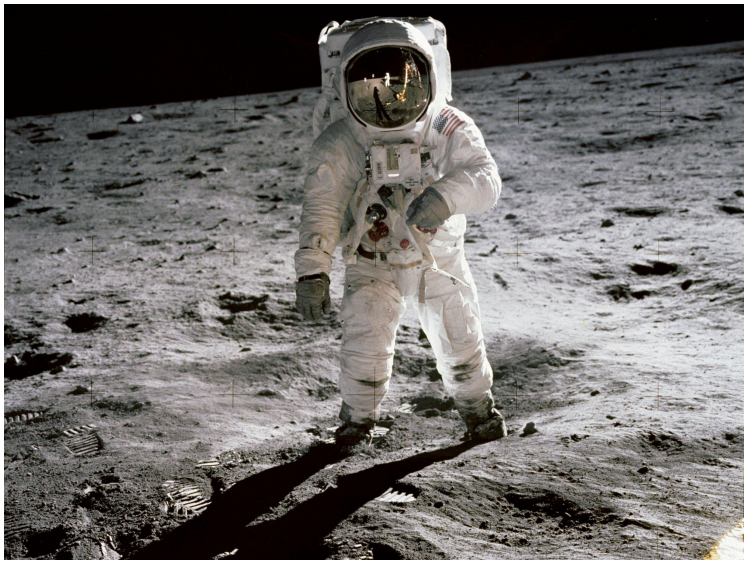
Labs for Foundations of Applied Mathematics

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.

Contents

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.

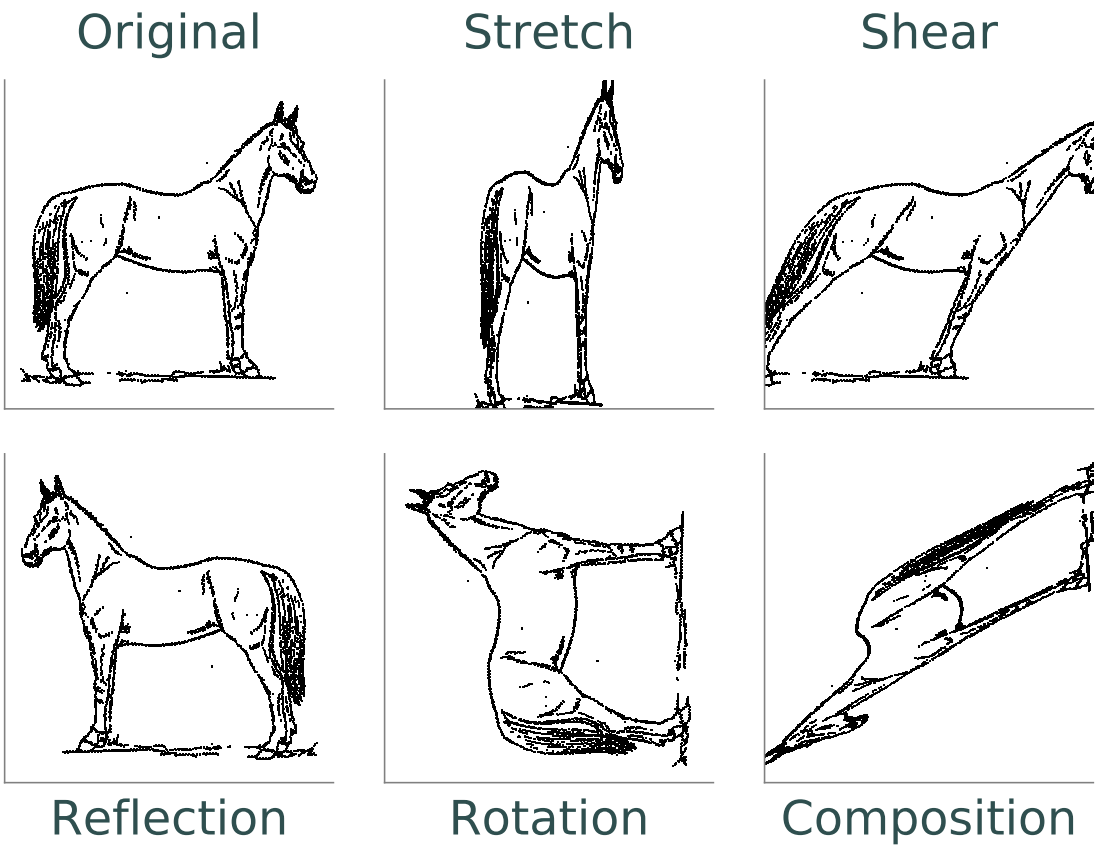


Figure 1.1: The points stored in `horse.npy` under various linear transformations.

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

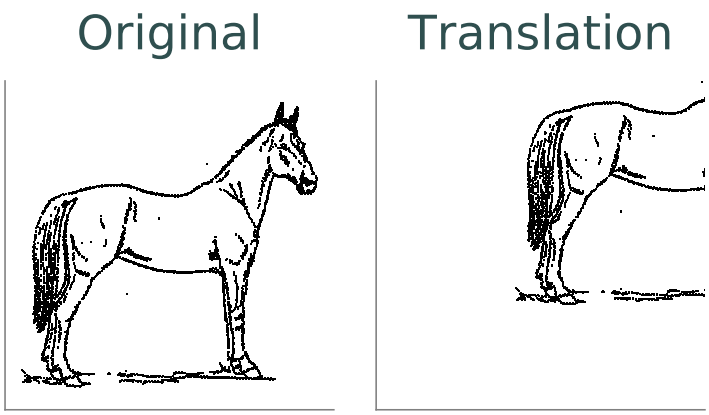
Let V, W, and Z be finite-dimensional vector spaces. If $L : V \to W$ and $K : W \to Z$ are linear transformations with matrix representations A and B, respectively, then the *composition* function $KL : V \to Z$ is also a linear transformation, and its matrix representation is the matrix product BA.

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*.

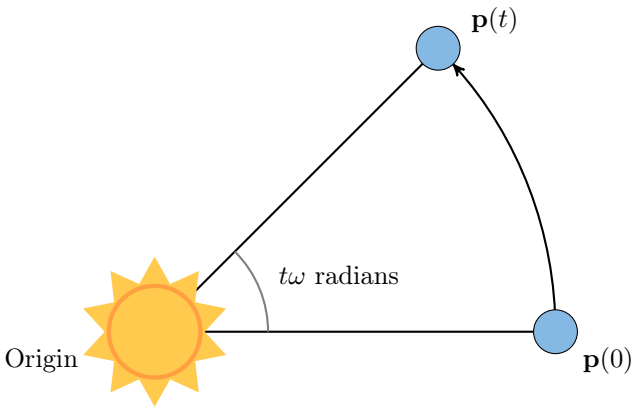
For example, if T is the translation with $\mathbf{b}=\left[\frac{3}{4},\frac{1}{2}\right]^{\mathsf{T}}$, then applying T to an image will shift it right by $\frac{3}{4}$ and up by $\frac{1}{2}$. This translation is illustrated below.



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.

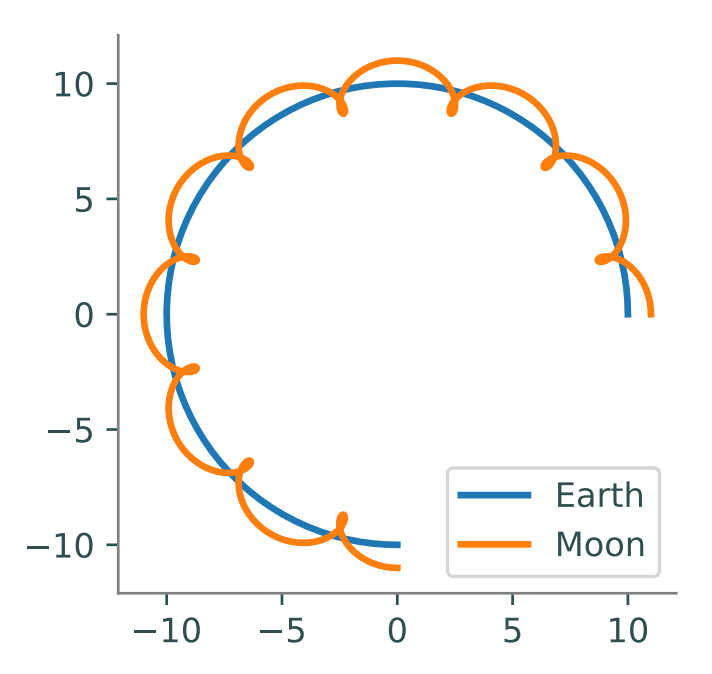
Problem 2. The moon orbits the earth while the earth orbits the sun. Assuming circular orbits, we can compute the trajectories of both the earth and the moon using only linear and affine transformations.

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

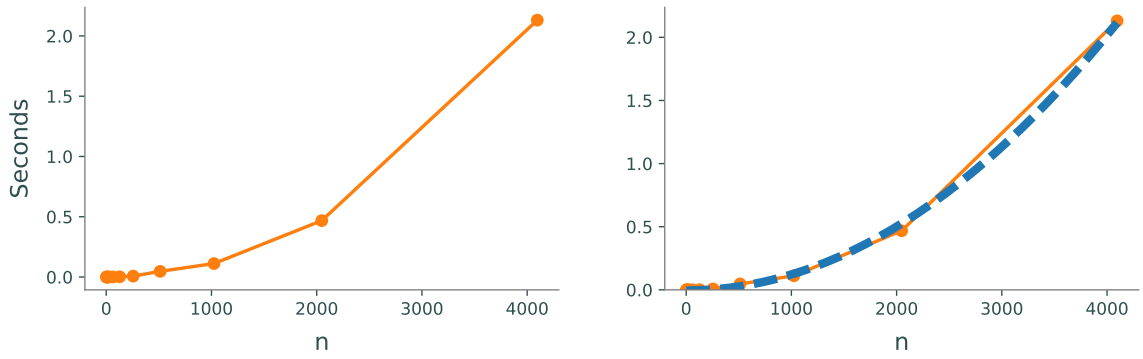
Most algorithms have at least one input that dictates the size of the problem to be solved. For example, the following functions take in a single integer n and produce a random vector of length n as a list or a random $n \times n$ matrix as a list of lists.

```
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:

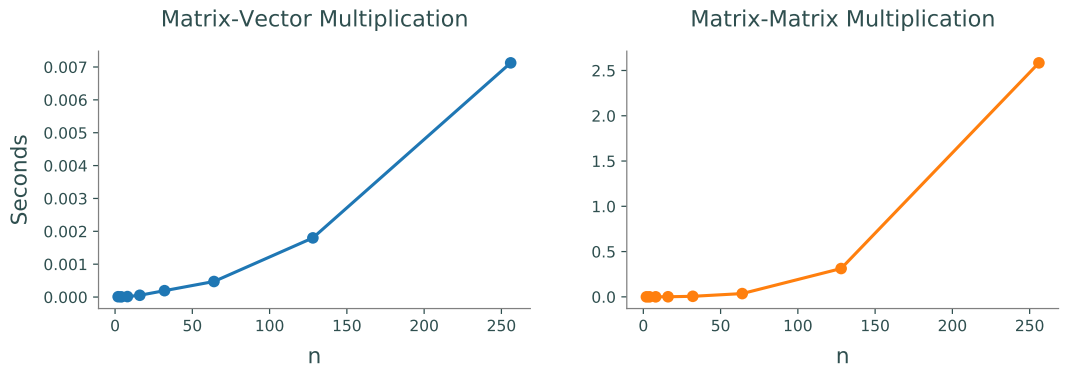
$$y_i = \sum_{k=1}^{n} a_{ik}x_k \qquad\qquad c_{ij} = \sum_{k=1}^{n} a_{ik}b_{kj}$$

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()
```

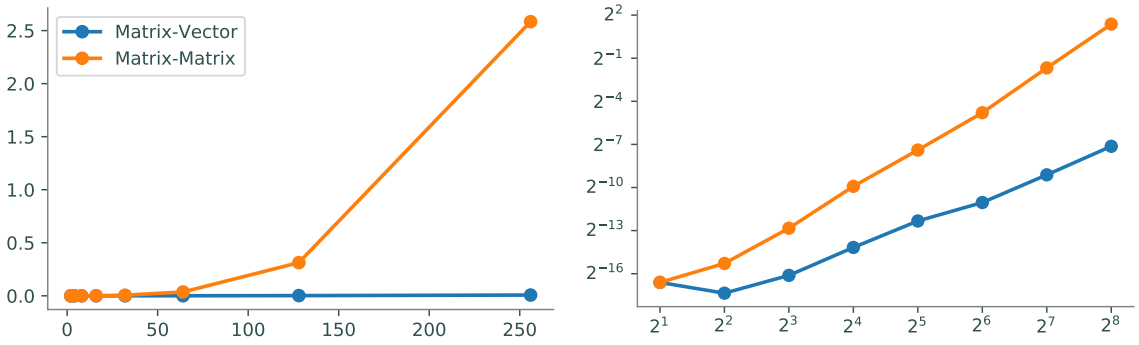


Figure 1.5

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.]]
```

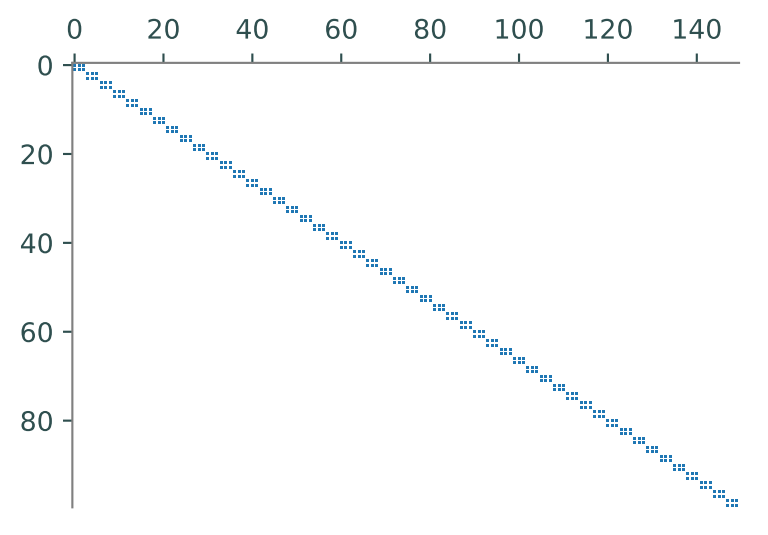
- **BSR Format**: Many sparse matrices can be formulated as block matrices, and a block matrix can be stored efficiently as a `bsr_matrix`. Use `sparse.bmat()` or `sparse.block_diag()` to create a block matrix quickly.

```
# 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.

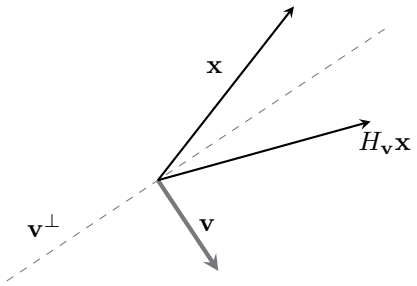


Figure 3.1: The vector $\mathbf{v}$ defines the orthogonal complement $\mathbf{v}^\perp$, which in this case is a line. Applying the Householder transformation $H_\mathbf{v}$ to $\mathbf{x}$ reflects $\mathbf{x}$ across $\mathbf{v}^\perp$.

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 $\mathbf{x}_k$).

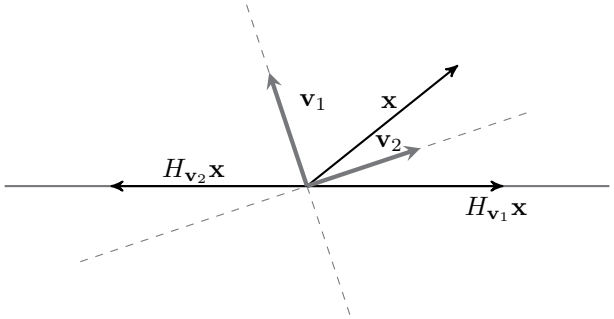


Figure 3.2: There are two reflections that map $\mathbf{x}$ into the span of $\mathbf{e}_1$, defined by the vectors $\mathbf{v}_1$ and $\mathbf{v}_2$. In this illustration, $H_{\mathbf{v}_2}$ is the more stable transformation since it reflects $\mathbf{x}$ further than $H_{\mathbf{v}_1}$.

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

1: **procedure** HOUSEHOLDER(A)
2: $m, n \leftarrow \text{shape}(A)$
3: $R \leftarrow \text{copy}(A)$
4: $Q \leftarrow I_m$ ▷ The $m \times m$ identity matrix.
5: **for** $k = 0 \dots n-1$ **do**
6: $\mathbf{u} \leftarrow \text{copy}(R_{k:,k})$
7: $u_0 \leftarrow u_0 + \text{sign}(u_0)\|\mathbf{u}\|$ ▷ u_0 is the first entry of $\mathbf{u}$.
8: $\mathbf{u} \leftarrow \mathbf{u}/\|\mathbf{u}\|$ ▷ Normalize $\mathbf{u}$.
9: $R_{k:,k:} \leftarrow R_{k:,k:} - 2\mathbf{u}\left(\mathbf{u}^\mathsf{T}R_{k:,k:}\right)$ ▷ Apply the reflection to R.
10: $Q_{k:,:} \leftarrow Q_{k:,:} - 2\mathbf{u}\left(\mathbf{u}^\mathsf{T}Q_{k:,:}\right)$ ▷ Apply the reflection to Q.
11: **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 $A = Q_1^\mathsf{T}Q_2^\mathsf{T}Q_3^\mathsf{T}HQ_3Q_2Q_1$, 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)
  $m, n \leftarrow \operatorname{shape}(A)$
  $H \leftarrow \operatorname{copy}(A)$
  $Q \leftarrow I_m$
  for $k = 0 \ldots n-3$ **do**
    $\mathbf{u} \leftarrow \operatorname{copy}(H_{k+1:,k})$
    $u_0 \leftarrow u_0 + \operatorname{sign}(u_0)\|\mathbf{u}\|$
    $\mathbf{u} \leftarrow \mathbf{u}/\|\mathbf{u}\|$
    $H_{k+1:,k:} \leftarrow H_{k+1:,k:} - 2\mathbf{u}(\mathbf{u}^\mathsf{T} H_{k+1:,k:})$ ▷ 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 $\mathbf{e}_1$.

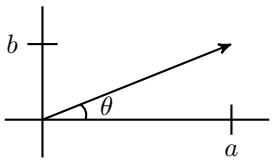


Figure 3.3: Rotating clockwise by θ sends the vector $[a, b]^\mathsf{T}$ to the span of $\mathbf{e}_1$.

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.

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 $G(i-1, i, \theta)$.

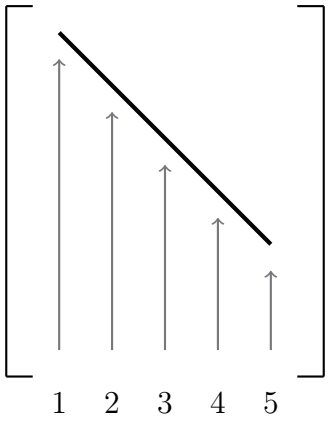


Figure 3.4: The order in which to zero out subdiagonal entries in the Givens triangularization algorithm. The heavy black line is the main diagonal of the matrix. Entries should be zeroed out from bottom to top in each column, beginning with the leftmost column.

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 $\widehat{b} \approx -3$.

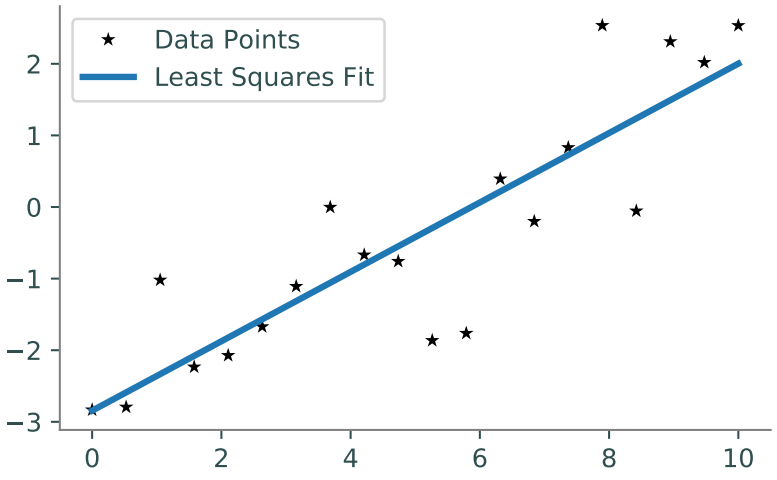


Figure 4.1

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.

$$p_n(x) = c_n x^n + c_{n-1}x^{n-1} + \cdots + c_2 x^2 + c_1 x + c_0 = \sum_{i=0}^{n} c_i x^i$$

Note that the polynomial is uniquely determined by its $n+1$ coefficients $\{c_i\}_{i=0}^n$. Ideally, then, we seek the set of coefficients $\{c_i\}_{i=0}^n$ 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 (10.5) 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 (10.5) 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.

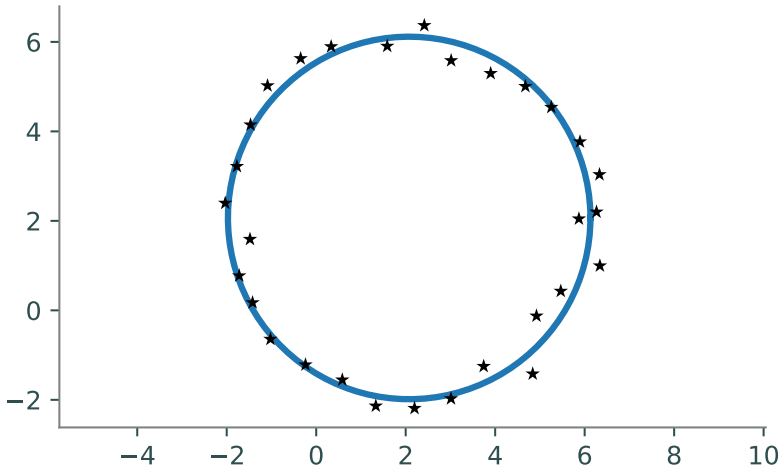
$$\begin{bmatrix} 2x_1 & 2y_1 & 1 \\ 2x_2 & 2y_2 & 1 \\ \vdots & \vdots & \vdots \\ 2x_m & 2y_m & 1 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix} = \begin{bmatrix} x_1^2 + y_1^2 \\ x_2^2 + y_2^2 \\ \vdots \\ x_m^2 + y_m^2 \end{bmatrix} \tag{4.6}$$

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)
  $m, n \leftarrow \text{shape}(A)$ ▷ A is square so $m = n$.
  $\mathbf{x}_0 \leftarrow \text{random}(n)$ ▷ A random vector of length n
  $\mathbf{x}_0 \leftarrow \mathbf{x}_0/\|\mathbf{x}_0\|$ ▷ Normalize $\mathbf{x}_0$
  for $k = 1,\ 2,\ \ldots,\ N-1$ **do**
    $\mathbf{x}_{k+1} \leftarrow A\mathbf{x}_k$
    $\mathbf{x}_{k+1} \leftarrow \mathbf{x}_{k+1}/\|\mathbf{x}_{k+1}\|$
  return $\mathbf{x}_N^\mathsf{T}A\mathbf{x}_N,\ \mathbf{x}_N$

[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.

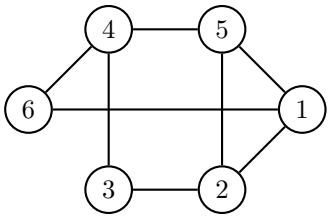
5 Image Segmentation

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.*

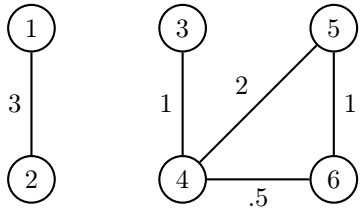
Graphs as Matrices

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).

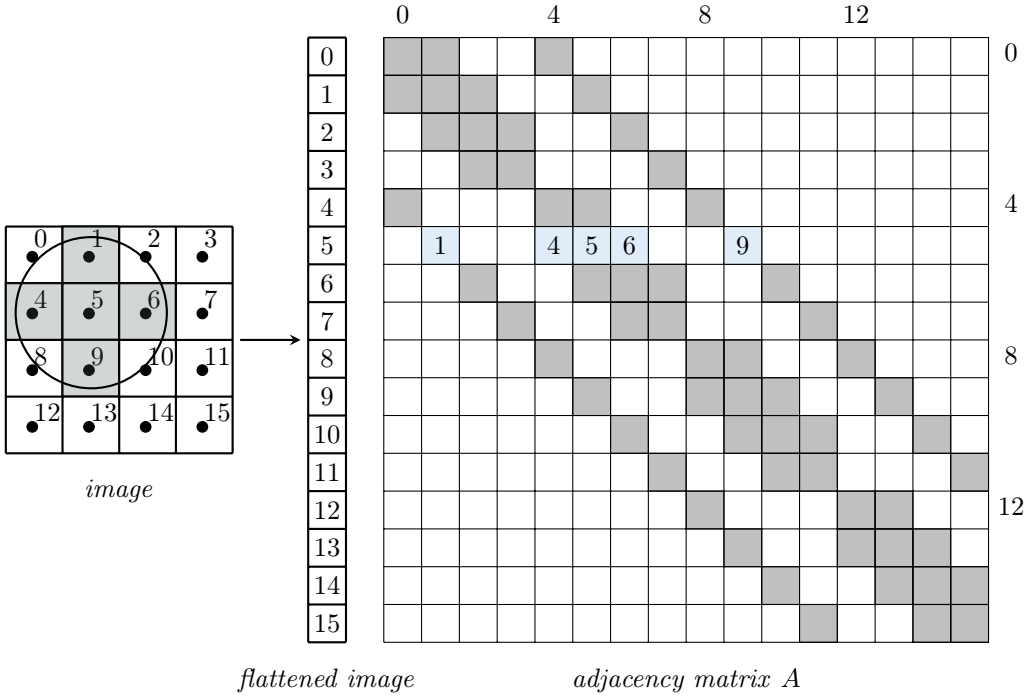


Figure 5.3: The grid on the left represents a 4×4 ($m \times n$) image with 16 pixels. On the right is the corresponding 16×16 ($mn \times mn$) adjacency matrix with all nonzero entries shaded. For example, in row 5, entries 1, 4, 5, 6, and 9 are nonzero because those pixels are within radius $r = 1.2$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

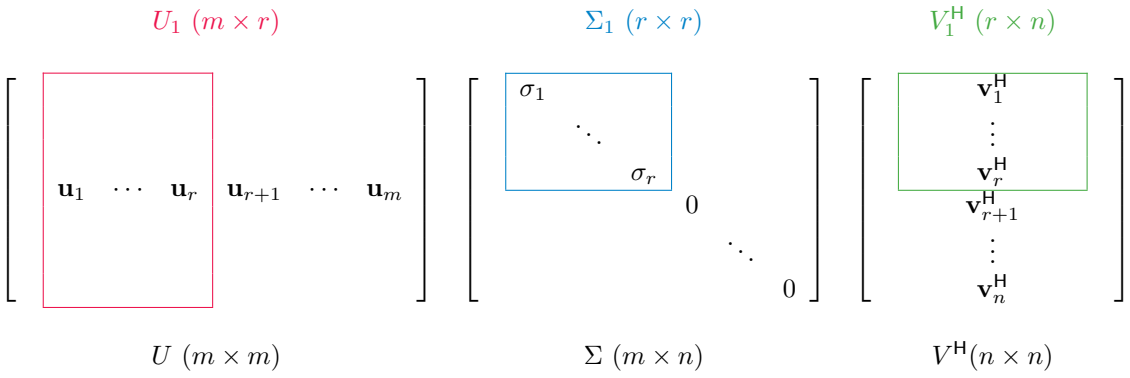
6 The SVD and Image Compression

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

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

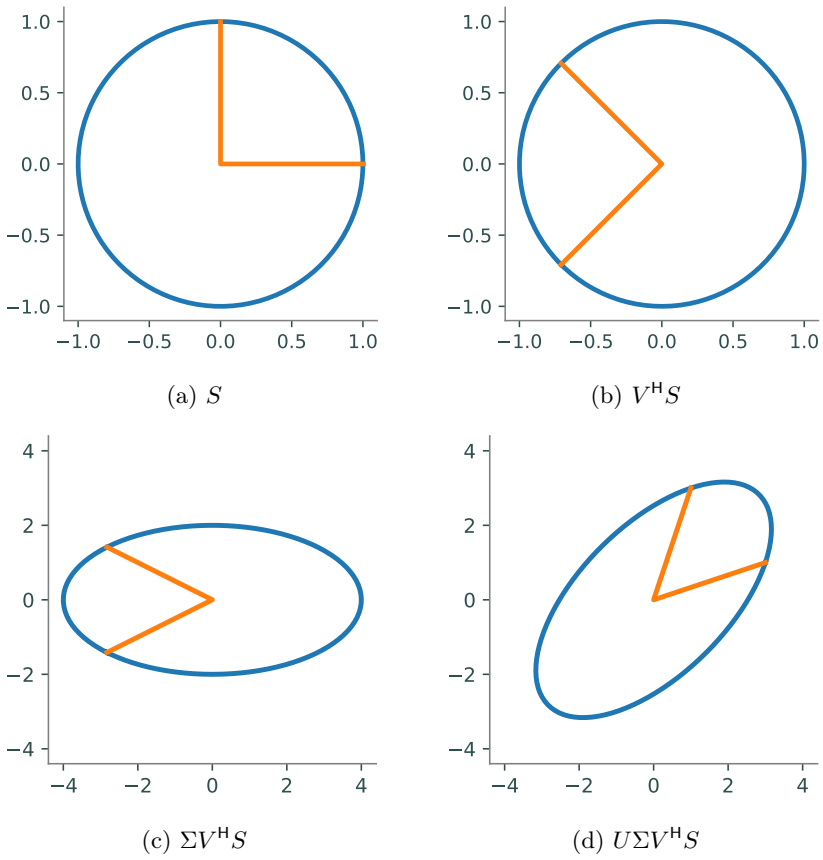
so that plotting the first row of S against the second row of S displays the unit circle, and plotting the first row of E against its second row displays the standard basis vectors in $\mathbb{R}^2$.

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

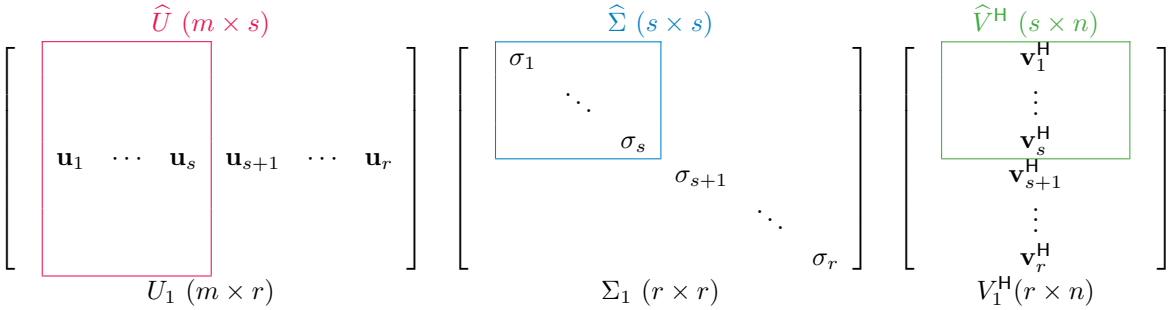
Low-Rank Matrix Approximations

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.

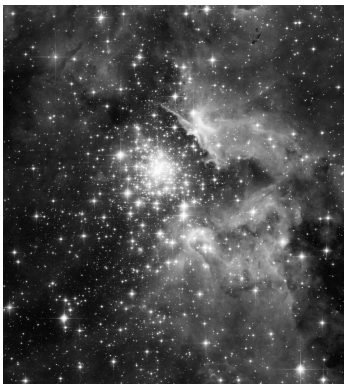
1. Compute the compact SVD of A, then use (6.2) to compute the lowest rank approximation A_s of A with 2-norm error less than ϵ. Avoid calculating the SVD more than once. (Hint: `np.argmax()`, `np.where()`, and/or fancy indexing may be useful.)
2. As in the previous problem, also return the number of 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 $\|A - A_s\|_2 < \epsilon$.

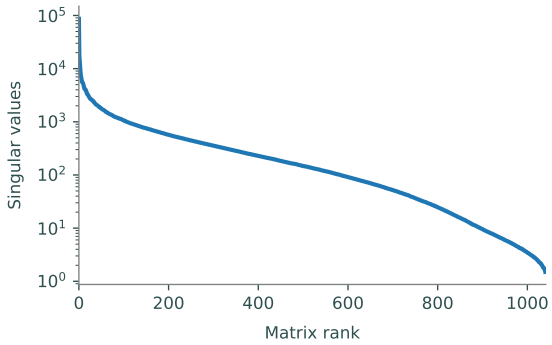
Image Compression

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.



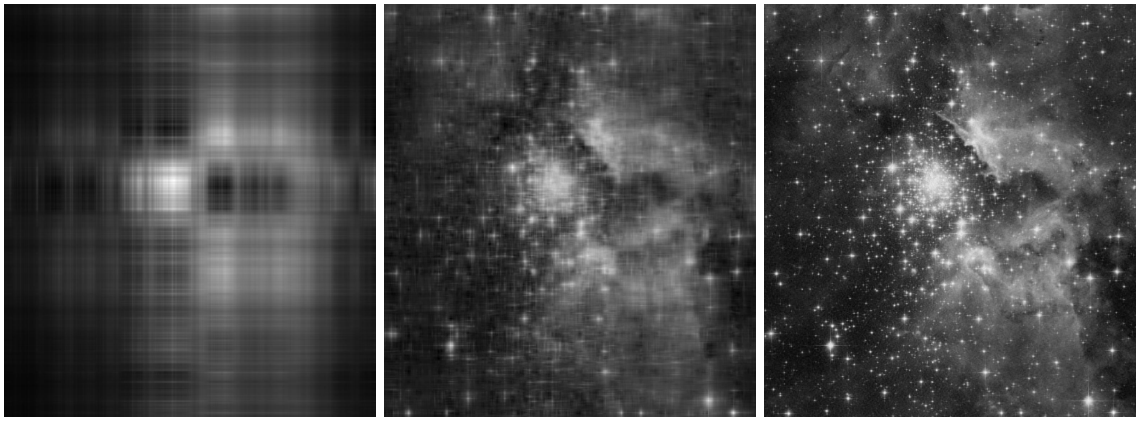
(a) NGC 3603 (Hubble Space Telescope).



(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

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

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 Differentiation

Lab Objective: *The derivative is critically important in many applications. Depending on the application and on the available information, the derivative may be calculated symbolically, numerically, or with differentiation software. In this lab we explore these three ways to take a derivative, discuss what settings they are each appropriate for, and demonstrate their strengths and weaknesses.*

Symbolic Differentiation

The derivative of a known mathematical function can be calculated symbolically with SymPy. This method is the most precise way to take a derivative, but it is computationally expensive and requires knowing the closed form formula of the function. Use `sy.diff()` to take a symbolic derivative.

```
>>> import sympy as sy

>>> x = sy.symbols('x')
>>> sy.diff(x**3 + x, x)     # Differentiate x^3 + x with respect to x.
3*x**2 + 1
```

Problem 1. Write a function that defines $f(x) = (\sin(x) + 1)^{\sin(\cos(x))}$ and takes its symbolic derivative with respect to x using SymPy. Lambdify the resulting function so that it can accept NumPy arrays and return the resulting function handle.

To check your function, plot f and its derivative f' over the domain $[-\pi, \pi]$. It may be helpful to move the bottom spine to 0 so you can see where the derivative crosses the x-axis.

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

>>> ax = plt.gca()
>>> ax.spines["bottom"].set_position("zero")
```

Numerical Differentiation

One definition for the derivative of a function $f : \mathbb{R} \to \mathbb{R}$ at a point x_0 is

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

Since this definition relies on h approaching 0, choosing a small, fixed value for h approximates $f'(x_0)$.

$$f'(x_0) \approx \frac{f(x_0 + h) - f(x_0)}{h} \tag{8.1}$$

This quotient is called the *first order forward difference quotient*. Using the points x_0 and $x_0 - h$ in place of $x_0 + h$ and x_0, respectively, results in the *first order backward difference quotient*.

$$f'(x_0) \approx \frac{f(x_0) - f(x_0 - h)}{h} \tag{8.2}$$

Forward difference quotients use values of f at x_0 and points greater than x_0, while backward difference quotients use the values of f at x_0 and points less than x_0. A *centered difference quotient* uses points on either side of x_0, and typically results in a better approximation than the one-sided quotients. Adding (8.1) and (8.2) yields the *second order centered difference quotient*.

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

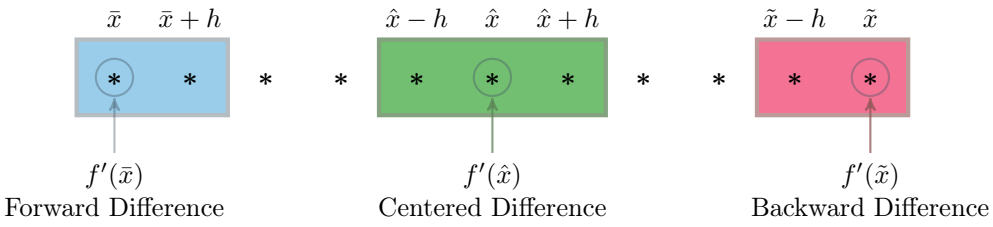


Figure 8.1

> **Note**
>
> The finite difference quotients in this section all approximate the first derivative of a function. The terms *first order* and *second order* refers to how quickly the approximation converges on the actual value of $f'(x_0)$ as h approaches 0, not to how many derivatives are being taken.
>
> There are finite difference quotients for approximating higher order derivatives, such as f'' or f'''. For example, the following is a centered difference quotient for the second derivative.
>
> $$f''(x_0) \approx \frac{f(x_0 - h) - 2f(x_0) + f(x_0 + h)}{h^2}$$
>
> This particular quotient is important for finite difference methods that approximate numerical solutions to certain partial differential equations.

While we do not derive them here, there are other finite difference quotients that use more points to approximate the derivative, some of which are listed below. Using more points generally results in better convergence properties.

Type	Order	Formula
Forward	1	$\frac{f(x_0+h)-f(x_0)}{h}$
	2	$\frac{-3f(x_0)+4f(x_0+h)-f(x_0+2h)}{2h}$
Backward	1	$\frac{f(x_0)-f(x_0-h)}{h}$
	2	$\frac{3f(x_0)-4f(x_0-h)+f(x_0-2h)}{2h}$
Centered	2	$\frac{f(x_0+h)-f(x_0-h)}{2h}$
	4	$\frac{f(x_0-2h)-8f(x_0-h)+8f(x_0+h)-f(x_0+2h)}{12h}$

Table 8.1: Common finite difference quotients for approximating $f'(x_0)$.

Problem 2. Write a function for each of the finite difference quotients listed in Table 8.1. Each function should accept a function handle f, an array of points `x`, and a float h; each should return an array of the difference quotients evaluated at each point in `x`.

To test your functions, approximate the derivative of $f(x) = (\sin(x)+1)^{\sin(\cos(x))}$ at each point of a domain over $[-\pi, \pi]$. Plot the results and compare them to the results of Problem 1.

Convergence of Finite Difference Quotients

Finite difference quotients are typically derived using Taylor's formula. This method also shows how the accuracy of the approximation increases as $h \to 0$.

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

where $R_2(h) = h^2 \int_0^1 (1-t)f''(x_0+th)\,dt$. Thus the absolute error of the first order forward difference quotient is

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

If f'' is continuous, then for any $\delta > 0$, setting $M = \sup_{x \in (x_0-\delta, x_0+\delta)} f''(x)$ guarantees that

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

whenever $|h| < \delta$. That is, the error decreases at the same rate as h. If h gets twice as small, the error does as well. This is what is meant by a *first order* approximation. In a *second order* approximation, the absolute error is $O(h^2)$, meaning that if h gets twice as small, the error gets four times smaller.

Note

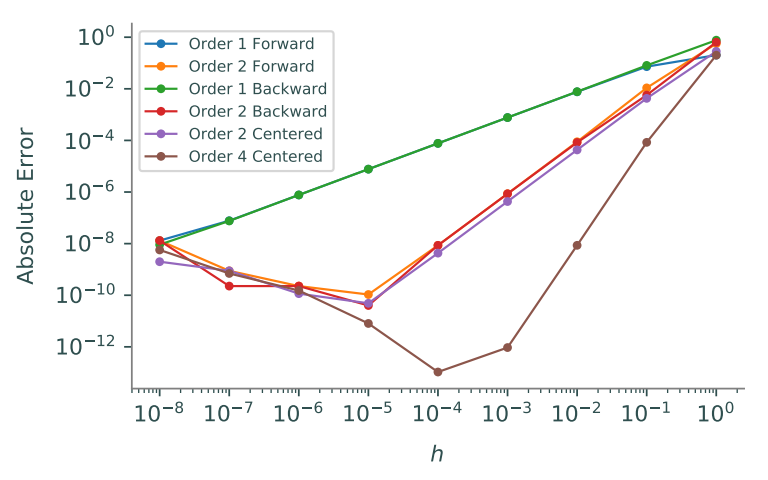
The notation $O(f(n))$ is commonly used to describe the temporal or spatial complexity of an algorithm. In that context, a $O(n^2)$ algorithm is much worse than a $O(n)$ algorithm. However, when referring to error, a $O(h^2)$ algorithm is **better** than a $O(h)$ algorithm because it means that the accuracy improves faster as h decreases.

Problem 3. Write a function that accepts a point x_0 at which to compute the derivative of $f(x) = (\sin(x) + 1)^{\sin(\cos(x))}$. Use your function from Problem 1 to compute the exact value of $f'(x_0)$. Then use each your functions from Problem 2 to get an approximate derivative $\tilde{f}'(x_0)$ for $h = 10^{-8}, 10^{-7}, \dots, 10^{-1}, 1$. Track the absolute error $|f'(x_0) - \tilde{f}'(x_0)|$ for each trial, then plot the absolute error against h on a log-log scale (use `plt.loglog()`).

Instead of using `np.linspace()` to create an array of h values, use `np.logspace()`. This function generates logarithmically spaced values between two powers of 10.

```
>>> import numpy as np
>>> np.logspace(-3, 0, 4)           # Get 4 values from 1e-3 to 1e0.
array([ 0.001,  0.01 ,  0.1  ,  1.   ])
```

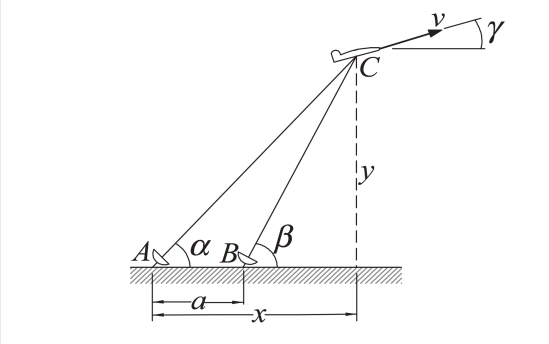
For $x_0 = 1$, your plot should resemble the following figure.



ACHTUNG!

Mathematically, choosing smaller h values results in tighter approximations of $f'(x_0)$. However, Problem 3 shows that when h gets too small, the error stops decreasing. This numerical error is due to the denominator in each finite difference quotient becoming very small. The optimal value of h is usually one that is small, but not too small.

Problem 4. The radar stations A and B, separated by the distance $a = 500$ m, track a plane C by recording the angles α and β at one-second intervals. Your goal, back at air traffic control, is to determine the speed of the plane.



Let the position of the plane at time t be given by $(x(t), y(t))$. The speed at time t is the magnitude of the velocity vector, $\|\frac{d}{dt}(x(t), y(t))\| = \sqrt{x'(t)^2 + y'(t)^2}$. The closed forms of the functions $x(t)$ and $y(t)$ are unknown (and may not exist at all), but we can still use numerical methods to estimate $x'(t)$ and $y'(t)$. For example, at $t = 3$, the second order centered difference quotient for $x'(t)$ is

$$x'(3) \approx \frac{x(3+h) - x(3-h)}{2h} = \frac{1}{2}(x(4) - x(2)).$$

In this case $h = 1$ since data comes in from the radar stations at 1 second intervals.

Successive readings for α and β at integer times $t = 7, 8, \ldots, 14$ are stored in the file `plane.npy`. Each row in the array represents a different reading; the columns are the observation time t, the angle α (in degrees), and the angle β (also in degrees), in that order. The Cartesian coordinates of the plane can be calculated from the angles α and β as follows.

$$x(\alpha, \beta) = a\frac{\tan(\beta)}{\tan(\beta) - \tan(\alpha)} \qquad y(\alpha, \beta) = a\frac{\tan(\beta)\tan(\alpha)}{\tan(\beta) - \tan(\alpha)}$$

Load the data, convert α and β to radians, then compute the coordinates $x(t)$ and $y(t)$ at each given t. Approximate $x'(t)$ and $y'(t)$ using a forward difference quotient for $t = 7$, a backward difference quotient for $t = 14$, and a centered difference quotient for $t = 8, 9, \ldots, 13$ (see Figure 8.1). Return the values of the speed $\sqrt{x'(t)^2 + y'(t)^2}$ at each t.[a]
(Hint: `np.deg2rad()` will be helpful.)

[a] This problem originates from *Numerical Methods in Engineering with Python 3* by Jaan Kiusalaas.

Numerical Differentiation in Higher Dimensions

Finite difference quotients can also be used to approximate derivatives in higher dimensions. The *Jacobian matrix* of a function $f : \mathbb{R}^n \to \mathbb{R}^m$ at a point $\mathbf{x}_0 \in \mathbb{R}^n$ is the $m \times n$ matrix J whose entries are given by

$$J_{ij} = \frac{\partial f_i}{\partial x_j}(\mathbf{x}_0).$$

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

$$J = \left[\begin{array}{c|c|c} \frac{\partial f}{\partial x_1} & \frac{\partial f}{\partial x_2} & \frac{\partial f}{\partial x_3} \end{array}\right] = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \frac{\partial f_1}{\partial x_3} \\ \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \frac{\partial f_2}{\partial x_3} \end{bmatrix}, \quad \text{where} \quad f(\mathbf{x}) = \begin{bmatrix} f_1(\mathbf{x}) \\ f_2(\mathbf{x}) \end{bmatrix}, \quad \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}.$$

The difference quotients in this case resemble directional derivatives. The first order forward difference quotient for approximating a partial derivative is

$$\frac{\partial f}{\partial x_j}(\mathbf{x}_0) \approx \frac{f(\mathbf{x}_0 + h\mathbf{e}_j) - f(\mathbf{x}_0)}{h},$$

where $\mathbf{e}_j$ is the j^{th} standard basis vector. The second order centered difference approximation is

$$\frac{\partial f}{\partial x_j}(\mathbf{x}_0) \approx \frac{f(\mathbf{x}_0 + h\mathbf{e}_j) - f(\mathbf{x}_0 - h\mathbf{e}_j)}{2h}. \tag{8.4}$$

Problem 5. Write a function that accepts a function $f : \mathbb{R}^n \to \mathbb{R}^m$, a point $\mathbf{x}_0 \in \mathbb{R}^n$, and a float h. Approximate the Jacobian matrix of f at $\mathbf{x}$ using the second order centered difference quotient in (8.4).
(Hint: the standard basis vector $\mathbf{e}_j$ is the jth column of the $n \times n$ identity matrix I.)

To test your function, define a simple function like $f(x, y) = [x^2, x^3 - y]^\mathsf{T}$ where the Jacobian is easy to find analytically, then check the results of your function against SymPy or your own scratch work.

Autograd

Autograd is a package that allows for efficient automatic differentiation of NumPy and some SciPy code. It has the ability to handle taking the derivative of functions that contain almost all NumPy structures[1], including `if` statements, `while` loops and recursion. It is very beneficial when calculating derivatives of unconventional or very complex functions. Due to this feature, it is extremely useful in many applications such as machine learning and neural networks.

Autograd is installed by running `pip install autograd` in the terminal. See `https://github.com/HIPS/autograd` for more complete installation instructions.

To support most of the NumPy features, 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 same way NumPy is used.

The function `grad()` returns a function that is the gradient of the original function, if the original function returns a scalar. This new function accepts the same parameters as the original function. The following code computes the derivative of $e^{\sin(\cos(x))}$ at $x = 1$ using autograd.

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

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

>>> g = lambda x: anp.exp(anp.sin(anp.cos(x)))
>>> grad_g = grad(g)
>>> grad_g(1.)
-1.2069777039799139
```

For multivariate functions, the parameter `argnum` specifies the variable with respect to which the gradient is computed.

```
>>> f = lambda x,y: 3*x*y+2*y- x

# Take the gradient with respect to the first variable x.
>>> grad_f = grad(f, argnum=0)
>>> grad_f(.25,.5)
array(0.5)

# Take the gradient with respect to the second variable y.
>>> grad_f = grad(f, argnum=1)
>>> grad_f(.25,.5)
array(2.75)
```

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

```
from autograd import multigrad

>>> grad_f = multigrad(f, argnums=[0,1])
>>> grad_f(.25,.5)
(array(0.5),array(2.75))
```

Problem 6. Compute the derivative of $f(x) = \ln\sqrt{\sin(\sqrt{x})}$ at $x = \frac{\pi}{4}$ using SymPy, the second order centered difference quotient and autograd. Print the computation time and error for each method. Do not include initializations of functions or variables in the computation time. Return the value of the autograd approximation.

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

As seen 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 computation time than SymPy.

Autograd can differentiate a function as many times as desired.

```
>>> f = lambda x: anp.sin(x)+3**anp.cos(x)

# Calculate the first derivative.
>>> grad_f = grad(f)

# Calculate the second derivative and so forth.
>>> grad_f2 = grad(grad_f)
>>> grad_f3 = grad(grad_f2)
>>> df3(1.)
array(2.683445898750351)
```

The main advantage of using autograd in differentiation is that it can differentiate many structures in Python functions. In fact, it can handle functions that include loops, `if` statements and recursion. For example, the following code computes the Taylor series of e^x evaluated at $x = 2$.

```
import numpy as np

# Define the Taylor series.
# Note that this function does not account for array broadcasting.
>>> def taylor_exp(x, tol=.0001):
...     result = 0
...     cur_term = x
...     i = 0
...     while anp.abs(cur_term) >= tol:
# Autograd's version of NumPy doesn't have the math attribute so use NumPy.
...         cur_term = x**i/np.math.factorial(i)
...         result += cur_term
...         i += 1
...     return result

# Compute the gradient.
>>> d_taylor_exp = grad(taylor_exp)
# Note that differentiation in autograd only works with float values.
>>> d_taylor_exp(2.)
array(7.388994708994709)
```

Problem 7. Write a function that uses autograd to take the first and second derivatives of the Taylor series of $\sin(x)$. Plot the original function along with its two derivatives on the interval $[-\pi, \pi]$.

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

>>> grad_f = elementwise_grad(f)
```

```
>>> grad_f(anp.array([1.,2.,3.]))
array([-1.13338111, -1.04855565, -1.04224253])
```

While the `grad()` function can only find the gradient of functions that output scalars, `jacobian()` can find the gradient of vectors. The following example 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 8.

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 using SymPy, the second order centered difference quotient and autograd. Print the time it takes to compute each Jacobian evaluated at $(x,y) = (1,1)$. Do not include the initialization of any variables or functions in the computation time. Return the value of the autograd approximation.

See `https://github.com/HIPS/autograd` for more examples with autograd.

9 Newton's Method

Lab Objective: *Newton's method, the classical method for finding the zeros of a function, is one of the most important algorithms of all time. In this lab, we implement Newton's method in arbitrary dimensions and use it to solve a few interesting problems. We also explore in some detail the convergence (or lack of convergence) of the method under various circumstances.*

Iterative Methods

An *iterative method* is an algorithm that must be applied repeatedly to obtain a result. The general idea behind any iterative method is to make an initial guess at the solution to a problem, apply a few easy computations to better approximate the solution, use that approximation as the new initial guess, and repeat until done. More precisely, let F be some function used to approximate the solution to a problem. Starting with an initial guess of x_0, compute

$$x_{k+1} = F(x_k) \tag{9.1}$$

for successive values of k to generate a sequence $\{x_k\}_{k=0}^{\infty}$ that hopefully converges to the true solution. If the terms of the sequence are vectors, they are denoted by $\mathbf{x}_k$.

In the best case, the iteration converges to the true solution x, written $\lim_{k\to\infty} x_k = x$ or $x_k \to x$. In the worst case, the iteration continues forever without approaching the solution. In practice, iterative methods require carefully chosen *stopping criteria* to guarantee that the algorithm terminates at some point. The general approach is to continue iterating until the difference between two consecutive approximations is sufficiently small, and to iterate no more than a specific number of times. That is, choose a very small $\epsilon > 0$ and an integer $N \in \mathbb{N}$, and update the approximation using (9.1) until either

$$|x_k - x_{k-1}| < \epsilon \qquad \text{or} \qquad k > N. \tag{9.2}$$

The choices for ϵ and N are significant: a "large" ϵ (such as 10^{-6}) produces a less accurate result than a "small" ϵ (such 10^{-16}), but demands less computations; a small N (10) also potentially lowers accuracy, but detects and halts nonconvergent iterations sooner than a large N (10,000). In code, ϵ and N are often named `tol` and `maxiters`, respectively (or similar).

While there are many ways to structure the code for an iterative method, probably the cleanest way is to combine a `for` loop with a `break` statement. As a very simple example, let $F(x) = \frac{x}{2}$. This method converges to $x = 0$ independent of starting point.

```
>>> F = lambda x: x / 2
>>> x0, tol, maxiters = 10, 1e-9, 8
>>> for k in range(maxiters):           # Iterate at most N times.
...     print(x0, end='  ')
...     x1 = F(x0)                     # Compute the next iteration.
...     if abs(x1 - x0) < tol:         # Check for convergence.
...         break                      # Upon convergence, stop iterating.
...     x0 = x1                        # Otherwise, continue iterating.
...
10  5.0  2.5  1.25  0.625  0.3125  0.15625  0.078125
```

In this example, the algorithm terminates after $N = 8$ iterations (the maximum number of allowed iterations) because the tolerance condition $|x_k - x_{k-1}| < 10^{-9}$ is not met fast enough. If N had been larger (say 40), the iteration would have quit early due to the tolerance condition.

Newton's Method in One Dimension

Newton's method is an iterative method for finding the zeros of a function. That is, if $f : \mathbb{R} \to \mathbb{R}$, the method attempts to find a $\bar{x}$ such that $f(\bar{x}) = 0$. Beginning with an initial guess x_0, calculate successive approximations for $\bar{x}$ with the recursive sequence

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}. \tag{9.3}$$

The sequence converges to the zero $\bar{x}$ of f if three conditions hold:

1. f and f' exist and are continuous,
2. $f'(\bar{x}) \neq 0$, and
3. x_0 is "sufficiently close" to $\bar{x}$.

In applications, the first two conditions usually hold. If $\bar{x}$ and x_0 are not "sufficiently close," Newton's method may converge very slowly, or it may not converge at all. However, when all three conditions hold, Newton's method converges quadratically, meaning that the maximum error is squared at every iteration. This is very quick convergence, making Newton's method as powerful as it is simple.

Problem 1. Write a function that accepts a function f, an initial guess x_0, the derivative f', a stopping tolerance defaulting to 10^{-5}, and a maximum number of iterations defaulting to 15. Use Newton's method as described in (9.3) to compute a zero $\bar{x}$ of f. Terminate the algorithm when $|x_k - x_{k-1}|$ is less than the stopping tolerance or after iterating the maximum number of allowed times. Return the last computed approximation to $\bar{x}$, a boolean value indicating whether or not the algorithm converged, and the number of iterations completed.

Test your function against functions like $f(x) = e^x - 2$ (see Figure 9.1) or $f(x) = x^4 - 3$. Check that the computed zero $\bar{x}$ satisfies $f(\bar{x}) \approx 0$. Also consider comparing your function to `scipy.optimize.newton()`, which accepts similar arguments.

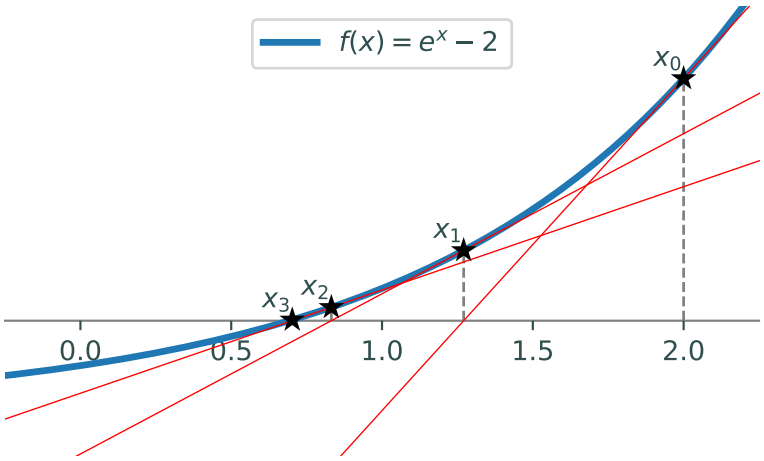


Figure 9.1: Newton's method approximates the zero of a function (blue) by choosing as the next approximation the x-intercept of the tangent line (red) that goes through the point $(x_k, f(x_k))$. In this example, $f(x) = e^x - 2$, which has a zero at $\bar{x} = \log(2)$. Setting $x_0 = 2$ and using (9.3) to iterate, we have $x_1 = x_0 - \frac{f(x_0)}{f'(x_0)} = 2 - \frac{e^2-2}{e^2} \approx 1.2707$. Similarly, $x_2 \approx 0.8320$, $x_3 \approx .7024$, and $x_4 \approx 0.6932$. After only a few iterations, the zero $\log(2) \approx 0.6931$ is already computed to several digits of accuracy.

Note

Newton's method can be used to find zeros of functions that are hard to solve for analytically. For example, the function $f(x) = \frac{\sin(x)}{x} - x$ is not continuous on any interval containing 0, but it can be made continuous by defining $f(0) = 1$. Newton's method can then be used to compute the zeros 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 (so $r = .05$ corresponds to 5% interest). In addition, 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

$$P_1[(1 + r)^{N_1} - 1] = P_2[1 - (1 + r)^{-N_2}].$$

Write a function that, given N_1, N_2, P_1, and P_2, uses Newton's method to determine r. For the initial guess, use $r_0 = 0.1$.
(Hint: Construct $f(r)$ such that when $f(r) = 0$, the equation is satisfied. Also compute $f'(r)$.)

To test your function, if $N_1 = 30, N_2 = 20, P_1 = 2000$, and $P_2 = 8000$, then $r \approx 0.03878$. (From Atkinson, page 118).

Backtracking

Newton's method may not converge for a variety of reasons. One potential problem occurs when the step from x_k to x_{k+1} is so large that the zero is stepped over completely. *Backtracking* is a strategy that combats the problem of overstepping by moving only a fraction of the full step from x_k to x_{k+1}. This suggests a slight modification to (9.3).

$$x_{k+1} = x_k - \alpha \frac{f(x_k)}{f'(x_k)}, \qquad \alpha \in (0, 1] \tag{9.4}$$

Note that setting $\alpha = 1$ results in the exact same method defined in (9.3), but for $\alpha \in (0, 1)$, only a fraction of the step is taken at each iteration.

Problem 3. Modify your function from Problem 1 so that it accepts a parameter α that defaults to 1. Incorporate (9.4) to allow for backtracking.

To test your modified function, consider $f(x) = x^{1/3}$. The command `x**(1/3.)` fails when `x` is negative, so the function can be defined with NumPy as follows.

```
import numpy as np
f = lambda x: np.sign(x) * np.power(np.abs(x), 1./3)
```

With $x_0 = .01$ and $\alpha = 1$, the iteration should **not** converge. However, setting $\alpha = .4$, the iteration should converge to a zero that is close to 0.

The backtracking constant α is significant, as it can result in faster convergence or convergence to a different zero (see Figure 9.2). However, it is not immediately obvious how to choose an optimal value for α.

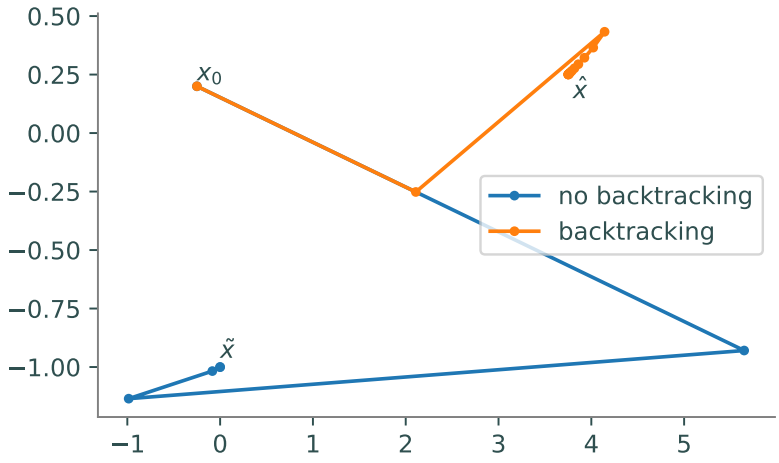


Figure 9.2: Starting at the same initial value but using different backtracking constants can result in convergence to two different solutions. The blue line converges to $\tilde{\mathbf{x}} = (0, -1)$ with $\alpha = 1$ in 5 iterations of Newton's method while the orange line converges to $\hat{\mathbf{x}} = (3.75, .25)$ with $\alpha = 0.4$ in 15 iterations. Note that the points in this example are 2-dimensional, which is discussed in the next section.

Problem 4. Write a function that accepts the same arguments as your function from Problem 3 except for α. Use Newton's method to find a zero of f using various values of α in the interval $(0, 1]$. Plot the values of α against the number of iterations performed by Newton's method. Return a value for α that results in the lowest number of iterations.

A good test case for this problem is the function $f(x) = x^{1/3}$ discussed in Problem 3. In this case, your plot should show that the optimal value for α is actually closer to .3 than to .4.

Newton's Method in Higher Dimensions

Newton's method can be generalized to work on functions with a multivariate domain and range. Let $f : \mathbb{R}^n \to \mathbb{R}^n$ be given by $f(\mathbf{x}) = [f_1(\mathbf{x})\ f_2(\mathbf{x})\ \dots\ f_k(\mathbf{x})]^\mathsf{T}$, with $f_i : \mathbb{R}^n \to \mathbb{R}$ for each i. The derivative $Df : \mathbb{R}^n \to \mathbb{R}^{n\times n}$ is the $n \times n$ Jacobian matrix of f.

$$Df = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_n}{\partial x_1} & \cdots & \frac{\partial f_n}{\partial x_n} \end{bmatrix}$$

In this setting, Newton's method seeks a vector $\bar{\mathbf{x}}$ such that $f(\bar{\mathbf{x}}) = \mathbf{0}$, the vector of n zeros. With backtracking incorporated, (9.4) becomes the following.

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \alpha Df(\mathbf{x}_k)^{-1} f(\mathbf{x}_k). \tag{9.5}$$

Note that if $n = 1$, (9.5) is exactly (9.4) because in that case, $Df(x)^{-1} = 1/f'(x)$.

This vector version of Newton's method terminates when the maximum number of iterations is reached or the difference between successive approximations is less than a predetermined tolerance ϵ with respect to a vector norm, that is, $||\mathbf{x}_k - \mathbf{x}_{k-1}|| < \epsilon$.

Problem 5. Modify your function from Problems 1 and 3 so that it can compute a zero of a function $f : \mathbb{R}^n \to \mathbb{R}^n$ for any $n \in \mathbb{N}$. Take the following tips into consideration.

- If $n > 1$, f should be a function that accepts a 1-D NumPy array with n entries and returns another NumPy array with n entries. Similarly, Df should be a function that accepts a 1-D array with n entries and returns a $n \times n$ array. In other words, f and Df are callable functions, but $f(\mathbf{x})$ is a vector and $Df(\mathbf{x})$ is a matrix.
- `np.isscalar()` may be useful for determining whether or not $n > 1$.
- Instead of computing $Df(\mathbf{x}_k)^{-1}$ directly at each step, solve the system $Df(\mathbf{x}_k)\mathbf{y}_k = f(\mathbf{x}_k)$ and set $\mathbf{x}_{k+1} = \mathbf{x}_k - \alpha\mathbf{y}_k$. Always avoid taking matrix inverses when possible.
- The stopping criterion now requires using a norm function instead of `abs()`.

After your modifications, carefully verify that your function still works in the case that $n = 1$, and that your functions from Problems 2 and 4 also still work correctly. In addition, your function from Problem 4 should also work for any $n \in N$.

Problem 6. 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

$$\begin{aligned}\gamma xy - x(1+y) &= 0\\ -xy + (\delta - y)(1+y) &= 0,\end{aligned}$$

where γ and δ are parameters that depend on various physical features of the system.

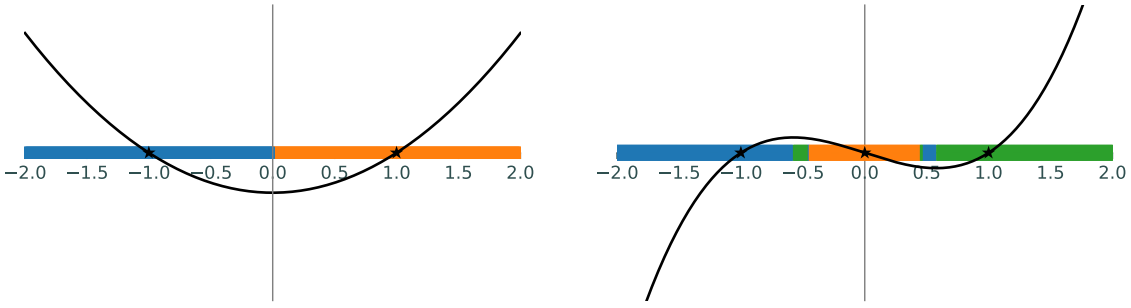
For this problem, assume the typical values $\gamma = 5$ and $\delta = 1$, for which the system has solutions at $(x, y) = (0, 1), (0, -1)$, and $(3.75, .25)$. Write a function that finds an initial point $\mathbf{x}_0 = (x_0, y_0)$ such that Newton's method converges to either $(0, 1)$ or $(0, -1)$ with $\alpha = 1$, and to $(3.75, .25)$ with $\alpha = 0.55$. As soon as a valid $\mathbf{x}_0$ is found, return it (stop searching).
(Hint: search within the rectangle $[-\frac{1}{4}, 0] \times [0, \frac{1}{4}]$.)

(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

When a function f has many zeros, the zero that Newton's method converges to depends on the initial guess x_0. For example, the function $f(x) = x^2 - 1$ has zeros 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 9.3a). The regions $(-\infty, 0)$ and $(0, \infty)$ are called the *basins of attraction* of f. Starting in one basin of attraction leads to finding one zero, while starting in another basin yields a different zero.

When f is a polynomial of degree greater than 2, the basins of attraction are much more interesting. For example, the basis of attraction for $f(x) = x^3 - x$ are shown in Figure 9.3b. The basin for the zero at the origin is connected, but the other two basins are disconnected and share a kind of symmetry.



(a) Basins of attraction for $f(x) = x^2 - 1$.

(b) Basins of attraction for $f(x) = x^3 - x$.

Figure 9.3: Basins of attraction with $\alpha = 1$. Since choosing a different value for α can change which zero Newton's method converges to, the basins of attraction may change for other values of α.

It can be shown that Newton's method converges in any Banach space with only slightly stronger hypotheses than those discussed previously. In particular, Newton's method can be performed over the complex plane $\mathbb{C}$ to find imaginary zeros of functions. Plotting the basins of attraction over $\mathbb{C}$ yields some interesting results.

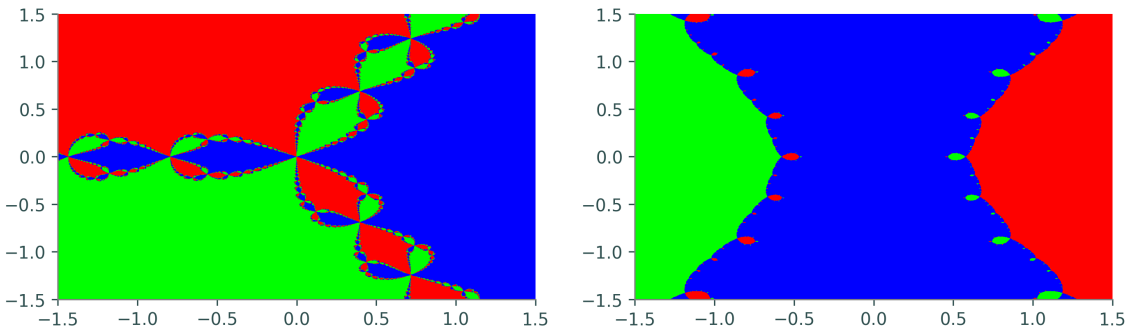
The zeros of $f(x) = x^3 - 1$ are 1, and $-\frac{1}{2} \pm \frac{\sqrt{3}}{2}i$. To plot the basins of attraction for $f(x) = x^3 - 1$ on the square complex domain $X = \{a+bi \mid a \in [-\frac{3}{2}, \frac{3}{2}], b \in [-\frac{3}{2}, \frac{3}{2}]\}$, create an initial grid of complex points in this domain using `np.meshgrid()`.

```
>>> x_real = np.linspace(-1.5, 1.5, 500)    # Real parts.
>>> x_imag = np.linspace(-1.5, 1.5, 500)    # Imaginary parts.
>>> X_real, X_imag = np.meshgrid(x_real, x_imag)
>>> X_0 = X_real + 1j*X_imag                # Combine real and imaginary parts.
```

The grid X_0 is a 500×500 array of complex values to use as initial points for Newton's method. Array broadcasting makes it easy to compute an iteration of Newton's method at every grid point.

```
>>> f = lambda x: x**3 - 1
>>> Df = lambda x: 3*x**2
>>> X_1 = X_0 - f(X_0)/Df(X_0)
```

After enough iterations, the (i, j)th element of the grid X_k corresponds to the zero of f that results from using the (i, j)th element of X_0 as the initial point. For example, with $f(x) = x^3 - 1$, each entry of X_k should be close to 1, $-\frac{1}{2} + \frac{\sqrt{3}}{2}i$, or $-\frac{1}{2} - \frac{\sqrt{3}}{2}i$. Each entry of X_k can then be assigned a value indicating which zero it corresponds to. Some results of this process are displayed below.



(a) Basins of attraction for $f(x) = x^3 - 1$.

(b) Basins of attraction for $f(x) = x^3 - x$.

Figure 9.4

Note

Notice that in some portions of Figure 9.4a, 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 kind of fractal is called a *Newton fractal*.

Newton fractals show that the long-term behavior of Newton's 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 phenomenon is called *chaos* in mathematics.

Problem 7. Write a function that accepts a function $f : \mathbb{C} \to \mathbb{C}$, its derivative $f' : \mathbb{C} \to \mathbb{C}$, an array `zeros` of the zeros of f, bounds $[r_{\min}, r_{\max}, i_{\min}, i_{\max}]$ for the domain of the plot, an integer `res` that determines the resolution of the plot, and number of iterations `iters` to run the iteration. Compute and plot the basins of attraction of f in the complex plane over the specified domain in the following steps.

1. Construct a `res`$\times$`res` grid X_0 over the domain $\{a + bi \mid a \in [r_{\min}, r_{\max}], b \in [i_{\min}, i_{\max}]\}$.
2. Run Newton's method (without backtracking) on X_0 `iters` times, obtaining the `res`$\times$`res` array X_k. To avoid the additional computation of checking for convergence at each step, do not use your function from Problem 5.
3. X_k cannot be directly visualized directly because its values are complex. Solve this issue by creating another `res`$\times$`res` array Y. To compute the (i, j)th entry $Y_{i,j}$, determine which zero of f is closest to the (i, j)th entry of X_k. Set $Y_{i,j}$ to the index of this zero in the array `zeros`. If there are R distinct zeros, each $Y_{i,j}$ should be one of $0, 1, \ldots, R - 1$. (Hint: `np.argmin()` may be useful.)
4. Use `plt.pcolormesh()` to visualize the basins. Recall that this function accepts three array arguments: the x-coordinates (in this case, the real components of the initial grid), the y-coordinates (the imaginary components of the grid), and an array indicating color values (Y). Set `cmap="brg"` to get the same color scheme as in Figure 9.4.

Test your function using $f(x) = x^3 - 1$ and $f(x) = x^3 - x$. The resulting plots should resemble Figures 9.4a and 9.4b, respectively.

10 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. Both of these concepts are important for answering the crucial question, "is my computer telling the truth?" In this lab, we examine the conditioning of common linear algebra problems, including computing polynomial roots and matrix eigenvalues. We also present an example to demonstrate how two different algorithms for the same problem may not have the same level of stability.*

Conditioning

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

$$\hat{\kappa}(\mathbf{x}) = \lim_{\delta \to 0^+} \sup_{\|\mathbf{h}\| < \delta} \frac{\|f(\mathbf{x}+\mathbf{h}) - f(\mathbf{x})\|}{\|\mathbf{h}\|}. \tag{10.1}$$

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.

$$\kappa(\mathbf{x}) = \lim_{\delta \to 0^+} \sup_{\|\mathbf{h}\| < \delta} \left(\frac{\|f(\mathbf{x}+\mathbf{h}) - f(\mathbf{x})\|}{\|f(\mathbf{x})\|} \Big/ \frac{\|\mathbf{h}\|}{\|\mathbf{x}\|} \right) = \frac{\|\mathbf{x}\|}{\|f(\mathbf{x})\|} \hat{\kappa}(\mathbf{x}). \tag{10.2}$$

A function with a large condition number is called *ill-conditioned*. Small changes to the input of an ill-conditioned function may produce large changes in output. It is important to know if a function is ill-conditioned because floating point representation almost always introduces some input error, and therefore the outputs of ill-conditioned functions cannot be trusted.

The *condition number* of a matrix A, $\kappa(A) = \|A\|\|A^{-1}\|$, 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. Recall that if σ is a singular value of A, $\frac{1}{\sigma}$ is a singular value of A^{-1}. Thus, we have that

$$\kappa(A) = \frac{\sigma_{\max}}{\sigma_{\min}}, \tag{10.3}$$

which is also a valid equation for non-square matrices.

Achtung!

Ill-conditioned matrices can wreak havoc in even simple applications. For example, the matrix

$$A = \begin{bmatrix} 1 & 1 \\ 1 & 1.0000000001 \end{bmatrix}$$

is extremely ill-conditioned, with $\kappa(A) \approx 4 \times 10^{10}$. Solving the systems $A\mathbf{x} = \mathbf{b}_1$ and $A\mathbf{x} = \mathbf{b}_2$ can result in wildly different answers, even when $\mathbf{b}_1$ and $\mathbf{b}_2$ are extremely close.

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

>>> A = np.array([[1, 1], [1, 1+1e-10]])
>>> np.linalg.cond(A)
39999991794.058899

# Set up and solve a simple system of equations.
>>> b1 = np.array([2, 2])
>>> x1 = la.solve(A, b1)
>>> print(x1)
[ 2.  0.]

# Solve a system with a very slightly different vector b.
>>> b2 = np.array([2, 2+1e-5])
>>> la.norm(b1 - b2)
>>> x2 = la.solve(A, b2)
>>> print(x2)
[-99997.99172662  99999.99172662]   # This solution is hugely different!
```

If you find yourself working with matrices that have large condition numbers, check your math carefully or try to reformulate the problem entirely.

Note

An *orthonormal matrix* U has orthonormal columns and satisfies $U^\mathsf{T}U = I$ and $\|U\|_2 = 1$. If U is square, then $U^{-1} = U^\mathsf{T}$ and U^T is also orthonormal. Therefore $\kappa(U) = \|U\|_2\|U^{-1}\|_2 = 1$. Even if U is not square, all of its singular values are equal to 1, and again $\kappa(U) = \sigma_{\max}/\sigma_{\min} = 1$.

The condition number of a matrix cannot be less than 1 since $\sigma_{\max} \geq \sigma_{\min}$ by definition. Thus orthonormal matrices are, in a sense, the best kind of matrices for computations. This is one of the main reasons why numerical algorithms based on the QR decomposition or the SVD are so important.

Problem 1. Write a function that accepts a matrix A and computes its condition number using (10.3). Use `scipy.linalg.svd()`, or `scipy.linalg.svdvals()` to compute the singular values of A. Avoid computing A^{-1}. If the smallest singular value is 0, return ∞ (`np.inf`).

Validate your function by comparing it to `np.linalg.cond()`. Check that orthonormal matrices have a condition number of 1 (use `scipy.linalg.qr()` to generate an orthonormal matrix) and that singular matrices have a condition number of ∞ according to your function.

The Wilkinson Polynomial

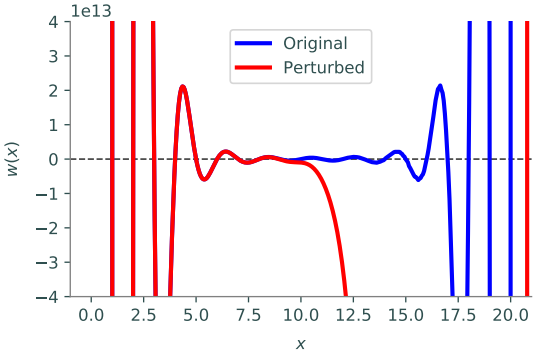
Let $f : \mathbb{C}^{n+1} \to \mathbb{C}^n$ be the function that maps a collection of $n+1$ coefficients $(c_n, c_{n-1}, \dots, c_0)$ to the n roots of the polynomial $c_n x^n + c_{n-1}x^{n-1} + \dots + c_2 x^2 + c_1 x + c_0$. Finding polynomial roots is an extremely ill-conditioned problem in general, so the condition number of f is likely very large. To see this, consider the *Wilkinson polynomial*, made famous by James H. Wilkinson in 1963.

$$w(x) = \prod_{r=1}^{20}(x - r) = x^{20} - 210x^{19} + 20615x^{18} - 1256850x^{17} + \cdots$$

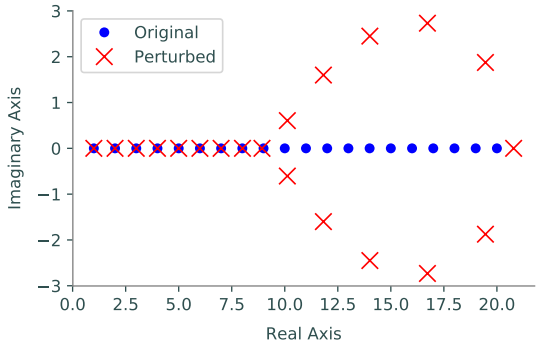
Let $\tilde{w}(x)$ be $w(x)$ where the coefficient on x^{19} is very slightly perturbed from -210 to -210.0000001. The following code computes and compares the roots of $\tilde{w}(x)$ and $w(x)$ using NumPy and SymPy.

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

# 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)))[0]
>>> w_coeffs = np.array(w.all_coeffs())
>>> print(w_coeffs[:6])
[1 -210 20615 -1256850 53327946 -1672280820]

# Perturb one of the coefficients very slightly.
>>> h = np.zeros(21)
>>> h[1]=1e-7
>>> new_coeffs = w_coeffs - h
>>> print(new_coeffs[:6])
[1 -210.000000100000 20615 -1256850 53327946 -1672280820]

# Use NumPy to compute the roots of the perturbed polynomial.
>>> new_roots = np.roots(np.poly1d(new_coeffs))
```

Figure 10.1a plots $w(x)$ and $\tilde{w}(x)$ together, and Figure 10.1b and compares 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.

Figure 10.1

Figure 10.1 clearly indicates that a very small change in just a single coefficient drastically changes the nature of the polynomial and its roots. To quantify the difference, estimate the condition numbers (this example uses the L^∞ norm to compute $\hat{\kappa}$ and κ).

```
# Sort the roots to ensure that they are in the same order.
>>> w_roots = np.sort(w_roots)
>>> new_roots = np.sort(new_roots)

# Estimate the absolute condition number in the infinity norm.
>>> k = la.norm(new_roots - w_roots, np.inf) / la.norm(h, 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.

1. Computing the quotients in (10.1) and (10.2) for a fixed perturbation $\mathbf{h}$ only approximates the condition number. The true 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 there is no way to be sure.

2. This example assumes that NumPy's root-finding algorithm, `np.roots()`, is *stable*, so that the difference between `w_roots` and `new_roots` is due to the difference in coefficients, and not to problems with `np.roots()`. We will return to this issue in the next section.

Even with these caveats, it is apparent that root finding is a difficult problem to solve correctly. Always check your math carefully when dealing with polynomial roots.

Problem 2. Write a function that carries out the following experiment 100 times.

1. Randomly perturb the true coefficients of the Wilkinson polynomial by replacing each coefficient c_i with $c_i * r_i$, 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.
   (Hint: use a pixel marker, `marker=','`, to avoid overcrowding the figure.)
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 10.2. Finally, return the average computed absolute and relative condition numbers.

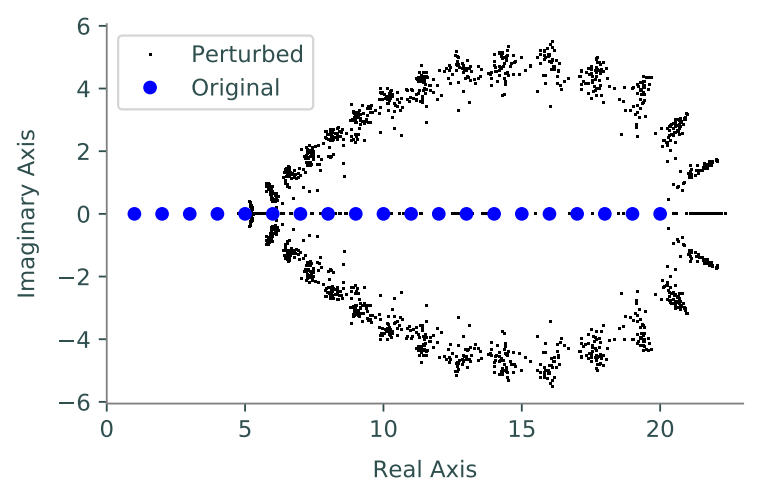


Figure 10.2: This figure replicates Figure 12.1 on p. 93 of *Numerical Linear Algebra* by Lloyd N. Trefethen and David Bau III.

Calculating Eigenvalues

Let $f : M_n(\mathbb{C}) \to \mathbb{C}^n$ be the function that maps an $n \times n$ matrix with complex entries to its n eigenvalues. This problem is well-conditioned for symmetric matrices, but it 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 $\tilde{A} = A + H$ is a pertubation of A and $\tilde{\boldsymbol{\lambda}}$ are its eigenvalues, then the condition numbers of f can be estimated by

$$\hat{\kappa}(A) = \frac{\|\boldsymbol{\lambda} - \tilde{\boldsymbol{\lambda}}\|}{\|H\|}, \qquad \kappa(A) = \frac{\|A\|}{\|\boldsymbol{\lambda}\|}\hat{\kappa}(A). \tag{10.4}$$

Problem 3. Write a function that accepts a matrix A and estimates the condition number of the eigenvalue problem using (10.4). For the perturbation H, construct a matrix with complex entries where the real and imaginary parts are drawn from normal distributions centered at 0 with standard deviation $\sigma = 10^{-10}$.

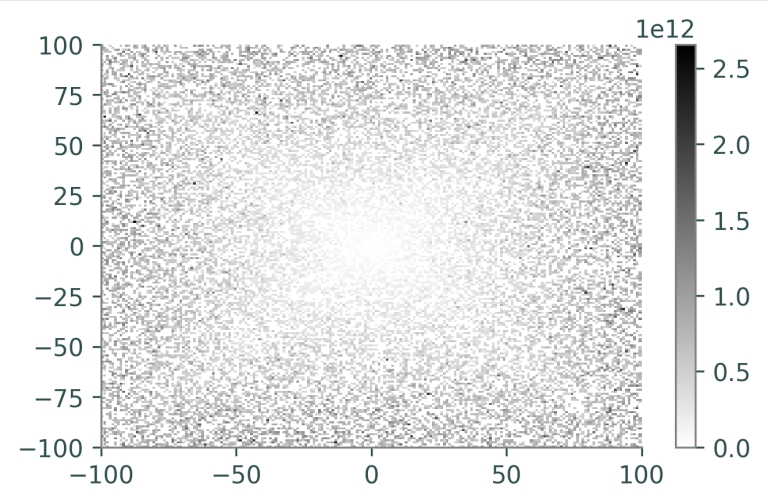
```
reals = np.random.normal(0, 1e-10, A.shape)
imags = np.random.normal(0, 1e-10, A.shape)
H = reals + 1j*imags
```

Use `scipy.linalg.eig()` or `scipy.linalg.eigvals()` to compute the eigenvalues of A and $A + H$, and 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 bounds $[x_{\min}, x_{\max}, y_{\min}, y_{\max}]$ and an integer `res`. Use your function from Problem 3 to compute the relative condition number of the eigenvalue problem for the 2×2 matrix

$$\begin{bmatrix} 1 & x \\ y & 1 \end{bmatrix}$$

at every point of an evenly spaced `res`$\times$`res` grid over the domain $[x_{\min}, x_{\max}] \times [y_{\min}, y_{\max}]$. Plot these estimated relative condition numbers using `plt.pcolormesh()` and the colormap `cmap='gray_r'`. With `res=200`, your plot should look similar to the following figure.



Problem 4 shows that the conditioning of the eigenvalue problem depends heavily on the matrix, and that it is difficult to know a priori how bad the problem will be. Luckily, most real-world problems requiring eigenvalues are symmetric. In their book on Numerical Linear Algebra, L. Trefethen and D. Bau III summed up the issue of conditioning and eigenvalues when they stated, "*if the answer is highly sensitive to perturbations, you have probably asked the wrong question.*"

Stability

The *stability* of an algorithm is measured by the error in its output. Let $f : \mathbb{R}^m \to \mathbb{R}^n$ be a problem to be solved, as in the previous section, and let $\tilde{f}$ be an actual algorithm for solving the problem. 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 called *stable* if its relative forward error is small.[1]

As an example, consider again NumPy's root-finding algorithm that we used to investigate the Wilkinson polynomial. The exact roots of $w(x)$ are clearly $1, 2, \ldots, 20$. Had we not known this, we could have tried computing the roots from the coefficients using `np.roots()` (without perturbing the coefficients at all).

```
# w_coeffs holds the coefficients and w_roots holds the true roots.
>>> computed_roots = np.sort(np.roots(np.poly1d(w_coeffs)))
>>> print(computed_roots[:6])       # The computed roots are close to integers.
[ 1.          2.          3.          3.99999999  5.00000076  5.99998749]

# Compute the forward error.
>>> forward_error = la.norm(w_roots - computed_roots)
>>> print(forward_error)
0.020612653126379665

# Compute the relative forward error.
>>> forward_error / la.norm(w_roots)
0.00038476268486104599              # The error is nice and small.
```

This analysis suggests that `np.roots()` is a stable algorithm, so large condition numbers of Problem 2 really are due to the poor conditioning of the problem, not the way in which the problem was solved.

> **Note**
>
> Conditioning is a property of a **problem** to be solved, such as finding the roots of a polynomial or calculating eigenvalues. Stability is a property of an **algorithm** to solve a problem, such as `np.roots()` or `scipy.linalg.eig()`. If a problem is ill-conditioned, any algorithm used to solve that problem may result in suspicious solutions, even if that algorithm is stable.

Least Squares

The *ordinary least squares* (OLS) 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 $A^\mathsf{H}A\mathbf{x} = A^\mathsf{H}\mathbf{b}$, called the *normal equations*. A common application of least squares is polynomial approximation. Given a set of m data points $\{(x_k, y_k)\}_{k=1}^m$, the goal is to find the set of coefficients $\{c_i\}_{i=0}^n$ such that

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

[1] See the Additional Material section for alternative (and more rigorous) definitions of algorithmic stability.

for all k, with the smallest possible error. These m linear equations yield the following linear system.

$$A\mathbf{x} = \begin{bmatrix} x_1^n & x_1^{n-1} & \cdots & x_1^2 & x_1 & 1 \\ x_2^n & x_2^{n-1} & \cdots & x_2^2 & x_2 & 1 \\ x_3^n & x_3^{n-1} & \cdots & x_3^2 & x_3 & 1 \\ \vdots & \vdots & & \vdots & \vdots & \vdots \\ x_m^n & x_m^{n-1} & \cdots & x_m^2 & x_m & 1 \end{bmatrix} \begin{bmatrix} c_n \\ c_{n-1} \\ \vdots \\ c_2 \\ c_1 \\ c_0 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_m \end{bmatrix} = \mathbf{b} \tag{10.5}$$

Problem 5. Write a function that accepts an integer n. Solve for the coefficients of the polynomial of degree n that best fits the data found in `stability_data.npy`. Use two approaches to get the least squares solution:

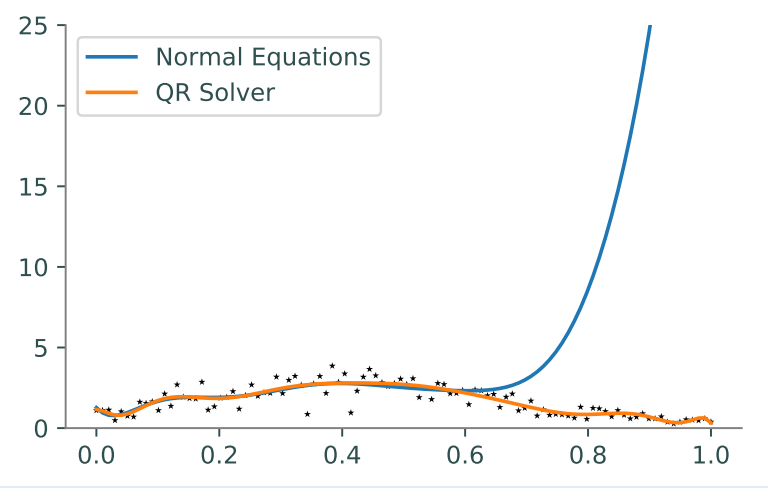
1. Use `la.inv()` to solve the normal equations: $\mathbf{x} = (A^\mathsf{T}A)^{-1}A^\mathsf{T}\mathbf{b}$. Although this approach seems intuitive, it is actually highly unstable and can return an answer with a very large forward error.
2. Use `la.qr()` with `mode='economic'` and `la.solve_triangular()` to solve the system $R\mathbf{x} = Q^\mathsf{T}\mathbf{b}$, which is equivalent to solving the normal equations. This algorithm has the advantage of being stable.

Load the data and set up the system (10.5) with the following code.

```
xk, yk = np.load("stability_data.npy").T
A = np.vander(xk, n+1)
```

Plot the resulting polynomials together with the raw data points. Return the forward error $\|A\mathbf{x} - \mathbf{b}\|_2$ of both approximations.
(Hint: The function `np.polyval()` will be helpful for plotting the resulting polynomials.)

Test your function using various values of n, taking special note of what happens for values of n near 14 (pictured below).



Catastrophic Cancellation

When a computer takes the difference of two very similar numbers, the result is often stored with a small number of significant digits and the tiniest bit of information is lost. However, these small errors can propagate into large errors later down the line. This phenomenon is called *catastrophic cancellation*, and is a common cause for numerical instability.

Catastrophic cancellation is a potential problem whenever floats or large integers that are very close to one another are subtracted. This problem can be avoided by either rewriting the program to not use subtraction, or by increasing the number of significant digits that the computer tracks.

For example, consider the simple problem of computing $\sqrt{a} - \sqrt{b}$. The computation can be done directly with subtraction, or by performing the equivalent division

$$\sqrt{a} - \sqrt{b} = (\sqrt{a} - \sqrt{b})\frac{\sqrt{a} + \sqrt{b}}{\sqrt{a} + \sqrt{b}} = \frac{a - b}{\sqrt{a} + \sqrt{b}}.$$

```
>>> from math import sqrt           # np.sqrt() fails for very large numbers.

>>> a = 10**20 + 1
>>> b = 10**20
>>> sqrt(a) - sqrt(b)               # Do the subtraction directly.
0.0                                 # a != b, so information has been lost.

>>> (a - b) / (sqrt(a) + sqrt(b))   # Use the alternative formulation.
5e-11                               # Much better!
```

In this example, a and b are distinct enough that the computer can still tell that $a - b = 1$, but $\sqrt{a}$ and $\sqrt{b}$ are so close to each other that $\sqrt{a} - \sqrt{b}$ is computed as 0.

Problem 6. Let $I(n) = \int_0^1 x^n e^{x-1} dx$. It can be shown that for a positive integer n,

$$I(n) = (-1)^n !n + (-1)^{n+1}\frac{n!}{e}, \tag{10.6}$$

where $!n = n! \sum_{k=0}^{n} \frac{(-1)^k}{k!}$ is the *subfactorial* of n. Write a function to do the following.

1. Use SymPy's `sy.integrate()` to evaluate the integral form of $I(n)$ for $n = 5, 10, \dots, 50$. Convert the symbolic results of each integration to a float. Since this is done symbolically, these values can be accepted as the true values of $I(n)$.
   (Hint: be careful that the values of n in the integrand are actual integers, not floats.)

2. Use (10.6) to compute $I(n)$ for the same values of n. Use `sy.subfactorial()` to compute $!n$ and `sy.factorial()` to compute $n!$.
   (Hint: be careful to only pass actual integers to these functions.)

3. Plot the relative forward error of the results computed in step 2 at each of the given values of n. Use a log scale on the y-axis. Is (10.6) a stable way to compute $I(n)$? Why?

The examples presented in this lab are just a few of the ways that a mathematical problem can turn into a computational train wreck. Always use stable algorithms when possible, and remember to check if problems are well conditioned or not.

Additional Material

Other Notions of Stability

The definition of stability can be made more rigorous in the following way. Let f be a problem to solve and $\tilde{f}$ an algorithm to solve it. If for every $\mathbf{x}$ in the domain there exists a $\tilde{\mathbf{x}}$ such that

$$\frac{\|\tilde{\mathbf{x}} - \mathbf{x}\|}{\|\mathbf{x}\|} \quad \text{and} \quad \frac{\|\tilde{f}(\mathbf{x}) - f(\tilde{\mathbf{x}})\|}{\|f(\tilde{\mathbf{x}})\|}$$

are small (close to $\epsilon_{\text{machine}} \approx 10^{-16}$), then $\tilde{f}$ is called stable. In other words, "A stable algorithm gives nearly the right answer to nearly the right question" (Trefethen, Bao, 104). Note carefully that the quantity on the right is slightly different from the plain forward error introduced earlier.

Stability is desirable, but plain stability isn't the best possible condition. For example, if for every input $\mathbf{x}$ there exists a $\tilde{\mathbf{x}}$ such that $\|\tilde{\mathbf{x}} - \mathbf{x}\|/\|\mathbf{x}\|$ is small and $\tilde{f}(\mathbf{x}) = f(\tilde{\mathbf{x}})$ exactly, then $\tilde{f}$ is called *backward stable*. Thus "A backward stable algorithm gives exactly the right answer to nearly the right question" (Trefethen, Bao, 104). Backward stable algorithms are generally more trustworthy than stable algorithms, but they are also less common.

Stabilty of Linear System Solvers

The algorithms presented so far in this manual have different levels of stability. The LU decomposition (with pivoting) is usually very good, but there are some pathological examples of matrices that can cause it to break down. Even so, `scipy.linalg.solve()` uses the LU decomposition. The QR decomposition (also with pivoting) is generally considered to be a better option than the LU decomposition and is more stable. However, solving a linear system using the SVD is even more stable than using the QR decomposition. For this reason, `scipy.linalg.lstsq()` uses the SVD.

11 Monte Carlo Integration

Lab Objective: *Many important integrals cannot be evaluated symbolically because the integrand has no antiderivative. Traditional numerical integration techniques like Newton-Cotes formulas and Gaussian quadrature usually work well for one-dimensional integrals, but rapidly become inefficient in higher dimensions. Monte Carlo integration is an integration strategy that has relatively slow convergence, but that does extremely well in high-dimensional settings compared to other techniques. In this lab we implement Monte Carlo integration and apply it to a classic problem in statistics.*

Volume Estimation

Since the area of a circle of radius r is $A = \pi r^2$, one way to numerically estimate π is to compute the area of the unit circle. Empirically, we can estimate the area by randomly choosing points in a domain that encompasses the unit circle. The percentage of points that land within the unit circle approximates the percentage of the area of the domain that the unit circle occupies. Multiplying this percentage by the total area of the sample domain gives an estimate for the area of the circle.

Since the unit circle has radius $r = 1$, consider the square domain $\Omega = [-1, 1] \times [-1, 1]$. The following code samples 2000 uniformly distributed random points in Ω, determines what percentage of those points are within the unit circle, then multiplies that percentage by 4 (the area of Ω) to get an estimate for π.

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

# Get 2000 random points in the 2-D domain [-1,1]x[-1,1].
>>> points = np.random.uniform(-1, 1, (2,2000))

# Determine how many points are within the circle.
>>> lengths = la.norm(points, axis=0)
>>> num_within = np.count_nonzero(lengths < 1)

# Estimate the circle's area.
>>> 4 * (num_within / 2000)
3.198
```

The estimate $\pi \approx 3.198$ isn't perfect, but it only differs from the true value of π by about 0.0564. On average, increasing the number of sample points decreases the estimate error.

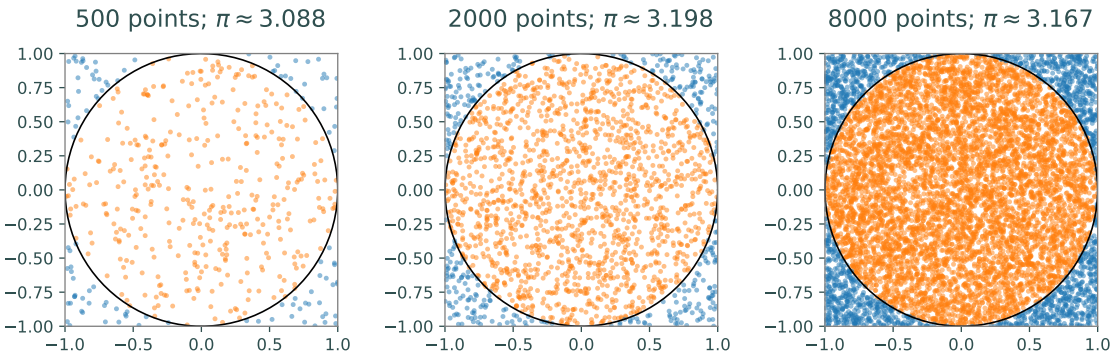


Figure 11.1: Estimating the area of the unit circle using random points.

Problem 1. The n-dimensional *open unit ball* is the set $U_n = \{\mathbf{x} \in \mathbb{R}^n \mid \|\mathbf{x}\|_2 < 1\}$. Write a function that accepts an integer n and a keyword argument N defaulting to 10^4. Estimate the volume of U_n by drawing N points over the n-dimensional domain $[-1,1]\times[-1,1]\times\cdots\times[-1,1]$. (Hint: the volume of $[-1,1]\times[-1,1]\times\cdots\times[-1,1]$ is 2^n.)

When $n = 2$, this is the same experiment outlined above so your function should return an approximation of π. The volume of the U_3 is $\frac{4}{3}\pi \approx 4.18879$, and the volume of U_4 is $\frac{\pi^2}{2} \approx 4.9348$. Try increasing the number of sample points N to see if your estimates improve.

Integral Estimation

The strategy for estimating π can be formulated as an integral problem. Define $f : \mathbb{R}^2 \to \mathbb{R}$ by

$$f(\mathbf{x}) = \begin{cases} 1 & \text{if } \|\mathbf{x}\|_2 < 1 \text{ } (\mathbf{x} \text{ is within the unit circle}) \\ 0 & \text{otherwise,} \end{cases}$$

and let $\Omega = [-1,1]\times[-1,1]$ as before. Then

$$\int_{-1}^{1}\int_{-1}^{1} f(x,y)\,dx\,dy = \int_{\Omega} f(\mathbf{x})\,dV = \pi.$$

To estimate the integral we chose N random points $\{\mathbf{x}_i\}_{i=1}^N$ in Ω. Since f indicates whether or not a point lies within the unit circle, the total number of random points that lie in the circle is the sum of the $f(\mathbf{x}_i)$. Then the average of these values, multiplied by the volume $V(\Omega)$, is the desired estimate.

$$\int_{\Omega} f(\mathbf{x})\,dV \approx V(\Omega)\frac{1}{N}\sum_{i=1}^{N} f(\mathbf{x}_i) \tag{11.1}$$

This remarkably simple equation can be used to estimate the integral of any function $f : \mathbb{R}^n \to \mathbb{R}$ over any domain $\Omega \subset \mathbb{R}^n$ and called the general formula for *Monte Carlo integration*.

The intuition behind (11.1) is that $\frac{1}{N}\sum_{i=1}^{N} f(\mathbf{x}_i)$ approximates the average value of f on Ω, and multiplying the approximate average value by the volume of Ω yields the approximate integral of f over Ω. This is a little easier to see in one dimension: for a single-variable function $f : \mathbb{R} \to \mathbb{R}$, the Average Value Theorem states that the average value of f over an interval $[a, b]$ is given by

$$f_{avg} = \frac{1}{b-a}\int_a^b f(x)\,dx.$$

Then using the approximation $f_{avg} \approx \frac{1}{N}\sum_{i=1}^{N} f(x_i)$, the previous equation becomes

$$\int_a^b f(x)\,dx = (b-a)f_{avg} \approx V(\Omega)\frac{1}{N}\sum_{i=1}^{N} f(x_i), \tag{11.2}$$

which is (11.1) in one dimension. In this setting $\Omega = [a, b]$ and hence $V(\Omega) = b - a$.

Problem 2. Write a function that accepts a function $f : \mathbb{R} \to \mathbb{R}$, bounds of integration a and b, and an integer N defaulting to 10^4. Use `np.random.uniform()` to sample N points over the interval $[a, b]$, then use (11.2) to estimate the integral

$$\int_a^b f(x)\,dx.$$

Test your function on the following integrals, or on other integrals that you can check by hand.

$$\int_{-4}^{2} x^2\,dx = 24 \qquad \int_{-2\pi}^{2\pi} \sin(x)\,dx = 0 \qquad \int_1^{10} \frac{1}{x}dx = \log(10) \approx 2.30259$$

$$\int_1^5 \left|\sin(10x)\cos(10x) + \sqrt{x}\sin(3x)\right|\,dx \approx 4.502$$

ACHTUNG!

Be careful not to use Monte Carlo integration to estimate integrals that do not converge. For example, since $1/x$ approaches ∞ as x approaches 0 from the right, the integral

$$\int_0^1 \frac{1}{x}\,dx$$

does not converge. Even so, attempts at Monte Carlo integration still return a finite value. Use various numbers of sample points to see whether or not the integral estimate is converging.

```
>>> for N in [5000, 7500, 10000]:
...     print(np.mean(1. / np.random.uniform(0, 1, N)), end='\t')
...
11.8451683722    25.5814419888    7.64364735049    # No convergence.
```

Integration in Higher Dimensions

The implementation of (11.1) for a function $f : \mathbb{R}^n \to \mathbb{R}$ with $n > 1$ introduces a few tricky details, but the overall procedure is the same for the case when $n = 1$. We consider only the case where $\Omega \subset \mathbb{R}^n$ is an n-dimensional box $[a_1, b_1] \times [a_2, b_2] \times \cdots \times [a_n, b_n]$.

1. If $n = 1$ then Ω is a line, so $V(\Omega) = b_1 - a_1$. If $n = 2$ then Ω is a rectangle, and hence $V(\Omega) = (b_1 - a_1)(b_2 - a_2)$, the product of the side lengths. The volume of a higher-dimensional box Ω is also the product of the side lengths.

$$V(\Omega) = \prod_{i=1}^{n} (b_i - a_i) \tag{11.3}$$

2. It is easy to sample uniformly over an interval $[a, b]$ with `np.random.uniform()`, or even over the n-dimensional cube $[a, b] \times [a, b] \times \cdots \times [a, b]$ (such as in Problem 1). However, if $a_i \neq a_j$ or $b_i \neq b_j$ for any $i \neq j$, the samples need to be constructed in a slightly different way.

   The interval $[0, 1]$ can be transformed to the interval $[a, b]$ by scaling it so that it is the same length as $[a, b]$, then shifting it to the appropriate location.

$$[0, 1] \xrightarrow{\text{scale by } b-a} [0, b - a] \xrightarrow{\text{shift by } a} [a, b]$$

   This suggests a strategy for sampling over $[a_1, b_1] \times [a_2, b_2] \times \cdots \times [a_n, b_n]$: sample uniformly from the n-dimensional box $[0, 1] \times [0, 1] \times \cdots \times [0, 1]$, multiply the ith component of each sample by $b_i - a_i$, then add a_i to that component.

$$[0, 1] \times \cdots \times [0, 1] \xrightarrow{\text{scale}} [0, b_1 - a_1] \times \cdots \times [0, b_n - a_n] \xrightarrow{\text{shift}} [a_1, b_1] \times \cdots \times [a_n, b_n] \tag{11.4}$$

Problem 3. Write a function that accepts a function $f : \mathbb{R}^n \to \mathbb{R}$, a list of lower bounds $[a_1, a_2, \ldots, a_n]$, a list of upper bounds $[b_1, b_2, \ldots, b_n]$, and an integer N defaulting to 10^4. Use (11.1), (11.3), and (11.4) with N sample points to estimate the integral

$$\int_\Omega f(\mathbf{x})\, dV,$$

where $\Omega = [a_1, b_1] \times [a_2, b_2] \times \cdots \times [a_n, b_n]$.
(Hint: use a list comprehension to calculate all of the $f(\mathbf{x}_i)$ quickly.)

Test your function on the following integrals.

$$\int_0^1 \int_0^1 x^2 + y^2 \, dx \, dy = \frac{2}{3} \qquad \int_{-2}^1 \int_1^3 3x - 4y + y^2 \, dx \, dy = 54$$

$$\int_{-4}^4 \int_{-3}^3 \int_{-2}^2 \int_{-1}^1 x + y - wz^2 \, dx \, dy \, dz \, dw = 0$$

Note carefully how the order of integration defines the domain. In the last example, the x-y-z-w domain is $[-1, 1] \times [-2, 2] \times [-3, 3] \times [-4, 4]$, so the lower and upper bounds passed to your function should be $[-1, -2, -3, -4]$ and $[1, 2, 3, 4]$, respectively.

Convergence

Monte Carlo integration has some obvious pros and cons. On the one hand, it is difficult to get highly precise estimates. In fact, 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 dividing the error by 10 requires using 100 times more sample points.

On the other hand, the convergence rate is independent of the number of dimensions of the problem. That is, the error converges at the same rate whether integrating a 2-dimensional function or a 20-dimensional function. This gives Monte Carlo integration a huge advantage over other methods, and makes it especially useful for estimating integrals in high dimensions where other methods become computationally infeasible.

Problem 4. The probability density function of the joint distribution of n independent normal random variables, each with mean 0 and variance 1, is the function $f : \mathbb{R}^n \to \mathbb{R}$ defined by

$$f(\mathbf{x}) = \frac{1}{(2\pi)^{n/2}} e^{-\frac{\mathbf{x}^T\mathbf{x}}{2}}.$$

Though this is a critical distribution in statistics, f does not have a symbolic antiderivative.

Integrate f several times to study the convergence properties of Monte Carlo integration.

1. Let $n = 4$ and $\Omega = [-\frac{3}{2}, \frac{3}{4}] \times [0, 1] \times [0, \frac{1}{2}] \times [0, 1] \subset \mathbb{R}^4$. Define f and Ω so that you can integrate f over Ω using your function from Problem 3.

2. Use `scipy.stats.mvn.mvnun()` to get the "exact" value of $F = \int_\Omega f(\mathbf{x})\, dV$. As an example, the following code computes the integral over $[-1, 1] \times [-1, 3] \times [-2, 1] \subset \mathbb{R}^3$.

```
>>> from scipy import stats

# Define the bounds of integration.
>>> mins = np.array([-1, -1, -2])
>>> maxs = np.array([ 1,  3,  1])

# The distribution has mean 0 and covariance I (the nxn identity).
>>> means, cov = np.zeros(3), np.eye(3)

# Compute the integral with SciPy.
>>> stats.mvn.mvnun(mins, maxs, means, cov)[0]
0.4694277116055261
```

3. Use `np.logspace()` to get 20 **integer** values of N that are roughly logarithmically spaced from 10^1 to 10^5. For each value of N, use your function from Problem 3 to compute 25 estimates of the integral with N samples, and average these estimates to obtain $\tilde{F}(N)$. Compute the relative error $\frac{|F - \tilde{F}(N)|}{|F|}$ for each value of N.

4. Plot the relative error against the sample size N on a log-log scale. Also plot the line $1/\sqrt{N}$ for comparison. Your results should be similar to Figure 11.2.

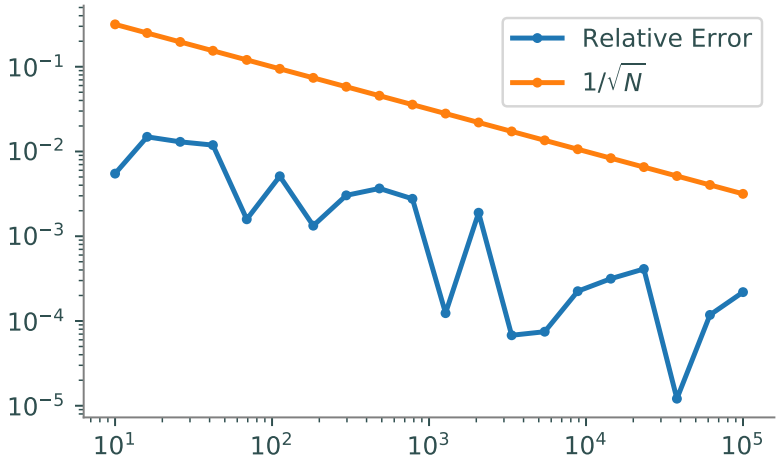


Figure 11.2: Monte Carlo integration converges at the same rate as $1/\sqrt{N}$ where N is the number of samples used in the estimate. However, the convergence is independent of dimension, which is why this strategy is so commonly used for high-dimensional integration.

12 Importance Sampling

Lab Objective: *Though Monte Carlo integration is a useful strategy for estimating integrals, the standard implementation suffers slow convergence and can be inaccurate. This typically occurs when the domain of integration is very small, making it unlikely that very many, if any, randomly chosen points will lie inside of it. Importance sampling remedies this problem by choosing the sample points more intelligently. This situation happens most frequently when trying to approximate integrals of probability distributions, so we focus on integrating common probability density functions.*

Monte Carlo Simulation

The standard procedure of Monte Carlo integration is not always the most efficient or accurate way to estimate an integral. Consider the probability density function (p.d.f) of the standard normal distribution in one dimension.

$$f_X(t) = \frac{e^{-t^2/2}}{\sqrt{2\pi}} \tag{12.1}$$

The probability that a random draw from the standard normal distribution is greater than 3 is given by the following integral.

$$\int_3^\infty f_X(t)\,dt = \frac{1}{\sqrt{2\pi}} \int_3^\infty e^{-t^2/2}\,dt \tag{12.2}$$

If $h : \mathbb{R} \to \mathbb{R}$ is the indicator function defined by

$$h(t) = \begin{cases} 1 & \text{if } t > 3 \\ 0 & \text{if } t \leq 3, \end{cases}$$

then (12.2) can be rewritten as follows.

$$\int_3^\infty f_X(t)\,dt = \int_{-\infty}^\infty h(t) f_X(t)\,dt. \tag{12.3}$$

Note that this process can be generalized to any domain of integration by redefining the indicator function h to match different bounds of integration.

We can now easily estimate this same probability using Monte Carlo simulation. Given a random collection of draws $\{x_i\}_{i=1}^N$ from the standard normal distribution, we can estimate the integral from (12.3) as follows.

$$\int_{-\infty}^{\infty} h(t) f_X(t)\, dt \approx \frac{1}{N} \sum_{i=1}^{N} h(x_i) \tag{12.4}$$

Statistics with SciPy

The `scipy.stats` module has many features for probability and statistics. One of the most effective uses of `scipy.stats` is to create an object for a particular distribution with the following methods:

Method	Description
`cdf()`	Calculate the cumulative probability evaluated up to a point.
`pdf()`	Calculate the probability of drawing a number from a distribution.
`rvs()`	Draw a random number from the distribution.

The following code shows how to appropriately use the methods of `stats` objects.

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

# Create an object for the standard normal distribution.
>>> F = stats.norm()
# loc is the mean and scale is the standard deviation.
>>> G = stats.norm(loc=3, scale=2)

# Calculate the probability of drawing a 1 from the normal distribution.
>>> F.pdf(1)
0.24197072451914337

# Draw a number at random from the normal distribution.
>>> F.rvs()
0.95779975

# Specifying a size returns a numpy.ndarray.
>>> F.rvs(size=2)
array([-0.40375954, 1.10956538])
```

Use `np.linspace()` and `pdf()` in order to plot a distribution.

```
>>> from matplotlib import pyplot as plt
# Create a linspace for our graph.
>>> X = np.linspace(-4, 4, 100)
# Use the normal distribution created previously.
>>> plt.plot(X, F.pdf(X))
>>> plt.show()
```

Object	Description
`norm()`	The normal distribution.
`gamma()`	The gamma distribution.
`multivariate_normal()`	The normal distribution in higher dimensions.
`beta()`	The beta distribution.

See Appendix **??** for a more thorough treatment of `scipy.stats`.

Problem 1. Write a function that accepts an integer parameter N. Use (12.4) to estimate the probability that a random draw from the standard normal distribution is greater than 3 using N samples. Return the approximation. Your answer should approach 0.0013499 for sufficiently large samples.

In Monte Carlo integration, each random point that is in the region of interest (in this case a number greater than 3) increases the approximation, and each random point that is not in that region decreases the approximation. If draws in the region of interest are unlikely, then it is possible that no random draws end up within the region of interest. The Monte Carlo integration method returns an approximation of 0 for the integral in this case, which isn't ideal. So, while standard Monte Carlo integration can get the job done if enough points are used, getting a good approximation requires an unacceptably large number of sample points.

Importance Sampling

Importance sampling makes Monte Carlo integration more efficient in circumstances where random draws within the region of interest are unlikely. Note that in Monte Carlo integration, random points that are close to and within the bounds of integration are more likely to influence the approximation than points that are farther away. We call these closer points *important* points. In importance sampling, we call the distribution of the integral we want to estimate the *target distribution*, and we usually denote it f_X. The idea of importance sampling is to choose a new distribution, called the *importance distribution*, that generates more important points. The importance distribution is usually denoted g_Y. We then modify (12.4) to take advantage of the importance distribution as follows.

$$\int_{-\infty}^{\infty} h(t)f_X(t)\,dt \approx \frac{1}{N}\sum_{i=1}^{N}\frac{h(y_i)f_X(y_i)}{g_Y(y_i)} \tag{12.5}$$

The fraction $\frac{f_X}{g_Y}$ is called the *importance weight*. Because of this result, we can use samples $y_1, \cdots, y_N$ from any distribution with equation g_Y to estimate the integral of f_X, as long as we multiply $h(y_i)$ by the importance weight. Note that if the importance distribution is chosen to be the same as the target distribution, or in other words, if we draw from the same distribution we are trying to estimate, then $g_Y = f_X$ and the importance weight is 1. In this case, the importance sampling method reduces to the original Monte Carlo simulation given by (12.4).

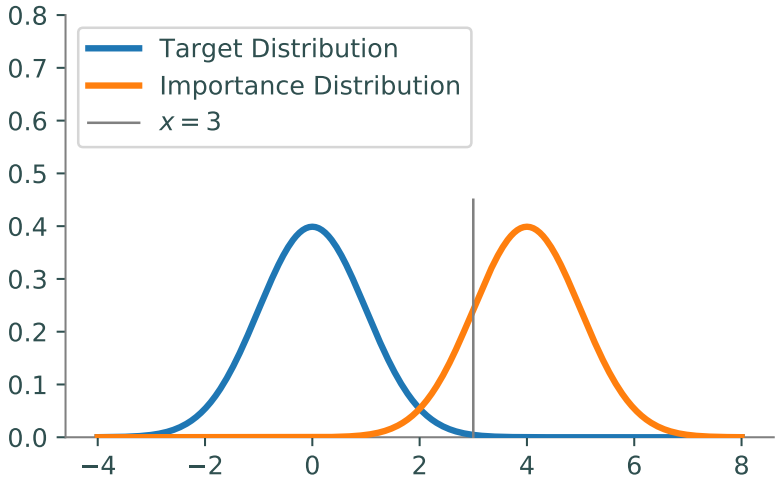


Figure 12.1: In our problem, we choose an importance distribution that will generate more samples that are greater than 3. Though not a perfect choice, choosing a normal distribution with $\mu = 4$ and $\sigma = 1$ will suffice.

> **Note**
>
> The derivation of (12.5) is based heavily on the *Law of the Unconscious Statistician*, an important idea in statistics. See the Additional Materials section for details.

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, the perfect answer is unnecessary. Close to perfect is good enough.

To solve the same problem as in Problem 1 using importance sampling, we choose a distribution that will generate more samples close to and greater than 3. We will choose g_Y to be the normal distribution with mean $\mu = 4$ and standard deviation $\sigma = 1$. Note that it is not necessary to choose an importance distribution of the same type as the target distribution.

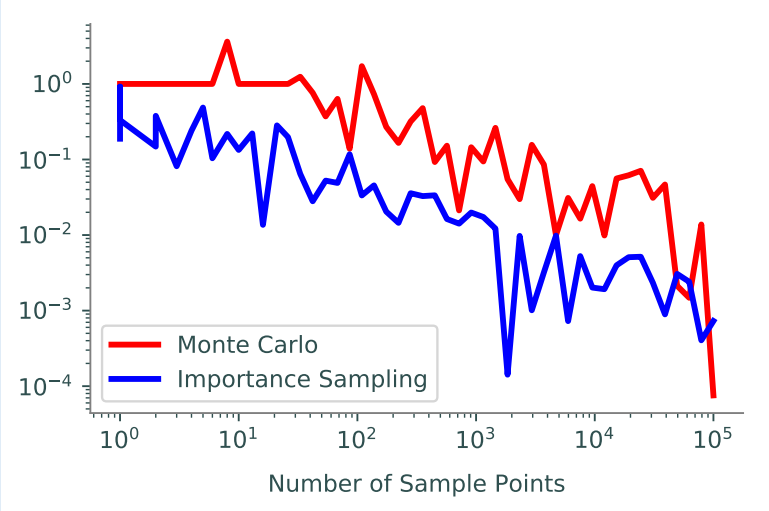
Figure 12.1 shows that a random draw from the importance distribution is far more likely to produce a number greater than 3 than a random draw from the target distribution. However, a draw greater than 3 from the importance distribution is accompanied by a low importance weight because it is so unlikely in the target distribution. Similarly, a draw less than 3 from the importance distribution has a higher importance weight because it is more likely in the target distribution.

Problem 2. Write a function that accepts a function handle f, representing the equation for the target distribution, a function handle g, representing the equation for the importance distribution, an indicator function h, a function that samples from the importance distribution, and an integer n representing the number of samples to use. Use (12.5) to approximate the integral of the target distribution and return this approximation.

To test your function, estimate the same integral as in Problem 1 using importance sampling. Choose the importance distribution to be a normal distribution with mean $\mu = 4$ and standard deviation $\sigma = 1$ as shown below. Your answer should approach 0.0013499 for large samples. When compared to Problem 1 this should give more consistent results.

```
# Choose the importance distribution with mean 4 and std dev 1
>>> G = stats.norm(loc=4, scale=1)
>>> g = G.pdf                    # Equation for importance distribution
>>> sampler = G.rvs              # Samples from importance distribution
```

Problem 3. Using the two previous problems, create a plot that compares the error of the traditional method of Monte Carlo integration to the error of the importance sampling method. Choose your target distribution to be the standard normal distribution, and estimate the probability that a random draw is greater than 3. Choose your importance distribution to be the same one you used to test Problem 2. You should calculate the errors for $n = 5000, 10000, \ldots, 500000$. Your plot should resemble the following figure.



To determine the error of your approximations, the following code returns the actual value of the probability:

```
>>> 1 - stats.norm.cdf(3)
```

Problem 3 shows that we can achieve the same results as traditional Monte Carlo with only a fraction of the samples if we choose an appropriate importance distribution. However, even though there is no correct choice for an importance distribution, there are choices that do not give a better approximation of an integral than the Monte Carlo method would without importance sampling. In Problem 2, we chose a normal distribution with $\mu = 4$ and $\sigma = 1$ to be our importance distribution to test the function. This produces more points larger than 3 to use for our integral estimation. If we had chosen a normal distribution that was less likely to produce points larger than 3, say for example a normal distribution with $\mu = 0$ and $\sigma = .5$, importance sampling would actually give a larger error than the traditional Monte Carlo method would alone. In addition, if we had chosen a normal distribution that produced hardly any points less than 3, the approximation using importance sampling would also be worse. We examine this further in the next problem.

Problem 4. Importance Sampling is only as good as the choice of g_Y. Repeat the previous problem of plotting the error for the estimates that a random draw from the standard normal distribution is greater than 3. Do this for various g_Y by creating 4 subplots. Each plot displays the error for traditional Monte Carlo as well as the errors of importance sampling for a specific g_Y. Each plot has a different g_Y, which will change the importance sampling error. In all cases let g_Y be a normal distribution with $\sigma = 1$, but let $\mu = -1, .25, 4, 7$.

Generalizing the Principles of Importance Sampling

Up to this point, the target distributions and the importance distributions have all been normal distributions. Importance sampling works for other types of distributions as well, and even works when the target distribution and the importance distribution are different from each other. The following problem is an example of this, and gives a potential real world application for importance sampling.

Problem 5. 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? This problem can be modeled using a gamma distribution. The following equation is for calculating the probability of the gamma distribution.

$$f_X(x) = \frac{x^{a-1}e^{-x/\theta}}{\Gamma(a)\theta^a}$$

The value a represents the number of calls we are waiting to receive. The value θ represents the the number of minutes it takes on average to receive one call. The variable x represents the number of minutes needed to wait to receive a calls given θ calls per minute. In the case of the above problem, $a = 9$, $\theta = .5$, and we want the probability that $x \geq 10$. Creating the gamma distribution object in `scipy.stats` is similar to creating the normal distribution object. It has the same methods as the normal distribution object.

```
# Create the gamma distribution object with a = 9, theta = .5
>>> F = stats.gamma(a=9, scale=.5)
```

Write a function that estimates and returns the probability of having to wait at least 10 minutes to receive 9 calls. Use a normal distribution with mean and standard deviation of your choosing as the importance distribution. Choose a large enough number of sample points so that the integral is estimated accurately. Your answer should approach 0.00208726.

In addition to single variable distributions, importance sampling can be used to approximate integrals of multivariate functions. The joint normal distribution of N independent random variables with mean $\mathbf{0}$ and covariance matrix I 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. Importance sampling can be used here to efficiently estimate the integral of this function. In the multivariate case, the importance distribution must also be multivariate. The multivariate normal distribution object in `scipy.stats` accepts a mean vector and a covariance matrix as parameters. The `pdf` and `rvs` methods work the same as in the single variable case, except that `pdf` accepts an array of size N and `rvs` returns an array of size n x N, where n is the number of samples to draw.

```
# Create a 2-dim multivariate normal object with a zero vector mean and cov ↩
    matrix I
>>> F = stats.multivariate_normal(mean=np.zeros(2), cov=np.eye(2))
>>> F.pdf(np.array([1,1]))
0.058549831524319168
>>> F.rvs(size=3)
array([[ 0.03429396,  0.13618787],
       [-0.12011818,  0,88691591],
       [-0.16356289,  0.53757853]])
```

Problem 6. Write a function that estimates and returns 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 equation of your target distribution. Create your own multivariate normal distribution with mean and covariance matrix of your choosing to serve as your importance distribution. As in the previous problem, choose a large enough number of sample points so that the integral is estimated accurately. Your answer should approach 0.02517149.

Hint: The indicator function may have to be coded differently from previous problems to accommodate for the fact that the sampler for the multivariate normal distribution returns a two dimensional array. Remember that when given an array of samples, the indicator function needs to return either a 0 or a 1 for each sample in the array.

Additional Material

Derivation of the importance sampling estimator

By the Law of the Unconscious Statistician (see Volume 2 §3.5), we can restate the integral from (12.2) as

$$\int_{-\infty}^{\infty} h(t) f_X(t)\, dt = E[h(X)].$$

Then we have

$$\begin{aligned} E[h(X)] &= \int_{-\infty}^{\infty} h(t) f_X(t)\, dt \\ &= \int_{-\infty}^{\infty} h(t) f_X(t) \left(\frac{g_Y(t)}{g_Y(t)}\right) dt \\ &= \int_{-\infty}^{\infty} \left(\frac{h(t) f_X(t)}{g_Y(t)}\right) g_Y(t)\, dt \\ &= E\left[\frac{h(Y) f_X(Y)}{g_Y(Y)}\right] \end{aligned}$$

and the corresponding estimator is

$$\begin{aligned} \widehat{E}[h(X)] &= \widehat{E}\left[\frac{h(Y) f_X(Y)}{g_Y(Y)}\right] \\ &= \frac{1}{N} \sum_{i=1}^{N} \frac{h(y_i) f_X(y_i)}{g_Y(y_i)} \end{aligned}$$

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, (12.5) 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

$$\begin{aligned}\widehat{E}_n[h(X)] &= \frac{\widehat{E}\left[\frac{h(Y)f(Y)}{g_Y(Y)}\right]}{\widehat{E}\left[\frac{f(Y)}{g_Y(Y)}\right]} \\ &= \frac{\frac{1}{N}\sum_{i=1}^{N}\frac{h(y_i)f(y_i)}{g_Y(y_i)}}{\frac{1}{N}\sum_{i=1}^{N}\frac{f(y_i)}{g_Y(y_i)}}\end{aligned}$$

13 Visualizing Complex-valued Functions

Lab Objective: *Functions that map from the complex plane into the complex plane are difficult to fully visualize because the domain and range are both 2-dimensional. However, such functions can be visualized at the expense of partial information. In this lab we present methods for analyzing complex-valued functions visually, including locating their zeros and poles in the complex plane. We recommend completing the exercises in a Jupyter Notebook.*

Representations of Complex Numbers

A complex number $z = x + iy$ can be written in *polar coordinates* as $z = re^{i\theta}$ where

- $r = |z| = \sqrt{x^2 + y^2}$ is the *magnitude* of z, and
- $\theta = \arg(z) = \arctan(y/x)$ is the *argument* of z, the angle in radians between z and 0.

Conversely, Euler's formula is the relation $re^{i\theta} = r\cos(\theta) + ir\sin(\theta)$. Then setting $re^{i\theta} = x + iy$ and equating real and imaginary parts yields the equations $x = r\cos(\theta)$ and $y = r\sin(\theta)$.

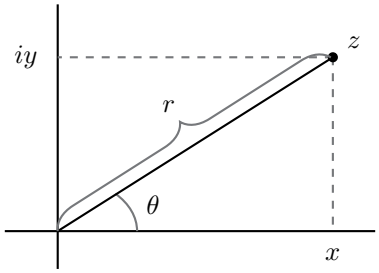


Figure 13.1: The complex number z can be represented in Cartesian coordinates as $z = x + iy$ and in polar coordinates as $z = re^{i\theta}$, when θ is in radians.

NumPy makes it easy to work with complex numbers and convert between coordinate systems. The function `np.angle()` returns the argument θ of a complex number (between $-\pi$ and π) and `np.abs()` (or `np.absolute()`) returns the magnitude r. These functions also operate element-wise on NumPy arrays.

```
>>> import numpy as np

>>> z = 2 - 2*1j                    # 1j is the imaginary unit i = sqrt(-1).
>>> r, theta = np.abs(z), np.angle(z)
>>> print(r, theta)                 # The angle is between -pi and pi.
2.82842712475 -0.785398163397

# Check that z = r * e^(i*theta)
>>> np.isclose(z, r*np.exp(1j*theta))
True

# These function also work on entire arrays.
>>> np.abs(np.arange(5) + 2j*np.arange(5))
array([ 0.        ,  2.23606798,  4.47213595,  6.70820393,  8.94427191])
```

Complex Functions

A function $f : \mathbb{C} \to \mathbb{C}$ is called a *complex-valued function*. Visualizing f is difficult because $\mathbb{C}$ has 2 real dimensions, so the graph of f should be 4-dimensional. However, since it is possible to visualize 3-dimensional objects, f can be visualized by ignoring one dimension. There are two main strategies for doing this: assign a color to each point $z \in \mathbb{C}$ corresponding to either the argument θ of $f(z)$, or to the magnitude r of $f(z)$. The graph that uses the argument is called a *complex color wheel graph*. Figure 13.2 displays the identity function $f(z) = z$ using these two methods.

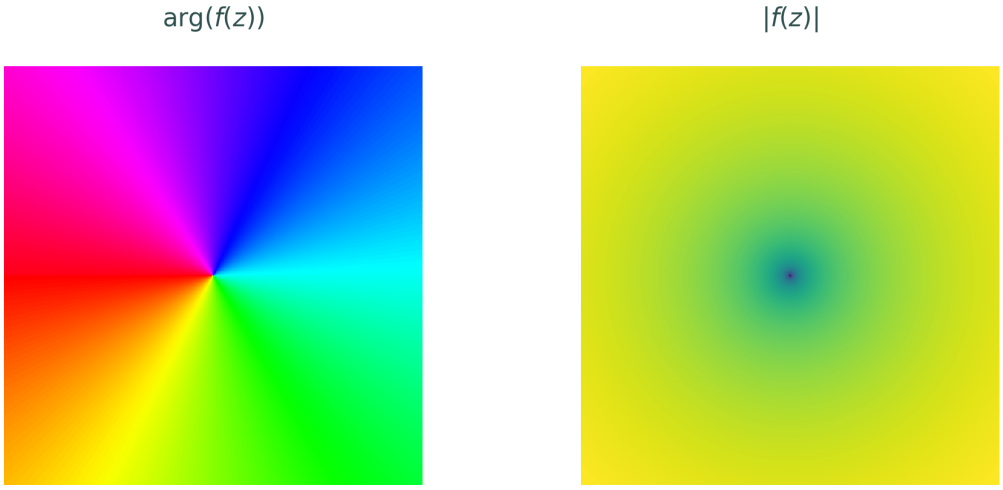


Figure 13.2: The identity function $f : \mathbb{C} \to \mathbb{C}$ defined by $f(z) = z$. On the left, the color at each point z represents the angle $\theta = \arg(f(z))$. As θ goes from $-\pi$ to π, the colors cycle smoothly counterclockwise from red to green to blue and back to red (this colormap is called `"hsv"`). On the right, the color represents the magnitude $r = |f(z)|$. The further a point is from the origin, the greater its magnitude (the colormap is the default, `"viridis"`).

The plots in Figure 13.2 use Cartesian coordinates in the domain and polar coordinates in the codomain. The procedure for plotting in this way is fairly simple. Begin by creating a grid of complex numbers: create the real and imaginary parts separately, then use `np.meshgrid()` to turn them into a single array of complex numbers. Pass this array to the function f, compute the angle and argument of the resulting array, and plot them using `plt.pcolormesh()`. The following code sets up the complex domain grid.

```
>>> x = np.linspace(-1, 1, 400)      # Real domain.
>>> y = np.linspace(-1, 1, 400)      # Imaginary domain.
>>> X, Y = np.meshgrid(x, y)         # Make grid matrices.
>>> Z = X + 1j*Y                     # Combine the grids into a complex array.
```

Visualizing the argument and the magnitude separately provides different perspectives of the function f. The angle plot is generally more useful for visualizing function behavior, though the magnitude plot often makes it easy to spot important points such as zeros and poles.

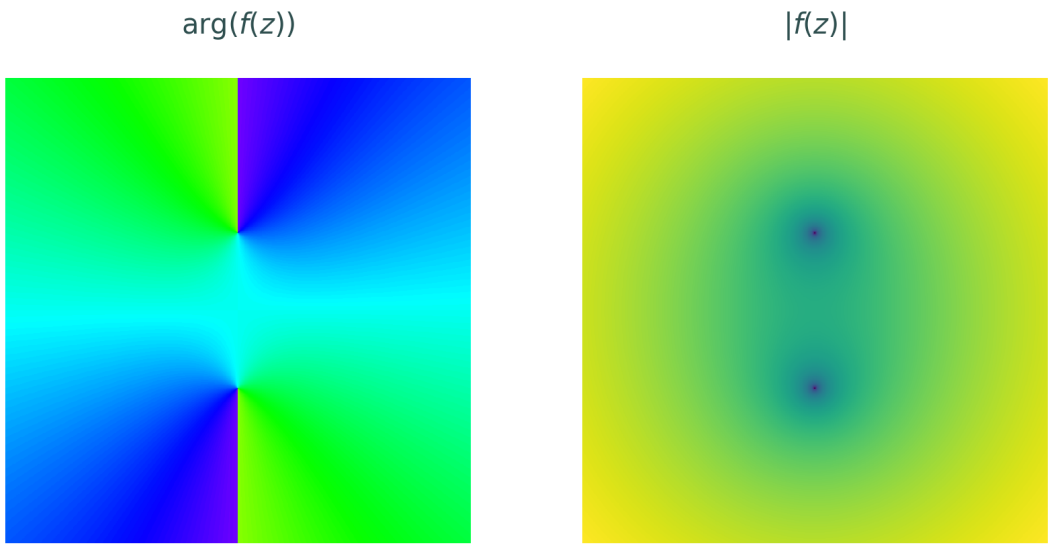


Figure 13.3: Plots of $f(z) = \sqrt{z^2+1}$ on $\{x+iy \mid x, y \in [-3, 3]\}$. Notice how a discontinuity is clearly visible in the angle plot on the left, but disappears from the magnitude plot on the right.

Problem 1. Write a function that accepts a function $f : \mathbb{C} \to \mathbb{C}$, bounds $[r_{\min}, r_{\max}, i_{\min}, i_{\max}]$ for the domain, an integer `res` that determines the resolution of the plot, and a string to set the figure title. Plot $\arg(f(z))$ and $|f(z)|$ on an equally-spaced `res`$\times$`res` grid over the domain $\{x + iy \mid x \in [r_{\min}, r_{\max}],\ y \in [i_{\min}, i_{\max}]\}$ in separate subplots.

1. For $\arg(f(z))$, set the `plt.pcolormesh()` keyword arguments `vmin` and `vmax` to $-\pi$ and π, respectively. This forces the color spectrum to work well with `np.angle()`. Use the colormap `"hsv"`, which starts and ends red, so that the color is the same for $-\pi$ and π.

2. For $|f(z)|$, set `norm=matplotlib.colors.LogNorm()` in `plt.pcolormesh()` so that the color scale is logarithmic. Use a sequential colormap like `"viridis"` or `"magma"`.

3. Set the aspect ratio to `"equal"` in each plot. Give each subplot a title, and set the overall figure title with the given input string.

Use your function to visualize $f(z) = z$ on $\{x+iy \mid x, y \in [-1, 1]\}$ and $f(z) = \sqrt{z^2+1}$ on $\{x+iy \mid x, y \in [-3, 3]\}$. Compare the resulting plots to Figures 13.2 and 13.3, respectively.

Interpreting Complex Plots

Plots of a complex function can be used to quickly identify important points in the function's domain.

Zeros

A complex number z_0 is called a *zero* of the complex-valued function f if $f(z_0) = 0$. The *mutliplicity* or *order* of z_0 is the largest integer n such that f can be written as $f(z) = (z - z_0)^n g(z)$ where $g(z_0) \neq 0$. In other words, f has a zero of order n at z_0 if the Taylor series of f centered at z_0 can be written as

$$f(z) = \sum_{k=n}^{\infty} a_k (z - z_0)^k \qquad \text{with } a_n \neq 0.$$

Angle and magnitude plots make it easy to locate a function's zeros and to determine their multiplicities.

Problem 2. Use your function from Problem 1 to plot the following functions on the domain $\{x+iy \mid x, y \in [-1, 1]\}$.

- $f(z) = z^n$ for $n = 2, 3, 4$.
- $f(z) = z^3 - iz^4 - 3z^6$. Compare the resulting plots to Figure 13.4.

Write a sentence or two about how the zeros of a function appear in angle and magnitude plots. How can you tell the multiplicity of the zero from the plot?

Problem 2 shows that in an angle plot of $f(z) = z^n$, the colors cycle n times counterclockwise around 0. This is explained by looking at z^n in polar coordinates.

$$z^n = (re^{i\theta})^n = r^n e^{i(n\theta)}$$

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. This is similar to taking a scalar-valued function $f : \mathbb{R} \to \mathbb{R}$ and replacing $f(x)$ with $f(nx)$.

Problem 2 also shows that the plot of $f(z) = z^3 - iz^4 - 3z^6$ looks very similar to the plot of $f(z) = z^3$ near the origin. This is because when z is close to the origin, z^4 and z^6 are much smaller in magnitude than z^3, and so the behavior of z^3 dominates the function. In terms of the Taylor series centered at $z_0 = 0$, the quantity $|z - z_0|^{n+k}$ is much smaller than $|z - z_0|^n$ for z close to z_0, and so the function behaves similar to $a_n(z - z_0)^n$.

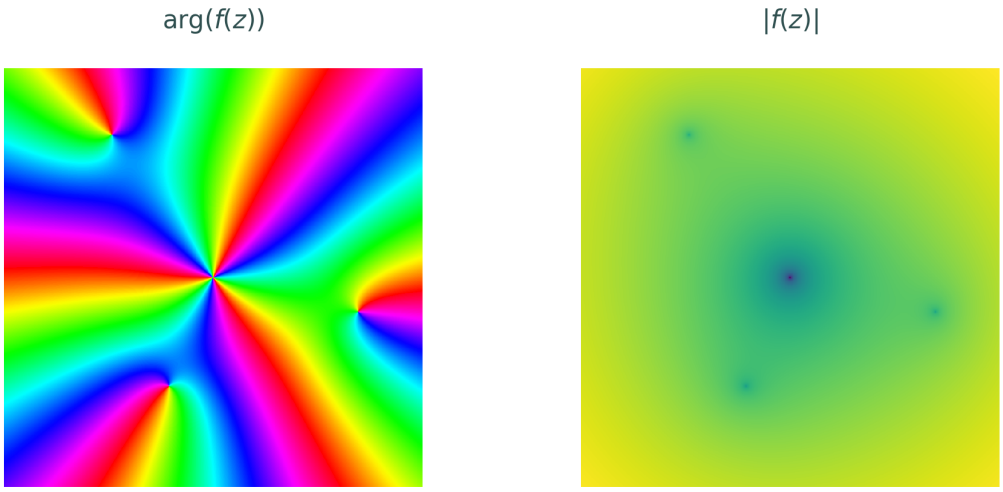


Figure 13.4: The angle plot of $f(z) = z^3 - iz^4 - 3z^6$ on $\{x + iy \mid x, y \in [-1, 1]\}$. The angle plot shows that $f(z)$ has a zero of order 3 at the origin and 3 distinct zeros of order 1 scattered around the origin. The magnitude plot makes it easier to pinpoint the location of the zeros.

Poles

A complex number z_0 is called a *pole* of the complex-valued function f if f can be written as $f(z) = g(z)/(z - z_0)$ where $g(z_0) \neq 0$. From this definition it is easy to see that $\lim_{z \to z_0} |f(z)| = \infty$, but knowing that $\lim_{z \to z_1} |f(z)| = \infty$ is not enough information to conclude that z_1 is a pole of f.

The *order* of z_0 is the largest integer n such that f can be written as $f(z) = g(z)/(z - z_0)^n$ with $g(z_0) \neq 0$. In other words, f has a pole of order n at z_0 if its Laurent series on a punctured neighborhood of z_0 can be written as

$$f(z) = \sum_{k=-n}^{\infty} a_k (z - z_0)^k \qquad \text{with } a_{-n} \neq 0.$$

Problem 3. Plot the following functions on domains that show all of its zeros and/or poles.

- $f(z) = z^{-n}$ for $n = 1, 2, 3$.
- $f(z) = z^2 + iz^{-1} + z^{-3}$.

Write a sentence or two about how the poles of a function appear in angle and magnitude plots. How can you tell the multiplicity of the poles from the plot?

Problem 3 shows that in angle plot of z^{-1}, the colors cycle n times clockwise around 0, as opposed to the counter-clockwise rotations seen around roots. 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.

From Problem 3 it is also clear that $f(z) = z^2 + iz^{-1} + z^{-3}$ behaves similarly to z^{-3} for z near the pole at $z_0 = 0$. 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 is why the order of a pole can be estimated by counting the number of times the colors circle a point in the clockwise direction.

Counting Zeros and Poles

The *Fundamental Theorem of Algebra* states that a polynomial f with highest degree n has exactly n zeros, counting multiplicity. For example, $f(z) = z^2 + 1$ has two zeros, and $f(z) = (z - i)^3$ has three zeros, all at $z_0 = i$ (that is, $z_0 = i$ is a zero with multiplicity 3).

The number of poles of function can also be apparent if it can be written as a quotient of polynomials. For example, $f(z) = z/(z+i)(z-i)^2$ has one zeros and three poles, counting multiplicity.

Problem 4. Plot the following functions and count the number and order of their zeros and poles. Adjust the bounds of each plot until you have found all zeros and poles.

- $f(z) = -4z^5 + 2z^4 - 2z^3 - 4z^2 + 4z - 4$
- $f(z) = z^7 + 6z^6 - 131z^5 - 419z^4 + 4906z^3 - 131z^2 - 420z + 4900$
- $f(z) = \frac{16z^4+32z^3+32z^2+16z+4}{16z^4-16z^3+5z^2}$

It is usually fairly easy to see how many zeros or poles a polynomial or quotient of polynomials has. However, it can be much more difficult to know how many zeros or poles a different function may or may not have without visualizing it.

Problem 5. Plot the following functions on the domain $\{x + iy \mid x, y \in [-8, 8]\}$. Explain carefully what each graph reveals about the function and why the function behaves that way.

- $f(z) = e^z$
- $f(z) = \tan(z)$

(Hint: use the polar coordinate representation to mathematically examine the magnitude and angle of each function.)

Essential Poles

A complex-valued function f 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,

$$e^{1/z} = \sum_{k=0}^{\infty} \frac{1}{n! z^n} = 1 + \frac{1}{z} + \frac{1}{2}\frac{1}{z^2} + \frac{1}{6}\frac{1}{z^3} + \dots.$$

An essential pole can be thought of as a pole of order ∞. Therefore, in an angle plot the colors cycle infinitely many times around an essential pole.

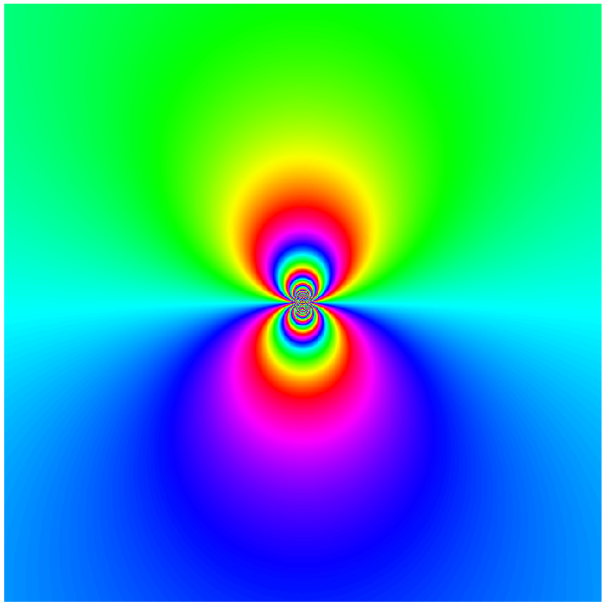


Figure 13.5: Angle plot of $f(z) = e^{1/z}$ on the domain $\{x + iy \mid x, y \in [-1, 1]\}$. The colors circle clockwise around the origin because it is a pole, not a zero. Because the pole is essential, the colors repeat infinitely many times.

Achtung!

Often, color plots like the ones presented in this lab can be deceptive because of a bad choice of domain. Be careful to validate your observations mathematically.

Problem 6. For each of the following functions, plot the function on $\{x + iy \mid x, y \in [-1, 1]\}$ and describe what this view of the plot seems to imply about the function. Then plot the function on a domain that allows you to see the true nature of the roots and poles and describe how it is different from what the original plot implied.

- $f(z) = 100z^2 + z$
- $f(z) = \sin\left(\frac{1}{100z}\right)$.

(Hint: zoom way in.)

14 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 14.1.

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 14.1 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

$$p_i(0) = \frac{1}{N} \qquad p_i(t+1) = \sum_{j \in \text{In}(i)} \frac{p_j(t)}{|\text{Out}(j)|}. \tag{14.1}$$

For example, in Figure 14.1 we have $N = 8$, and

$$p_6(t+1) = \frac{p_3(t)}{3} + \frac{p_4(t)}{3} + \frac{p_5(t)}{2}.$$

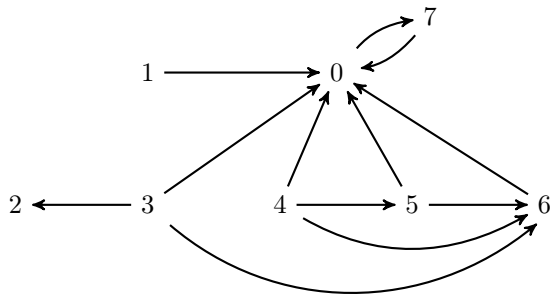


Figure 14.1: This directed graph describes the links between 8 webpages. In this example, $\text{In}(0) = \{1, 3, 4, 5, 6, 7\}$ and $\text{Out}(0) = \{7\}$.

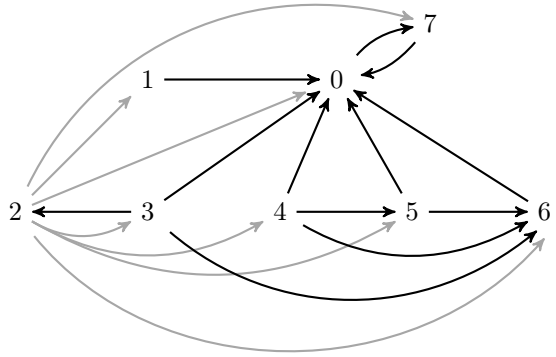


Figure 14.2: Here Figure 14.1 has been modified to guarantee that page 2 is no longer a sink. A new link has been added from page 2 to every other page (the added links are grey).

Refining the Model: Pages with No Outbound Links

A node with no outbound links, such as node 2 in Figure 14.1, 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 14.1 (where node 2 is a sink) to look like Figure 14.2.

Refining the Model: Adding Boredom

The equations in (14.1) 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 (14.1) then become

$$p_i(0) = \frac{1}{N} \qquad p_i(t+1) = d \sum_{j \in \text{In}(i)} \frac{p_j(t)}{|\text{Out}(j)|} + \frac{1-d}{N}. \tag{14.2}$$

Matrix Form of the PageRank Algorithm

We can rewrite (14.2) as the matrix equation

$$\mathbf{p}(0) = \frac{1}{N}\mathbf{1} \qquad \mathbf{p}(t+1) = dK\mathbf{p}(t) + \frac{1-d}{N}\mathbf{1} \tag{14.3}$$

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 14.3 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 14.1 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 14.1 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 (14.3). 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 14.2, 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 14.2, 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:

$$(I - dK)\mathbf{p} = \frac{1-d}{N}\mathbf{1}. \tag{14.4}$$

We can use SciPy's solver to find the page ranks of the network in Figure 14.2.

```
>>> 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 (14.4) 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 (14.3) 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 (14.3) for $\mathbf{p}(t+1)$ becomes

$$\mathbf{p}(t+1) = \Big(dK + \frac{1-d}{N}E\Big)\mathbf{p}(t).$$

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 14.1. 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 14.1.

```
>>> 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

15 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

$$A = S^{-1} \begin{bmatrix} M & \mathbf{0} \\ \mathbf{0} & N \end{bmatrix} S, \tag{15.1}$$

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

$$A^D = S^{-1} \begin{bmatrix} M^{-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} S. \tag{15.2}$$

Next, the *Schur decomposition* of A is given by

$$A = QTQ^{-1}, \tag{15.3}$$

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 (15.1). 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 (15.2) 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 (15.1) is given in Algorithm 15.1. Due to possible floating point arithmetic errors, consider all eigenvalues smaller than a certain tolerance to be 0.

Algorithm 15.1

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 15.1 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 15.1

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 15.1 for an example.

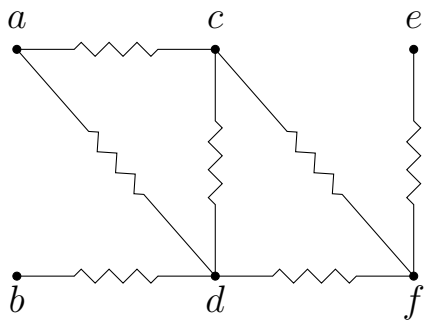


Figure 15.1: A graph with a resistor on each edge.

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,

$$R_{ij} = \begin{cases} (\widetilde{L}^j)^D_{ii} & \text{if } i \neq j \\ 0 & \text{if } i = j \end{cases}, \tag{15.4}$$

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 (15.4) 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 15.2.

[1]See Problem 1 of Image Segmentation for a refresher on adjacency matrices and the Laplacian.

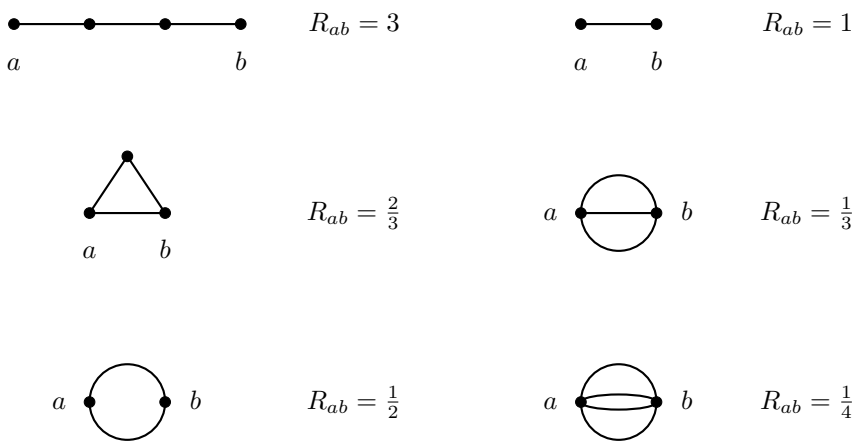


Figure 15.2: The effective resistance between two points for several simple graphs. Nodes that are farther apart have a larger effective resistance, while nodes that are nearer or better connected have a smaller effective resistance.

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 15.3 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.

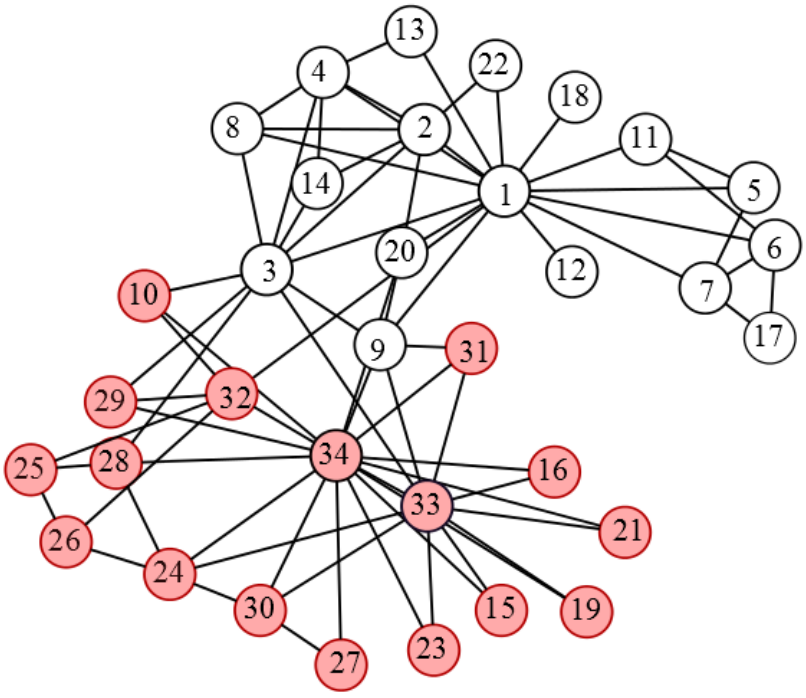


Figure 15.3: The social network contained in `social_network.csv`. Adapted from data by Wayne. W Zachary (see `https://en.wikipedia.org/wiki/Zachary%27s_karate_club`).

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

16 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 kth iteration of the iterative method for solving the problem $A\mathbf{x} = \mathbf{b}$ for $\mathbf{x}$. Furthermore, let x_i be the ith component of $\mathbf{x}$ so that $x_i^{(k)}$ is the ith component of $\mathbf{x}$ in the kth iteration. Like other iterative methods, there are two stopping parameters: a very small $\epsilon > 0$ and an integer $N \in \mathbb{N}$. Iterations continue until either

$$\|\mathbf{x}^{(k-1)} - \mathbf{x}^{(k)}\| < \epsilon \qquad \text{or} \qquad k > N. \tag{16.1}$$

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 equations.

$$\begin{array}{rcccccc} x_1^{(1)} &=& \tfrac{1}{2}(3 + x_3^{(0)}) &=& \tfrac{1}{2}(3+0) &=& \tfrac{3}{2} \\ x_2^{(1)} &=& \tfrac{1}{3}(3 + x_1^{(0)} - 2x_3^{(0)}) &=& \tfrac{1}{3}(3+0-0) &=& 1 \\ x_3^{(1)} &=& \tfrac{1}{3}(-1 - x_2^{(0)}) &=& \tfrac{1}{3}(-1-0) &=& -\tfrac{1}{3} \end{array}$$

Thus $\mathbf{x}^{(1)} = [\frac{3}{2}, 1, -\frac{1}{3}]^\mathsf{T}$. 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 (16.1) 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, $\mathbf{x}$ can be expressed 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.

$$\begin{aligned} \mathbf{x}^{(k+1)} &= D^{-1}(-(A - D)\mathbf{x}^{(k)} + \mathbf{b}) \\ &= D^{-1}(D\mathbf{x}^{(k)} - A\mathbf{x}^{(k)} + \mathbf{b}) \\ &= \mathbf{x}^{(k)} + D^{-1}(\mathbf{b} - A\mathbf{x}^{(k)}) \end{aligned} \tag{16.2}$$

There is a potential problem with (16.2): 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 `tol`, and a maximum number of iterations `maxiters`. Implement the Jacobi method using (16.2), returning the approximate solution to the equation $A\mathbf{x} = \mathbf{b}$.

Run the iteration until $\|\mathbf{x}^{(k-1)} - \mathbf{x}^{(k)}\|_\infty <$ `tol`, and only iterate at most `maxiters` times. Avoid using `la.inv()` to calculate D^{-1}, but use `la.norm()` to calculate the vector ∞-norm $\|\mathbf{x}\|_\infty = \sup |x_i|$.

Your function should be robust enough to accept systems of any size. To test your function, generate a random $\mathbf{b}$ with `np.random.random()` and use the following function to generate an $n \times n$ matrix A for which the Jacobi method is guaranteed to converge. Run the iteration, then check that $A\mathbf{x}^{(k)}$ and $\mathbf{b}$ are close using `np.allclose()`.

```
def diag_dom(n, num_entries=None):
    """Generate a strictly diagonally dominant (n, n) matrix.
    Parameters:
        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): A (n, n) 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
```

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

$$|a_{ii}| > \sum_{j \neq i} |a_{ij}| \quad \text{for all} \quad i = 1, 2, \ldots, n,$$

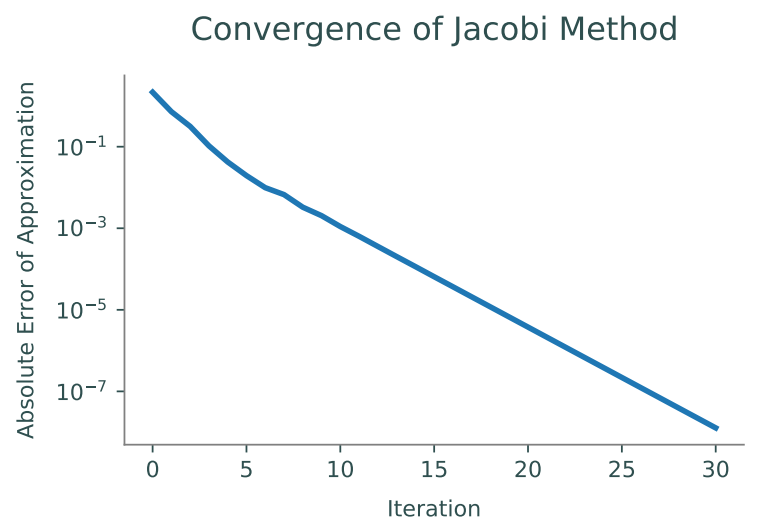
then A is called *strictly diagonally dominant* (`diag_dom()` in Problem 1 generates a strictly diagonally dominant $n \times n$ matrix). If this is the case,[1] then the Jacobi method always converges, regardless of the initial guess $\mathbf{x}_0$. This is a very different convergence result than many other iterative methods such as Newton's method where convergence is highly sensitive to 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 at each iteration.
3. If `plot` is True, produce a lin-log plot (use `plt.semilogy()`) of the error against iteration count. Remember to still return the approximate solution $\mathbf{x}$.

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. As an example, consider again the system from 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 as before.

$$x_1^{(1)} = \frac{1}{2}(3 + x_3^{(0)}) = \frac{1}{2}(3 + 0) = \frac{3}{2}$$

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 converges in less than half as many iterations as Jacobi does for this system.

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.

$$x_i^{(k+1)} = \frac{1}{a_{ii}} \left(b_i - \sum_{j<i} a_{ij} x_j^{(k)} - \sum_{j>i} a_{ij} x_j^{(k)} \right) \tag{16.3}$$

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 suggests the following simplification.

$$\begin{aligned} x_i^{(k+1)} &= \frac{1}{a_{ii}}\left(b_i - A_i^\mathsf{T}\mathbf{x}^{(k)} + a_{ii}x_i^{(k)}\right) \\ &= x_i^{(k)} + \frac{1}{a_{ii}}\left(b_i - A_i^\mathsf{T}\mathbf{x}^{(k)}\right) \end{aligned} \tag{16.4}$$

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 `tol`, a maximum number of iterations `maxiters`, and a keyword argument `plot` that defaults to `False`. Implement the Gauss-Seidel method using (16.4), 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 $\mathbf{x}^{(0)}$.

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.[2]

Problem 4. Write a new function that accepts a **sparse** matrix A, a vector $\mathbf{b}$, a convergence tolerance `tol`, and a maximum number of iterations `maxiters` (plotting the convergence is not required for this problem). Implement the Gauss-Seidel method using (16.4), 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]

# Multiply only the nonzero elements of the i-th row of A with the
# corresponding elements of x.
Aix = 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

There are many systems that meet the requirements for convergence with the Gauss-Seidel method, but for which convergence is still relatively slow. A slightly altered version of the Gauss-Seidel method, called *Successive Over-Relaxation* (SOR), can result in faster convergence. This is achieved by introducing a *relaxation factor* $\omega \geq 1$ and modifying (16.3) in the following way.

$$x_i^{(k+1)} = (1-\omega)x_i^{(k)} + \frac{\omega}{a_{ii}}\left(b_i - \sum_{j<i} a_{ij}x_j^{(k)} - \sum_{j>i} a_{ij}x_j^{(k)}\right)$$

Simplifying the equation results in the following.

$$x_i^{(k+1)} = x_i^{(k)} + \frac{\omega}{a_{ii}}\left(b_i - A_i^\mathsf{T}\mathbf{x}^{(k)}\right) \tag{16.5}$$

[2]See the lab on Linear Systems for a review of `scipy.sparse` matrices and syntax.

Note that when $\omega = 1$, SOR reduces to Gauss-Seidel. The relaxation factor ω weights the new iteration between the current best approximation and the next approximation in a way that can sometimes dramatically improve convergence.

Problem 5. Write a function that accepts a sparse matrix A, a vector $\mathbf{b}$, a relaxation factor ω, a convergence tolerance `tol`, and a maximum number of iterations `maxiters`. Implement SOR using (16.5), compute the approximate solution to the equation $A\mathbf{x} = \mathbf{b}$. Use the usual stopping criterion. Return the approximate solution $\mathbf{x}$ as well as the number of iterations computed. (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.

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \tag{16.6}$$

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 (16.6) 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 to approximate the partial derivatives,

$$\begin{aligned} 0 &= \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \\ &\approx \frac{U_{i+1,j} - 2U_{i,j} + U_{i-1,j}}{h^2} + \frac{U_{i,j+1} - 2U_{i,j} + U_{i,j-1}}{h^2} \\ &= \frac{1}{h^2}\left(-4U_{i,j} + U_{i+1,j} + U_{i-1,j} + U_{i,j+1} + U_{i,j-1}\right), \end{aligned} \tag{16.7}$$

where $h = x_{i+1} - x_i = y_{j+1} - y_j$ is the distance between the grid points in either direction. 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 (16.7), we have the following for an interior point $U_{i,j}$.

$$-4U_{i,j} + U_{i+1,j} + U_{i-1,j} + U_{i,j+1} + U_{i,j-1} = 0 \tag{16.8}$$

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, the neighbor $U_{3,0}$ of the gridpoint for $U_{3,1}$ is fixed at $U_{3,0} = 100$. In this case, (16.8) becomes

$$-4U_{3,1} + U_{2,1} + U_{3,2} + U_{4,1} = -100.$$

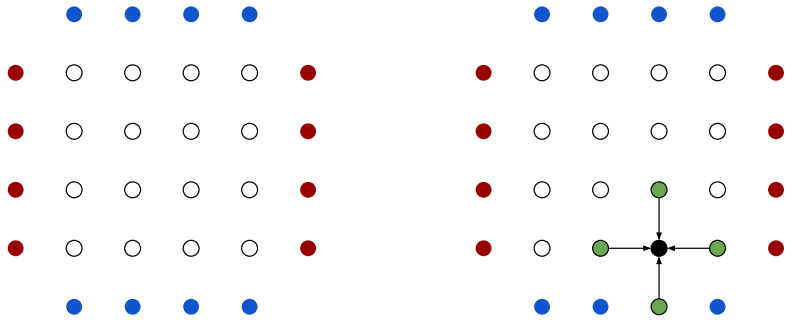


Figure 16.1: On the left, an example of a 6×6 grid ($n = 4$) where the red dots are hot boundary zones and the blue dots are cold boundary zones. On the right, the green dots are the neighbors of the interior black dot that are used to approximate the heat at the black dot.

The constants on the right side of (16.8) 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.

As an example, writing (16.8) for the 16 interior points of the grid in Figure 16.1 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 6. Write a function that accepts an integer n, a relaxation factor ω, a convergence tolerance `tol` that defaults to 10^{-8}, a maximum number of iterations `maxiters` 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 5. Also return the number of iterations computed.
(Hint: see Problem 5 of the Linear Systems lab for the construction of A. 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 `"coolwarm"` 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 7. To demonstrate how convergence is affected by the value of the relaxation factor ω in SOR, run your function from Problem 6 with $\omega = 1,\ 1.05,\ 1.1,\ \ldots, 1.9, 1.95$ and $n = 20$. Plot the number of computed iterations as a function of ω. Return the value of ω that results in the least number of iterations.

Note that the matrix A from Problem 6 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 `maxiters=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.

17 The Arnoldi Iteration

Lab Objective: *The Arnoldi Iteration is an efficient method for finding the eigenvalues of extremely large matrices. Instead of using standard methods, the iteration uses Krylov subspaces to approximate how a linear operator acts on vectors. With this approach, the Arnoldi Iteration facilitates the computation of eigenvalues for enormous matrices without needing to physically create the matrix in memory. We will explore this subject by implementing the Arnoldi iteration algorithm, using our implementation for eigenvalue computation, and then graphically representing the accuracy of our approximated eigenvalues.*

Krylov Subspaces

One of the biggest difficulties in numerical 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 that it can run on any linear operator without knowing the operator's underlying matrix representation. The outputs of the Arnoldi algorithm can then be used to approximate the eigenvalues of the matrix of the linear operator.

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, $A^n x$ frequently converges to a dominant eigenvector of A as n gets large, which fills the basis with many almost parallel vectors. This yields a basis prone to ill-conditioned computations and numerical instability.

The Arnoldi Iteration Algorithm

The Arnoldi iteration focuses on efficiently creating an orthonormal basis for $\mathcal{K}_n(A, \mathbf{x})$ 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. This process yields an orthonormal basis for $\mathcal{K}_n(A, \mathbf{x})$ that can be used for further computations.

The algorithm begins by initializing a matrix H which will be an upper Hessenberg matrix and a matrix Q which will be filled with the basis vectors of our Krylov subspace. It also requires an initial vector $\mathbf{b} \neq 0$ which is normalized to get $\mathbf{q}_1 = \mathbf{b}/\left\|\mathbf{b}\right\|$. This represents the basis for the initial Krylov subspace, $\mathcal{K}_1(A, \mathbf{b})$.

For the kth iteration, compute the next basis vector $\mathbf{q}_{k+1}$ by using the modified Gram-Schmidt process to make $A\mathbf{q}_k$ orthonormal to $\mathbf{q}_k$. This entails making each column of Q orthogonal to $\mathbf{q}_k$ before proceeding to the next iteration. The vectors $\{\mathbf{q}_i\}_{i=1}^{k}$ are then a basis for $\mathcal{K}_k(A, \mathbf{b})$. If $\|\mathbf{q}_{k+1}\|$ is below a certain tolerance, stop and return H and Q. Otherwise, normalize the new basis vector new $\mathbf{q}_{k+1}$ and continue to the next iteration.

Algorithm 17.1 The Arnoldi iteration. This algorithm accepts a square matrix A and a 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 an upper Hessenberg H and an orthonormal Q such that $H = Q^{\mathsf{H}}AQ$.

procedure ARNOLDI($\mathbf{b}$, A, k, `tol`)
  $Q \leftarrow$ empty(size($\mathbf{b}$), $k+1$) ▷ Some initialization steps
  $H \leftarrow$ zeros($k+1, k$)
  $Q_{:,0} \leftarrow \mathbf{b}/\left\|\mathbf{b}\right\|_2$
  for $j = 0 \dots k-1$ **do** ▷ Perform the actual iteration.
    $Q_{:,j+1} \leftarrow A(Q_{:,j})$
    for $i = 0 \dots j$ **do** ▷ Modified Gram-Schmidt.
      $H_{i,j} \leftarrow Q_{:,i}^{\mathsf{H}} Q_{:,j+1}$
      $Q_{:,j+1} \leftarrow Q_{:,j+1} - H_{i,j} Q_{:,i}$
    $H_{j+1,j} \leftarrow \left\|Q_{:,j+1}\right\|_2$ ▷ Set subdiagonal element of H.
    if $|H_{j+1,j}| <$ `tol` **then** ▷ Stop if $\left\|Q_{:,j+1}\right\|_2$ is small enough.
      return $H_{:j+1,:j+1}$, $Q_{:,:j+1}$
    $Q_{:,j+1} \leftarrow Q_{:,j+1}/H_{j+1,j}$ ▷ Normalize $\mathbf{q}_{j+1}$.
  return $H_{:-1,:}$, Q ▷ Return H_k and Q.

ACHTUNG!

If the starting vector $\mathbf{x}$ is an eigenvector of A with corresponding eigenvalue 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 $\mathbf{x}$. So, when $\mathbf{x}$ is normalized with $\mathbf{q}_1 = \mathbf{x}/\|\mathbf{x}\|$, $\mathbf{q}_2 = A\mathbf{q}_1 = \lambda\mathbf{q}_1$.

The vector $\mathbf{q}_2$ is supposed to be the next vector in the orthonormal basis for $\mathcal{K}_k(A, \mathbf{x})$, but it is not linearly independent of $\mathbf{q}_1$. In fact, $\mathbf{q}_1$ already spans $\mathcal{K}_k(A, \mathbf{x})$. Hence, the Gram-Schmidt process fails and results in a `ZeroDivisionError` or an extremely early termination of the algorithm. 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 L is some linear function, then we can modify the pseudocode above by replacing $AQ_{:,j}$ with $A_{mul}(Q_{:,j})$. This makes it possible to find the eigenvalues of an arbitrary linear transformation.

Problem 1. Write a function that accepts a starting vector $\mathbf{b}$ for the Arnoldi Iteration, a function handle L that describes a linear operator, the number of times n to perform the iteration, and a tolerance `tol` that defaults to 10^{-8}. Use Algorithm 17.1 to implement the Arnoldi Iteration with these parameters. Return the upper Hessenberg matrix H and the orthonormal matrix Q from the iteration.

Consider the following implementation details.

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. This function can be tested on a matrix A by passing in `A.dot` for a linear operator.
3. Remember to use complex inner products. Here is an example of how to evaluate $A^H A$:

```
b = A.conj() @ B
```

Test your function by comparing the resulting H with $Q^{\mathsf{H}} A Q$.

Finding Eigenvalues Using the 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

$$H_k = Q_k^{\mathsf{H}} A Q_k. \tag{17.1}$$

If $k < n$, then H_k is a low-rank approximation to A and the eigenvalues of H_k may be used as approximations for the eigenvalues of A. The eigenvalues of H_k are called *Ritz Values*, and we will later show that they converge quickly to the largest eigenvalues of A.

Problem 2. Write a function that accepts a function handle L that describes a linear operator, the dimension of the space `dim` that the linear operator works on, the number of times k to perform the Arnoldi Iteration, and the number of Ritz values n to return. Use the previous implementation of the Arnoldi Iteration and an eigenvalue function such as `scipy.linalg.eigs()` to compute the largest Ritz values of the given operator. Return the `n` largest Ritz values.

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 a vector $\mathbf{x} \in \mathbb{C}^{2^{20}}$, 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 very commonly in 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 from Problem 2 to approximate the eigenvalues of the Fast Fourier Transform. Set $k = 10$ and `dim` $= 2^{20}$. For the argument L, use the `scipy.fftpack.fft()`.

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.

```
>>> from scipy.sparse import linalg as spla
>>> B = np.random.random((100,100))
>>> spla.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 ])
```

Convergence

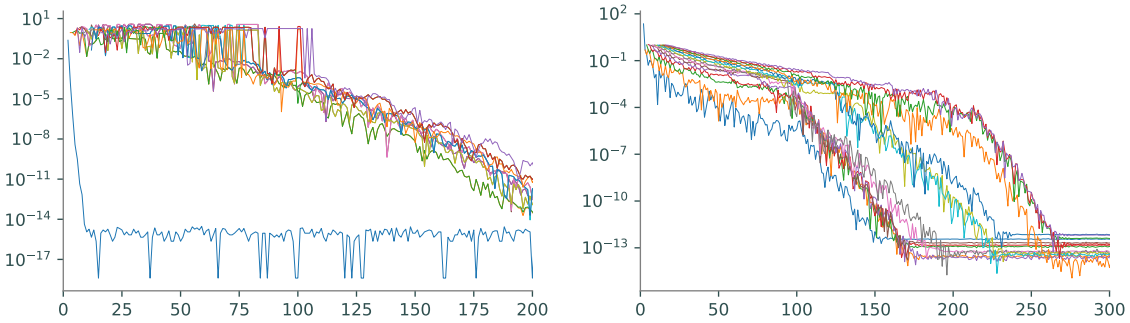
As more iterations of the Arnoldi method are performed, our approximations are of higher rank. Consequently, the Ritz values become more accurate approximations to the eigenvalues of the linear operator.

This technique converges quickly 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 17.1a.

However, Ritz values converge more slowly for matrices with random eigenvalues. Figure 17.1b plots convergence of the Ritz values for a matrix with eigenvalues uniformly distributed in $[0, 1)$.

Problem 4. Write a function that accepts a linear operator A, the number of Ritz values to plot n, and the the number of times to perform the Arnoldi iteration `iters`. Use these parameters to create a plot of the absolute error between the largest Ritz values of A and the largest eigenvalues of A.

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 $k = 0, 1, \dots,$ `iters`.
   (a) Use your Ritz function to find the n largest Ritz values of the operator. Note that for small k, the matrix H_k may not have this many eigenvalues. Due to this, the graphs of some eigenvalues have to begin after a few iterations.
   (b) Store the absolute error between the eigenvalues of A and the Ritz values of H. Make sure that the errors are stored in the correct order.
3. Iteratively plot the errors for each eigenvalue with the range of the iterations.



(a) (b)

Figure 17.1: These plots show the relative error of the ritz values as approximations to the eigenvalues of a matrix. The figure on the left plots the largest 15 Ritz values for a 500×500 matrix with random entries and demonstrates that the largest eigenvalue (the blue line) converges after 20 iterations. The figure at right plots the largest 15 Ritz values for a 500×500 matrix with uniformly distributed eigenvalues in $[0, 1)$ and demonstrates that all the eigenvalues take from 150 to 250 iterations to converge.

Hints: If $\tilde{\mathbf{x}}$ is an an approximation to $\mathbf{x}$, then the *absolute error* in the approximation is $\|\mathbf{x} - \tilde{\mathbf{x}}\|$.

Sort your eigenvalues from greatest to least. An example of how to do this is included:

```
# Evaluate the eigenvalues
eigvalues = la.eig(A)[0]
# Sort them from greatest to least (use np.abs to account for complex ↩
    parts)
eigvalues = eigvalues[np.sort(np.abs(eigvalues))[::-1]]
```

In addition, remember that certain eigenvalues of H will not appear until we are computing enough iterations in the Arnoldi algorithm. As a result, we will have to begin the graphs of several eigenvalues after we are computing sufficient iterations of the algorithm.

Run your function on these examples. The plots should be fairly similar to Figures 17.1b and 17.1a.

```
>>> 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 @ d @ la.inv(A)
>>> plot_ritz(B, 10, 175)
```

Additional Material

The Lanczos Iteration

The Lanczos iteration is a version of the Arnoldi iteration that is optimized to operate on symmetric matrices. If A is symmetric, then (**??**) 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).

Algorithm 17.2 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.

```
1:  procedure LANCZOS(b, A, k, tol)
2:      q_0 ← zeros(size(b))                          ▷ Some initialization
3:      q_1 ← b/‖b‖_2
4:      x ← empty(k)
5:      y ← empty(k)
6:      for i = 0...k−1 do                            ▷ Perform the iteration.
7:          z ← Aq_1                                  ▷ z is a temporary vector to store q_{i+1}.
8:          x[i] ← q_1^T z                            ▷ q_1 is used to store the previous q_i.
9:          z ← z − x[i]q_1 + y[i−1]q_0               ▷ q_0 is used to store q_{i−1}.
10:         y[i] = ‖z‖_2                              ▷ Initialize y[i].
11:         if y[i] < tol then                        ▷ Stop if ‖q_{i+1}‖_2 is too small.
12:             return x[: i+1], y[: i]
13:         z = z/y[i]
14:         q_0, q_1 = q_1, z                         ▷ Store new q_{i+1} and q_i on top of q_1 and q_0.
15:     return x, y[: −1]
```

As it is described in Algorithm 17.2, 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.

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 `scipy.sparse.linalg.eigsh()`.

18 GMRES

Lab Objective: *The Generalized Minimal Residuals (GMRES) algorithm is an iterative Krylov subspace method for efficiently solving large linear systems. In this lab we implement the basic GMRES algorithm, then make an improvement by using restarts. We then discuss the convergence of the algorithm and its relationship with the eigenvalues of a linear system. Finally, we introduce SciPy's version of GMRES.*

The GMRES Algorithm

GMRES is an iterative method that uses Krylov subspaces to reduce a high-dimensional problem to a sequence of smaller dimensional problems. Let A be an invertible $m \times m$ matrix and let $\mathbf{b}$ be a vector of length m. Let $\mathcal{K}_n(A, \mathbf{b})$ be the order-n Krylov subspace generated by A and $\mathbf{b}$. Instead of solving the system $A\mathbf{x} = \mathbf{b}$ directly, GMRES uses 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 terminates when this residual is smaller than some predetermined value. In many situations, this happens when n is much smaller than m.

The GMRES algorithm uses the Arnoldi iteration for numerical stability. The Arnoldi iteration produces H_n, an $(n+1) \times n$ upper Hessenberg matrix, and Q_n, a matrix whose columns make up an orthonormal basis of $\mathcal{K}_n(A, \mathbf{b})$, such that $AQ_n = Q_{n+1}H_n$. The GMRES algorithm finds the vector $\mathbf{x}_n$ which minimizes the norm $\|\mathbf{b} - A\mathbf{x}_n\|_2$, where $\mathbf{x}_n = Q_n\mathbf{y}_n + \mathbf{x}_0$ for some $\mathbf{y}_n \in \mathbb{R}^n$. Since the columns of Q_n are orthonormal, the residual can be equivalently computed as

$$\|\mathbf{b} - A\mathbf{x}_n\|_2 = \|Q_{n+1}(\beta\mathbf{e}_1 - H_n\mathbf{y}_n)\|_2 = \|H_n\mathbf{y}_n - \beta\mathbf{e}_1\|_2. \tag{18.1}$$

Here $\mathbf{e}_1$ is the vector $[1, 0, \dots, 0]^\mathsf{T}$ of length $n+1$ and $\beta = \|\mathbf{b} - A\mathbf{x}_0\|_2$, where $\mathbf{x}_0$ is an initial guess of the solution. Thus, to minimize $\|\mathbf{b} - A\mathbf{x}_n\|_2$, the right side of (18.1) can be minimized, and $\mathbf{x}_n$ can be computed as $\mathbf{x}_n = Q_n\mathbf{y}_n + \mathbf{x}_0$.

Algorithm 18.1 The GMRES algorithm. This algorithm operates on a vector $\mathbf{b}$ and a linear operator 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`)
  $Q \leftarrow$ empty(size($\mathbf{b}$), $k+1$) ▷ Initialization.
  $H \leftarrow$ zeros($k+1, k$)
  $r_0 \leftarrow \mathbf{b} - A(\mathbf{x}_0)$
  $Q_{:,0} = r_0 / \|r_0\|_2$
  for $j = 0 \dots k-1$ **do** ▷ Perform the Arnoldi iteration.
    $Q_{:,j+1} \leftarrow A(Q_{:,j})$
    for $i = 0 \dots j$ **do**
      $H_{i,j} \leftarrow Q_{:,i}^T Q_{:,j+1}$
      $Q_{:,j+1} \leftarrow Q_{:,j+1} - H_{i,j} Q_{:,i}$
    $H_{j+1,j} \leftarrow \|Q_{:,j+1}\|_2$
    if $|H_{j+1,j}| >$ `tol` **then** ▷ Avoid dividing by zero.
      $Q_{:,j+1} \leftarrow Q_{:,j+1} / H_{j+1,j}$
    $\mathbf{y} \leftarrow$ least squares solution to $\|H_{:j+2,:j+1}\mathbf{x} - \beta e_1\|_2$ ▷ β and $\mathbf{e}_1$ as in (18.1).
    `res` $\leftarrow \|H_{:j+2,:j+1}\mathbf{y} - \beta e_1\|_2$
    if `res` $<$ `tol` **then**
      return $Q_{:,:j+1}\mathbf{y} + \mathbf{x}_0$, `res`
  return $Q_{:,:j+1}\mathbf{y} + \mathbf{x}_0$, `res`

Problem 1. Write a function that accepts a matrix A, a vector $\mathbf{b}$, and an initial guess $\mathbf{x}_0$, a maximum number of iterations k defaulting to 100, and a stopping tolerance `tol` that defaults to 10^{-8}. Use Algorithm 18.1 to approximate the solution to $A\mathbf{x} = \mathbf{b}$ using the GMRES algorithm. Return the approximate solution and the residual at the approximate solution.

You may assume that A and $\mathbf{b}$ only have real entries. Use `scipy.linalg.lstsq()` to solve the least squares problem. Be sure to read the documentation so that you understand what the function returns.

Compare your function to the following code.

```
>>> A = np.array([[1,0,0],[0,2,0],[0,0,3]])
>>> b = np.array([1, 4, 6])
>>> x0 = np.zeros(b.size)
>>> gmres(A, b, x0, k=100, tol=1e-8)
(array([ 1.,  2.,  2.]), 7.174555448775421e-16)
```

Convergence of GMRES

One of the most important characteristics of GMRES is that it will always arrive at an exact solution (if one exists). At the n-th iteration, GMRES computes the best approximate solution to $A\mathbf{x} = \mathbf{b}$ for $\mathbf{x}_n \in \mathcal{K}_n$. If A is full rank, then $\mathcal{K}_m = \mathbb{F}^m$, so the m^{th} iteration will always return an exact answer. Sometimes, the exact solution $\mathbf{x} \in \mathcal{K}_n$ for some $n < m$, in this case x_n is an exact solution. In either case, the algorithm is convergent 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. Add a keyword argument `plot` defaulting to `False` to your function from Problem 1. If `plot=True`, keep track of the residuals at each step of the algorithm. At the end of the iteration, before returning the approximate solution and its residual error, create a figure with two subplots.

1. Make a scatter plot of the eigenvalues of A on the complex plane.
2. Plot the residuals versus the iteration counts using a log scale on the y-axis (use `ax.semilogy()`).

Problem 3. Use your function from Problem 2 to investigate how the convergence of GMRES relates to the eigenvalues of a matrix as follows. Define an $m \times m$ matrix

$$A_n = nI + P,$$

where I is the identity matrix and P is an $m \times m$ matrix with entries taken from a random normal distribution with mean 0 and standard deviation $1/(2\sqrt{m})$. Call your function from Problem 2 on A_n for $n = -4, -2, 0, 2, 4$. Use $m = 200$, let $\mathbf{b}$ be an array of all ones, and let $\mathbf{x}_0 = \mathbf{0}$.

Use `np.random.normal()` to create the matrix P. When analyzing your results, pay special attention to the clustering of the eigenvalues in relation to the origin. Compare your results with $n = 2$, $m = 200$ to Figure 18.1.

Ideas for this problem were taken from Example 35.1 on p. 271 of [**Trefethen1997**].

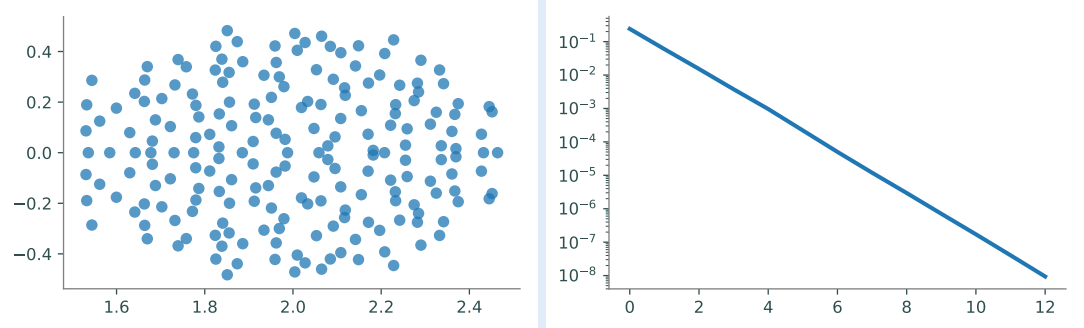


Figure 18.1: On the left, the eigenvalues of the matrix A_2 defined in Problem 3. On the right, the rapid convergence of the GMRES algorithm on A_2 with starting vector $\mathbf{b} = (1, 1, \ldots, 1)$.

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 temporally and spatially. 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 with an improved initial guess. The new initial guess is taken to be the vector that was found upon termination of the last GMRES iteration run. 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 4. Write a function that implements GMRES with restarts as follows.

1. Perform the GMRES algorithm for a maximum of k iterations.
2. If the desired tolerance was reached, terminate the algorithm. If not, repeat step 1 using x_k from the previous GMRES algorithm as a new initial guess x_0.
3. Repeat step 2 until the desired tolerance has been obtained or until a given maximum number of restarts has been reached.

Your function should accept all of the same inputs as the function you wrote in Problem 1 with the exception of k, which will now denote the number of iterations before restart (defaults to 5), and an additional parameter `restarts` which denotes the maximum number of restarts before termination (defaults to 50).

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
>>> from scipy.sparse import linalg as spla

>>> A = np.random.rand(300, 300)
>>> b = np.random(300)
>>> x, info = spla.gmres(A, b)
>>> print(info)
3000
```

The function outputs two objects: the approximate solution `x` and an integer `info` which gives information about the convergence of the algorithm. If `info=0` then convergence occured; if `info` is positive then it equals the number of iterations performed. In the previous case, the function performed 3000 iterations of GMRES before returning the approximate solution `x`. The following code verifies how close the computed value was to the exact solution.

```
>>> la.norm((A @ x) - b)
4.744196381683801
```

A better approximation can be obtained using GMRES with restarts.

```
# Restart after 1000 iterations.
>>> x, info = spla.gmres(A, b, restart=1000)
>>> info
0
>>> la.norm((A @ x) - b)
1.0280404494143551e-12
```

This time, the returned approximation $\mathbf{x}$ is about as close to a true solution as can be expected.

Problem 5. Plot the runtimes of your implementations of GMRES from Problems 1 and 4 and `scipy.sparse.linalg.gmres()` use the default tolerance and `restart=1000` with different matrices. Use the $m \times m$ matrix P with $m = 25, 50, \ldots 200$ and with entries taken from a random normal distribution with mean 0 and standard deviation $1/(2\sqrt{m})$. Use a vector of ones for $\mathbf{b}$ and a vector of zeros for $\mathbf{x}_0$. Use a single figure for all plots, plot the runtime on the y-axis and m on the x-axis.

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`.

$$A = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \end{bmatrix}$$

$$\texttt{A.sum(axis=0)} = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \end{bmatrix} = \begin{bmatrix} 4 & 8 & 12 & 16 \end{bmatrix}$$

$$\texttt{A.sum(axis=1)} = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \end{bmatrix} = \begin{bmatrix} 10 & 10 & 10 & 10 \end{bmatrix}$$