

COMP2870 Theoretical Foundations: Linear Algebra

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1 Introduction

1.1 Contents of this submodule

This part of the module will deal with numerical algorithms that involve matrices. The study of this type of problem is called *linear algebra*. We will approach these problems using a combination of theoretical ideas and practical solutions, thinking through the lens of real-world applications. As a consequence, to succeed in linear algebra, you will do some programming (using Python) and some pen-and-paper theoretical work, too.

1.1.1 Topics

We will have 7 double lectures, 3 tutorials, and 3 labs. We break up the topics as follows:

Lectures

1. Introduction and motivation, key problem statements (Week 4, Mon)
2. When can we solve systems of linear equations? (Week 4, Wed)
3. Direct methods for systems of linear equations (Week 5, Mon)
4. Iterative solution of linear equations (Week 5, Wed)
5. Complex numbers (Week 6, Mon)
6. Eigenvalues and eigenvectors (Week 6, Wed)
7. Practical solutions for eigenvalues and eigenvectors / Summary (Week 7, Mon)

Labs

1. Floating point numbers (Week 4)
2. When can we solve systems of linear equations? (Week 5)
3. Systems of linear equations (Week 6)
4. Eigenvalues and eigenvectors (Week 7)

Tutorials

1. Linear independence, span, basis (Week 5)
2. Solution of linear systems (Week 6)
3. Eigenvalue and eigenvectors (Week 7)

Later this term, week 11, you will complete a project based on the things you've learnt from this section of the module.

1.1.2 Learning outcomes

Candidates should be able to:

- explain practical challenges working with floating-point numbers;
- define and identify what it means for a set of vectors to be a basis, spanning set or linearly independent;
- apply direct and iterative solvers to solve systems of linear equations; implement methods using floating point numbers and investigate computational cost using computer experiments;
- apply algorithms to compute eigenvectors and eigenvalues of large matrices.

1.2 Textbooks and other resources

There are many textbooks and other external resources which could help your learning:

- [Introduction to Linear Algebra](#) (Fifth Edition), Gilbert Strang, Wellesley-Cambridge Press, 2016. with [MIT course material](#). *Strongly recommended book and YouTube lecture series*
- [Scientific Computing: An Introductory Survey](#), T.M. Heath, McGraw-Hill, 2002. Some lecture notes based on the book
- [Engineering Mathematics](#), K.A. Stroud, Macmillan, 2001. *available online*
- [Numerical Recipes in C++/C/FORTRAN](#): The Art of Scientific Computing, W.H. Press, S.A. Teukolsky, W.T. Vetterling and B.P. Flannery, Cambridge University Press, 2002/1993/1993. *A very practical view of the methods we develop in this module which could be used for library development*

Other links and resources are given at the end of each section of the notes.

1.3 Programming

This section of the notes links theoretical material with practical applications. We will have weekly lab sessions where you will see how the methods mentioned in the lecture notes work when implemented. More instructions on how we will do this will be covered in the lab sessions themselves.

An important theoretical aspect of translating the algorithms in linear algebra to computer implementations is the use of floating-point numbers. You will have already met floating-point numbers in your first year studies where you met how computer store numbers. You will already know that computer cannot store every possible real number exactly. The inexactness of floating-point numbers has real consequences when performing linear algebra computations.

Exploring and understanding the material in (Chapter 2) is really helpful for understanding many of the choices that we make when forming methods in linear algebra.

We will make extensive use of [Python](#) and [numpy](#) during this section of the module. It may help you to revise some of your notes from last year on these topics.

1.4 The big problems in linear algebra

We will cover two big linear algebra problems in this section of the module. Linear algebra can be defined as the study of problems involving matrices and vectors.

1.4.1 Reminder of matrices and vectors

There are two important objects we will work with that were defined in your first-year Theoretical Foundations module (COMP1870).

Definition 1.1. A *matrix* is a rectangular array of numbers called *entries* or *elements* of the matrix. A matrix with m rows and n columns is called an $m \times n$ matrix or m -by- n matrix. We may additionally say that the matrix is of order $m \times n$. If $m = n$, then we say that the matrix is *square*.

Example 1.1. A is a 3×4 matrix and B is a 3×4 matrix:

$$A = \begin{pmatrix} 10 & 1 & 0 & 9 \\ 12.4 & 6 & 1 & 0 \\ 1 & 3.14 & 1 & 0 \end{pmatrix} \quad B = \begin{pmatrix} 0 & 6 & 3 & 1 \\ 1 & 4 & 1 & 0 \\ 7 & 0 & 10 & 20 \end{pmatrix} \quad C = \begin{pmatrix} 4 & 1 & 8 & -1 \\ 1.5 & 1 & 3 & 4 \\ 6 & -4 & 2 & 8 \end{pmatrix}$$

Exercise 1.1.

1. Compute, if defined, $A + B$, $B + C$.
2. Compute, if defined, AB , BA , BC (here, by writing matrices next to each other we mean the matrix product).

When considering systems of linear equations, the entries of the matrix will always be real numbers (later we will explore using complex numbers (Chapter 6) too)

Definition 1.2. A *column vector*, often just called a *vector*, is a matrix with a single column. A matrix with a single row is a *row vector*. The entries of a vector are called *components*. A vector with n rows is called an n -vector.

Example 1.2. \vec{a} is a row vector, \vec{b} and \vec{c} are (column) vectors.

$$\vec{a} = \begin{pmatrix} 0 & 1 & 7 \end{pmatrix} \quad \vec{b} = \begin{pmatrix} 0 \\ 1 \\ 3.1 \\ 7 \end{pmatrix} \quad \vec{c} = \begin{pmatrix} 4 \\ 6 \\ -4 \\ 0 \end{pmatrix}.$$

Exercise 1.2.

1. Compute, if defined, $\vec{b} + \vec{c}$, $0.25\vec{c}$.
2. What is the meaning of $\vec{b}^T \vec{c}$? (Here, we are interpreting the vectors as matrices).
3. Compute, if defined, $B\vec{b}$.

Example 1.3 (Some special matrices). It will be helpful to remember some special matrices during this section of the module.

A **rotation matrix** is a 2×2 matrix given by

$$R(\theta) = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix}. \quad (1.1)$$

This matrix describes an anti-clockwise rotation by θ (in radians).

The **projection operator** maps vectors onto either lines or planes which pass through the origin ($\vec{0}$).

- For projection onto a line $L = \{\lambda\vec{a} : \lambda \in \mathbb{R}\}$, we can write this transformation as:

$$\vec{x} \mapsto \vec{a} \cdot \vec{x}\vec{a} = (\vec{a} \otimes \vec{a})\vec{x},$$

where \otimes is the *outer product*. For two n -vectors \vec{a} and \vec{b} , $\vec{a} \otimes \vec{b}$ is an $n \times n$ with entries:

$$(\vec{a} \otimes \vec{b})_{ij} = a_i b_j.$$

- For projection onto a plane $\Pi = \{\lambda\vec{a} + \mu\vec{b} : \lambda, \mu \in \mathbb{R}\}$, we can write the projection operator as:

$$\vec{x} \mapsto (\vec{a} \otimes \vec{a} + \vec{b} \otimes \vec{b})\vec{x}.$$

1.4.2 Systems of linear equations

Given an $n \times n$ matrix A and an n -vector \vec{b} , find the n -vector \vec{x} which satisfies:

$$A\vec{x} = \vec{b}. \quad (1.2)$$

We can also write (3.1) as a system of linear equations:

$$\begin{array}{ll} \text{Equation 1:} & a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \cdots + a_{1n}x_n = b_1 \\ \text{Equation 2:} & a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + \cdots + a_{2n}x_n = b_2 \\ \vdots & \\ \text{Equation i:} & a_{i1}x_1 + a_{i2}x_2 + a_{i3}x_3 + \cdots + a_{in}x_n = b_i \\ \vdots & \\ \text{Equation n:} & a_{n1}x_1 + a_{n2}x_2 + a_{n3}x_3 + \cdots + a_{nn}x_n = b_n. \end{array}$$

Notes:

- The values a_{ij} are known as **coefficients**.
- The **right hand side** values b_i are known and are given to you as part of the problem.
- $x_1, x_2, x_3, \dots, x_n$ are **not** known and are what you need to find to solve the problem.

Many computational algorithms require the solution of linear equations, e.g. in fields such as

- Scientific computation;
- Network design and optimisation;
- Graphics and visualisation;
- Machine learning.

Typically, these systems are *very* large ($n \approx 10^9$).

It is therefore important that this problem can be solved

- accurately: we are allowed to make small errors but not big errors;
- efficiently: we need to find the answer quickly;
- reliably: we need to know that our algorithm will give us an answer that we are happy with.

Example 1.4 (Temperature in a sealed room). Suppose we wish to estimate the temperature distribution inside an object:



Figure 1.1: Image showing temperature sample points and relations in a room.

We can place a network of points inside the object and use the following model: the temperature at each interior point is the average of its neighbours.

This example leads to the system:

$$\begin{pmatrix} 1 & -1/6 & -1/6 & 0 & -1/6 & 0 & 0 \\ -1/6 & 1 & -1/6 & -1/6 & 0 & -1/6 & 0 \\ -1/4 & -1/4 & 1 & 0 & -1/4 & -1/4 & 0 \\ 0 & -1/5 & 0 & 1 & 0 & -1/5 & 0 \\ -1/6 & 0 & -1/6 & 0 & 1 & -1/6 & -1/6 \\ 0 & -1/8 & -1/8 & -1/8 & -1/8 & 1 & -1/8 \\ 0 & 0 & 0 & 0 & -1/5 & -1/5 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \\ x_7 \end{pmatrix} = \begin{pmatrix} 400/6 \\ 100/6 \\ 0 \\ 0 \\ 100/6 \\ 0 \\ 0 \end{pmatrix}.$$

Example 1.5 (Traffic network). Suppose we wish to monitor the flow of traffic in a city centre:



Figure 1.2: Example network showing traffic flow in a city

As the above example shows, it is not necessary to monitor every single road. If we know all of the y values, we can calculate the x values!

This example leads to the system:

$$\begin{pmatrix} 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \\ x_7 \\ x_8 \end{pmatrix} = \begin{pmatrix} y_5 \\ y_{12} - y_6 \\ y_8 - y_7 \\ y_{11} - y_4 \\ y_{11} + y_{12} - y_{10} \\ y_9 \\ y_2 - y_3 \\ y_1 \end{pmatrix}.$$

1.4.3 Eigenvalues and eigenvectors

For this problem, we will think of a matrix A acting on functions \vec{x} :

$$\vec{x} \mapsto A\vec{x}.$$

We are interested in when the output vector $A\vec{x}$ is *parallel* to \vec{x} ?

Definition 1.3. We say that any vector \vec{x} , where $A\vec{x}$ is parallel to \vec{x} , is called an *eigenvector* of A . Here by parallel, we mean that there exists a number λ (can be positive, negative or zero) such that

$$A\vec{x} = \lambda\vec{x}. \quad (1.3)$$

We call the associated number λ an *eigenvalue* of A .

We will later see that an $n \times n$ square matrix always has n eigenvalues (which may not always be distinct).

To help with our intuition here, we start with some simple examples:

Example 1.6. Let A be the 2×2 matrix that scales any input vector by a in the x -direction and by b in the y -direction. We can write this matrix as

$$A = \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix},$$

since then for a 2-vector $\vec{x} = (x, y)^T$, we have

$$A\vec{x} = \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} ax + 0y \\ 0x + by \end{pmatrix} = \begin{pmatrix} ax \\ by \end{pmatrix}.$$

Then, we infer we have two eigenvalues and two eigenvectors: One eigenvalue is a with eigenvector $(1, 0)^T$ and the other is b with eigenvector $(0, 1)^T$ since:

$$\begin{aligned} \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} &= \begin{pmatrix} a \\ 0 \end{pmatrix} = a \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} &= \begin{pmatrix} 0 \\ b \end{pmatrix} = b \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \end{aligned}$$

Example 1.7. Let P be the 3×3 matrix that represents projection onto a plane π . What are the eigenvalues and eigenvectors of P ?

Sample plane and normal vector



- If \vec{x} is in the plane Π , then $P\vec{x} = \vec{x}$. This means that \vec{x} is an eigenvector and the associated eigenvalue is 1.
- If \vec{y} is perpendicular to the plane Π , then $P\vec{y} = \vec{0}$. This means that \vec{y} is an eigenvector and the associated eigenvalue is 0.

Let \vec{y} be perpendicular to Π (so that $P\vec{y} = \vec{0}$ and \vec{y} is an eigenvector of P), then for any number s , we can compute

$$P(s\vec{y}) = sP\vec{y} = s\vec{0} = \vec{0}.$$

This means that $s\vec{y}$ is also an eigenvector of P associated to the eigenvalue 0. As a consequence, when we compute eigenvectors, we need to take care to *normalise* the vector to ensure we get a unique answer.

We see we end up with a two-dimensional space of eigenvectors (i.e., the plane Π) associated to eigenvalue 1 and a one-dimensional space of eigenvectors (i.e., the line perpendicular to Π) eigenvalue 0. We use the term *eigenspace* the space of eigenvectors associated to a particular eigenvalue.

Example 1.8. Let A be the permutation matrix which takes an input two-vector and outputs a two-vector with the components swapped. The matrix is given by

$$A = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

What are the eigenvectors and eigenvalues of A ?

- Let $\vec{x} = (1, 1)^T$, then swapping the components of \vec{x} gives back the same vector \vec{x} . In equations, we can write $A\vec{x} = \vec{x}$. This means that \vec{x} is an eigenvector and the eigenvalue is 1.
- Let $\vec{x} = (-1, 1)^T$, then swapping the components of \vec{x} gives back $(1, -1)^T$, which we can see is $-\vec{x}$. In equations, we can write $A\vec{x} = -\vec{x}$. This means that \vec{x} is an eigenvector of A and the associated eigenvalue is -1 .

Here we see that again we actually have two one-dimensional eigenspaces.

1.5 Comments on these notes

There are two versions of these notes available: as an online website and as a pdf. I expect minor adjustments to be made to both throughout the progress of delivering the materials.

You can always find the latest versions at:

- <https://comp2870-2526.github.io/linear-algebra-notes/> (html version)
- <https://comp2870-2526.github.io/linear-algebra-notes/COMP2870-Theoretical-Foundations--Linear-Algebra.pdf> (pdf version)

Please either email me (T.Ranner@leeds.ac.uk) or use the [github repository](#) to report any corrections.

This version of the notes is 8f588b5+dirty.

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2 Floating point number systems

Module learning objective

Explain practical challenges working with floating-point numbers.

This topic will not be presented explicitly in lectures; instead, you will study the material yourself in Lab Session 1.

2.1 Finite precision number systems

Computers store numbers with **finite precision**, i.e. using a finite set of bits (binary digits), typically 32 or 64 of them. You learned how to store numbers as floating-point numbers last year in the module COMP1860 Building our Digital World.

You will recall that many numbers cannot be stored exactly.

- Some numbers cannot be represented precisely using **any** finite set of digits: e.g. $\sqrt{2} = 1.14142 \dots$, $\pi = 3.14159 \dots$, etc.
- Some cannot be represented precisely in a given number base:
e.g. $\frac{1}{9} = 0.111 \dots$ (decimal), $\frac{1}{5} = 0.00110011 \dots$ (binary).
- Others can be represented by a finite number of digits but only using more than are available: e.g. 1.526374856437 cannot be stored exactly using 10 decimal digits.

The inaccuracies inherent in finite precision arithmetic must be modelled in order to understand:

- how the numbers are represented (and the nature of associated limitations);
- the errors in their representation;
- the errors which occur when arithmetic operations are applied to them.

The examples shown here will be in **decimal** by the issues apply to any base, *e.g.* **binary**.

This is important when trying to solve problems with floating-point numbers, so that we learn how to avoid the key pitfalls.

2.2 Normalised systems

To understand how this works in practice, we introduce an abstract way to think about the practicalities of floating-point numbers, but our examples will have fewer digits.

Any finite precision number can be written using the floating point representation:

$$x = \pm 0.b_1 b_2 b_3 \dots b_{t-1} b_t \times \beta^e.$$

- The digits b_i are integers satisfying $0 \leq b_i \leq \beta - 1$.
- The **mantissa**, $b_1 b_2 b_3 \dots b_{t-1} b_t$, contains t digits.
- β is the **base** (always a positive integer).
- e is the integer **exponent** and is bounded ($L \leq e \leq U$).

(β, t, L, U) fully defines a finite precision number system.

Normalised finite precision systems will be considered here for which

$$b_1 \neq 0 \quad (0 < b_1 \leq \beta - 1).$$

Example 2.1.

1. In the case $(\beta, t, L, U) = (10, 4, -49, 50)$ (base 10),

$$10000 = .1000 \times 10^5, \quad 22.64 = .2264 \times 10^2, \quad 0.0000567 = .5670 \times 10^{-4}$$

2. In the case $(\beta, t, L, U) = (2, 6, -7, 8)$ (binary),

$$10000 = .100000 \times 2^5, \quad 1011.11 = .101111 \times 2^4,$$

$$0.000011 = .110000 \times 2^{-4}.$$

3. **Zero** is always taken to be a special case e.g., $0 = \pm 0.0 \dots 0 \times \beta^0$.

Our familiar floating point numbers can be represented using this format too:

1. The [IEEE single-precision standard](#) is $(\beta, t, L, U) = (2, 23, -127, 128)$. This is available via `numpy.single`.
2. The [IEEE double-precision standard](#) is $(\beta, t, L, U) = (2, 52, -1023, 1024)$. This is available via `numpy.double`.

```

1 import numpy as np
2
3 a = np.double(1.1)
4 print(type(a))
5 b = np.single(1.2)
6 print(type(b))
7 c = np.half(1.3)
8 print(type(c))

```

```

<class 'numpy.float64'>
<class 'numpy.float32'>
<class 'numpy.float16'>

```

You can create double-precision floating point numbers without using `numpy` (i.e. 64 bit with the same β, t, L, U as above) by calling the `float` function, or just giving the number in decimal format:

```

1 (np.double(5.1) == 5.1, np.double(5.1) == 5.1)

```

```
(np.True_, np.True_)
```

However, in some extreme edge cases, you are unlikely to meet, Python floats do not follow the IEEE double-precision standard in some extreme edge cases.

Example 2.2. Consider the number system given by $(\beta, t, L, U) = (10, 2, -1, 2)$ which gives

$$x = \pm.b_1 b_2 \times 10^e \text{ where } -1 \leq e \leq 2.$$

a. How many numbers can be represented by this normalised system?

- The sign can be positive or negative
- b_1 can take on the values 1 to 9 (9 options)
- b_2 can take on the values 0 to 9 (10 options)
- e can take on the values $-1, 0, 1, 2$ (4 options)

Overall this gives us:

$$2 \times 9 \times 10 \times 4 \text{ options} = 720 \text{ options.}$$

b. What are the two largest positive numbers in this system?

The largest value uses + as a sign, $b_1 = 9$, $b_2 = 9$ and $e = 2$ which gives

$$+0.99 \times 10^2 = 99.$$

The second largest value uses + as a sign, $b_1 = 9$, $b_2 = 8$ and $e = 2$ which gives

$$+0.98 \times 10^2 = 98.$$

- c. What are the two smallest positive numbers?

The smallest positive number has + sign, $b_1 = 1$, $b_2 = 0$ and $e = -1$ which gives

$$+0.10 \times 10^{-1} = 0.01.$$

The second smallest positive number has + sign, $b_1 = 1$, $b_2 = 1$ and $e = -1$ which gives

$$+0.11 \times 10^{-1} = 0.011.$$

- d. What is the smallest possible difference between two numbers in this system?

The smallest difference will be between numbers of the form $+0.10 \times 10^{-1}$ and $+0.11 \times 10^{-1}$ which gives

$$0.11 \times 10^{-1} - 0.10 \times 10^{-1} = 0.011 - 0.010 = 0.001.$$

Alternatively, we can brute-force search for this:

```
The minimum difference min_diff=0.0010
at x=+0.57 x 10^{-1} y=+0.58 x 10^{-1}.
```

Exercise 2.1. Consider the number system given by $(\beta, t, L, U) = (10, 3, -3, 3)$ which gives

$$x = \pm.b_1 b_2 b_3 \times 10^e \text{ where } -3 \leq e \leq 3.$$

- a. How many numbers can be represented by this normalised system?
- b. What are the two largest positive numbers in this system?
- c. What are the two smallest positive numbers?
- d. What is the smallest possible difference between two numbers in this system?
- e. What is the smallest possible difference in this system, x and y , for which $x < 100 < y$?

Example 2.3 (What about in Python). We find that even with double-precision floating point numbers, we see some funniness when working with decimals:

```

1 a = np.double(0.0)
2
3 # add 0.1 ten times to get 1?
4 for _ in range(10):
5     a = a + np.double(0.1)
6     print(a)
7
8 print("Is a = 1?", a == 1.0)

```

```

0.1
0.2
0.3000000000000004
0.4
0.5
0.6
0.7
0.799999999999999
0.899999999999999
0.999999999999999
Is a = 1? False

```

Why is this output not a surprise?

We also see that even adding up numbers can have different results depending on what order we add them:

```

1 x = np.double(1e30)
2 y = np.double(-1e30)
3 z = np.double(1.0)
4
5 print(f"(x + y) + z={:.16f}")

```

```
(x + y) + z=1.0000000000000000
```

```
1 print(f"x + (y + z)={:.16f}")
```

```
x + (y + z)=0.0000000000000000
```

2.3 Errors and machine precision

From now on $fl(x)$ will be used to represent the (approximate) stored value of x . The error in this representation can be expressed in two ways.

$$\begin{aligned}\text{Absolute error} &= |fl(x) - x| \\ \text{Relative error} &= \frac{|fl(x) - x|}{|x|}.\end{aligned}$$

The number $fl(x)$ is said to approximate x to t **significant digits** (or figures) if t is the largest non-negative integer for which

$$\text{Relative error} < 0.5 \times \beta^{1-t}.$$

It can be proved that if the relative error is equal to β^{-d} , then $fl(x)$ has d correct significant digits.

In the number system given by (β, t, L, U) , the nearest (larger) representable number to $x = 0.b_1 b_2 b_3 \dots b_{t-1} b_t \times \beta^e$ is

$$\tilde{x} = x + .\underbrace{000\dots01}_{t \text{ digits}} \times \beta^e = x + \beta^{e-t}$$

Any number $y \in (x, \tilde{x})$ is stored as either x or \tilde{x} by **rounding** to the nearest representable number, so

- the largest possible error is $\frac{1}{2}\beta^{e-t}$,
- which means that $|y - fl(y)| \leq \frac{1}{2}\beta^{e-t}$.

It follows from $y > x \geq .100\dots00 \times \beta^e = \beta^{e-1}$ that

$$\frac{|y - fl(y)|}{|y|} < \frac{1}{2} \frac{\beta^{e-t}}{\beta^{e-1}} = \frac{1}{2} \beta^{1-t},$$

and this provides a bound on the **relative error**: for any y

$$\frac{|y - fl(y)|}{|y|} < \frac{1}{2} \beta^{1-t}.$$

The last term is known as **machine precision** or **unit roundoff** and is often called eps . This is obtained in Python with

```

1  eps = np.finfo(np.double).eps
2  print(eps)

```

2.220446049250313e-16

Example 2.4.

1. The number system $(\beta, t, L, U) = (10, 2, -1, 2)$ gives

$$\text{eps} = \frac{1}{2}\beta^{1-t} = \frac{1}{2}10^{1-2} = 0.05.$$

2. The number system $(\beta, t, L, U) = (10, 3, -3, 3)$ gives

$$\text{eps} = \frac{1}{2}\beta^{1-t} = \frac{1}{2}10^{1-3} = 0.005.$$

3. The number system $(\beta, t, L, U) = (10, 7, 2, 10)$ gives

$$\text{eps} = \frac{1}{2}\beta^{1-t} = \frac{1}{2}10^{1-7} = 0.000005.$$

4. For some common types in python, we see the following values:

```

1  for dtype in [np.half, np.single, np.double]:
2      print(dtype.__name__, np.finfo(dtype).eps)

```

```

float16 0.000977
float32 1.1920929e-07
float64 2.220446049250313e-16

```

Machine precision epsilon (eps) gives us an upper bound for the error in the representation of a floating-point number in a particular system. We note that this is different to the smallest possible numbers that we can store!

```

1  eps = np.finfo(np.double).eps
2  print(f"eps={eps}")
3
4  smaller = eps
5  for _ in range(5):
6      smaller = smaller / 10.0
7  print(f"smaller={smaller}")

```

```

eps=np.float64(2.220446049250313e-16)
smaller=np.float64(2.2204460492503132e-17)
smaller=np.float64(2.220446049250313e-18)
smaller=np.float64(2.220446049250313e-19)
smaller=np.float64(2.2204460492503132e-20)
smaller=np.float64(2.2204460492503133e-21)

```

Arithmetic operations are usually carried out as though infinite precision is available, after which the result is rounded to the nearest representable number.

This approach means that arithmetic cannot be completely trusted and the usual rules do not necessarily apply!

Example 2.5. Consider the number system $(\beta, t, L, U) = (10, 2, -1, 2)$ and take

$$x = .10 \times 10^2, \quad y = .49 \times 10^0, \quad z = .51 \times 10^0.$$

- In exact arithmetic $x + y = 10 + 0.49 = 10.49$ and $x + z = 10 + 0.51 = 10.51$.
- In this number system rounding gives

$$fl(x + y) = .10 \times 10^2 = x, \quad fl(x + z) = .11 \times 10^2 \neq x.$$

(Note that $\frac{y}{x} < \text{eps}$ but $\frac{z}{x} > \text{eps}$.)

Evaluate the following expression in this number system.

$$x + (y + y), \quad (x + y) + y, \quad x + (z + z), \quad (x + z) + z.$$

(Also note the benefits of adding the *smallest* terms first!)

Exercise 2.2 (More examples).

1. Verify that a similar problem arises for the numbers

$$x = .85 \times 10^0, \quad y = .3 \times 10^{-2}, \quad z = .6 \times 10^{-2},$$

in the system $(\beta, t, L, U) = (10, 2, -3, 3)$.

2. Given the number system $(\beta, t, L, U) = (10, 3, -3, 3)$ and $x = .100 \times 10^3$, find nonzero numbers y and z from this system for which $fl(x + y) = x$ and $fl(x + z) > x$.

It is sometimes helpful to think of another machine precision epsilon in other way: **Machine precision epsilon** is the smallest positive number eps such that $1 + \text{eps} > 1$, i.e. it is half the difference between 1 and the next largest representable number.

Examples:

1. For the number system $(\beta, t, L, U) = (10, 2, -1, 2)$,

$$\begin{array}{r} .11 \times 10^1 \\ - .10 \times 10^1 \\ \hline .01 \times 10^1 \end{array} \quad \begin{array}{l} \leftarrow \text{next number} \\ \leftarrow 1 \\ \leftarrow 0.1 \end{array}$$

so $\text{eps} = \frac{1}{2}(0.1) = 0.05$.

2. Verify that this approaches gives the previously calculated value for eps in the number system given by $(\beta, t, L, U) = (10, 3, -3, 3)$.

2.4 Other “Features” of finite precision

When working with floating-point numbers there are other things we need to worry about, too!

Overflow The number is too large to be represented, e.g. multiply the largest representable number by 10. This gives `inf` (infinity) with `numpy.doubles` and is usually “fatal”.

Underflow The number is too small to be represented, e.g. divide the smallest representable number by 10. This gives 0 and may not be immediately obvious.

Divide by zero gives a result of `inf`, but $\frac{0}{0}$ gives `nan` (not a number)

Divide by inf gives 0.0 with no warning

2.5 Is this all academic?

No! There are many examples of major software errors that have occurred due to programmers not understanding the issues associated with computer arithmetic...

- In February 1991, a [basic rounding error](#) within software for the US Patriot missile system caused it to fail, contributing to the loss of 28 lives.
- In June 1996, the European Space Agency’s Ariane Rocket exploded shortly after take-off: the error was due to failing to [handle overflow correctly](#).
- In October 2020, a driverless car drove straight into a wall due to [faulty handling of a floating-point error](#).

2.6 Summary

- There is inaccuracy in almost all computer arithmetic.
- Care must be taken to minimise its effects, for example:
 - add the smallest terms in an expression first;
 - avoid taking the difference of two very similar terms;
 - even checking whether $a = b$ is dangerous!
- The usual mathematical rules no longer apply.
- There is no point in trying to compute a solution to a problem to a greater accuracy than can be stored by the computer.

2.6.1 Further reading

- David Goldberg, [What every computer scientist should know about floating-point arithmetic](#), ACM Computing Surveys, Volume 23, Issue 1, March 1991.
- John D Cook, [Floating point error is the least of my worries](#), *online*, November 2011.

3 Introduction to systems of linear equations

Module learning objective

Define and identify what it means for a set of vectors to be a basis, spanning set or linearly independent.

3.1 Definition of systems of linear equations

Given an $n \times n$ matrix A and an n -vector \vec{b} , find the n -vector \vec{x} which satisfies:

$$A\vec{x} = \vec{b}. \quad (3.1)$$

We can also write (3.1) as a system of linear equations:

$$\text{Equation 1: } a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \cdots + a_{1n}x_n = b_1$$

$$\text{Equation 2: } a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + \cdots + a_{2n}x_n = b_2$$

⋮

$$\text{Equation } i: \quad a_{i1}x_1 + a_{i2}x_2 + a_{i3}x_3 + \cdots + a_{in}x_n = b_i$$

⋮

$$\text{Equation } n: \quad a_{n1}x_1 + a_{n2}x_2 + a_{n3}x_3 + \cdots + a_{nn}x_n = b_n.$$

Notes:

- The values a_{ij} are known as **coefficients**.
- The **right-hand side** values b_i are known and are given to you as part of the problem.
- $x_1, x_2, x_3, \dots, x_n$ are **not** known and are what you need to find to solve the problem.

3.2 Can we do it?

Our first question might be: Is it possible to solve (3.1)?

We know a few simple cases where we can answer this question very quickly:

1. If $A = I_n$, the $n \times n$ *identity matrix*, then we *can* solve this problem:

$$\vec{x} = \vec{b}.$$

2. If $A = O$, the $n \times n$ *zero matrix*, and $\vec{b} \neq \vec{0}$, the zero vector, then there are no solutions to the problem:

$$O\vec{x} = \vec{0} \neq \vec{b} \quad \text{for any vector } \vec{x}.$$

3. If A is *invertible*, with inverse A^{-1} , then we *can* solve this problem:

$$\vec{x} = A^{-1}\vec{b}.$$

However, in general, this is a *terrible* idea and we will see algorithms that are more efficient than finding the inverse of A .

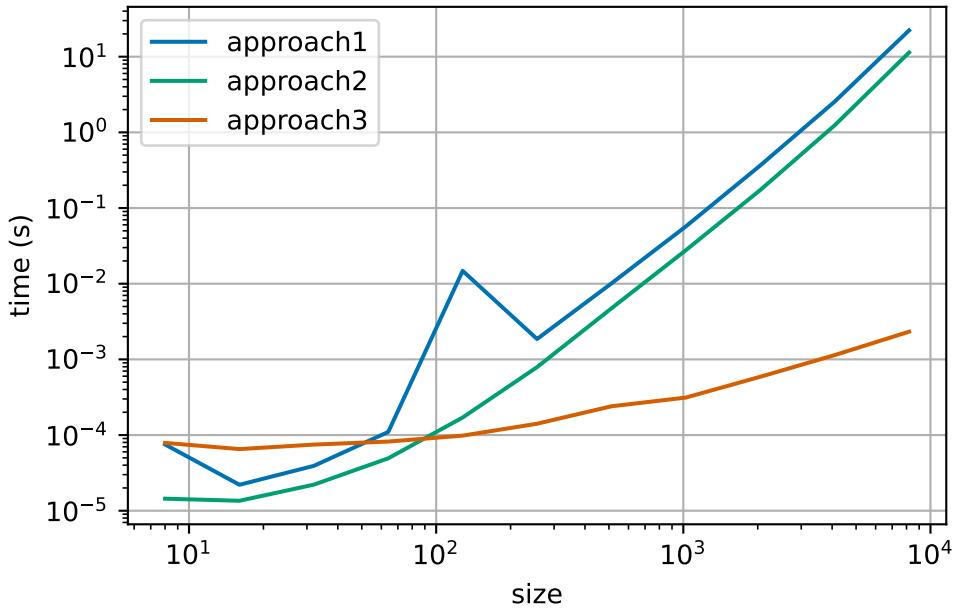
Remark 3.1. One way to solve a system of linear equations is to compute the inverse of A , A^{-1} , directly, then the solution is found through matrix multiplication: $\vec{x} = A^{-1}\vec{b}$. Here we compare two simple and one more specialised implementations:

```
1 def approach1(A, b):
2     """
3     Solve the system of linear equations Ax = b by applying the inverse of A
4     """
5     A_inv = np.linalg.inv(A)
6     x = A_inv @ b
7     return x
8
9
10 def approach2(A, b):
11     """
12     Solve the system of linear equations Ax = b through numpy's linear solver
13     """
14     x = np.linalg.solve(A, b)
15     return x
16
17
18 def approach3(A_sparse, b):
19     """
20     Solve the system of linear equations Ax = b through scipy's sparse linear
```

```

21     solver
22     """
23     x = sp.sparse.linalg.spsolve(A_sparse, b)
24     return x

```



There are tools to help us determine when a matrix is invertible which arise naturally when considering about what $A\vec{x} = \vec{b}$ means! We have to go back to the basic operations on vectors.

There are two fundamental operations you can do on vectors: addition and scalar multiplication. Consider the vectors:

$$\vec{a} = \begin{pmatrix} 2 \\ 1 \\ 2 \end{pmatrix}, \quad \vec{b} = \begin{pmatrix} 1 \\ 2 \\ 4 \end{pmatrix}, \quad \vec{c} = \begin{pmatrix} 4 \\ 2 \\ 6 \end{pmatrix}.$$

Then, we can easily compute the following *linear combinations*:

$$\vec{a} + \vec{b} = \begin{pmatrix} 3 \\ 3 \\ 6 \end{pmatrix} \tag{3.2}$$

$$\vec{c} - 2\vec{a} = \begin{pmatrix} 0 \\ 0 \\ 2 \end{pmatrix} \tag{3.3}$$

$$\vec{a} + 2\vec{b} + 2\vec{c} = \begin{pmatrix} 12 \\ 9 \\ 22 \end{pmatrix}. \tag{3.4}$$

Now if we write A for the 3×3 -matrix whose columns are $\vec{a}, \vec{b}, \vec{c}$:

$$A = \begin{pmatrix} \vec{a} & \vec{b} & \vec{c} \end{pmatrix} = \begin{pmatrix} 2 & 1 & 4 \\ 1 & 2 & 2 \\ 2 & 4 & 6 \end{pmatrix},$$

then the three equations (3.2), (3.3), (3.4), can be written as

$$\begin{aligned} \vec{a} + \vec{b} &= 1\vec{a} + 1\vec{b} + 0\vec{c} = A \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, \\ \vec{c} - 2\vec{a} &= -2\vec{a} + 0\vec{b} - 2\vec{c} = A \begin{pmatrix} -2 \\ 0 \\ 1 \end{pmatrix}, \\ \vec{a} + 2\vec{b} + 2\vec{c} &= 1\vec{a} + 2\vec{b} + 2\vec{c} = A \begin{pmatrix} 1 \\ 2 \\ 2 \end{pmatrix}. \end{aligned}$$

In other words,

We can write any linear combination of vectors as a matrix-vector multiply,

or if we reverse the process,

We can write matrix-vector multiplication as a linear combination of the columns of the matrix.

This rephrasing means that solving the system $A\vec{x} = \vec{b}$ is equivalent to finding a linear combination of the columns of A which is equal to \vec{b} . So, our question about whether we can solve (3.1), can also be rephrased as: does there exist a linear combination of the columns of A which is equal to \vec{b} ? We will next write this condition mathematically using the concept of *span*.

3.2.1 The span of a set of vectors

Definition 3.1. Given a set of vectors of the same size, $S = \{\vec{v}_1, \dots, \vec{v}_k\}$, we say the *span* of S is the set of all vectors which are linear combinations of vectors in S :

$$\text{span}(S) = \left\{ \sum_{i=1}^k x_i \vec{v}_i : x_i \in \mathbb{R} \text{ for } i = 1, \dots, k \right\}. \quad (3.5)$$

Example 3.1. Consider three new vectors

$$\vec{a} = \begin{pmatrix} 2 \\ 3 \end{pmatrix} \quad \vec{b} = \begin{pmatrix} -1 \\ 2 \end{pmatrix} \quad \vec{c} = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

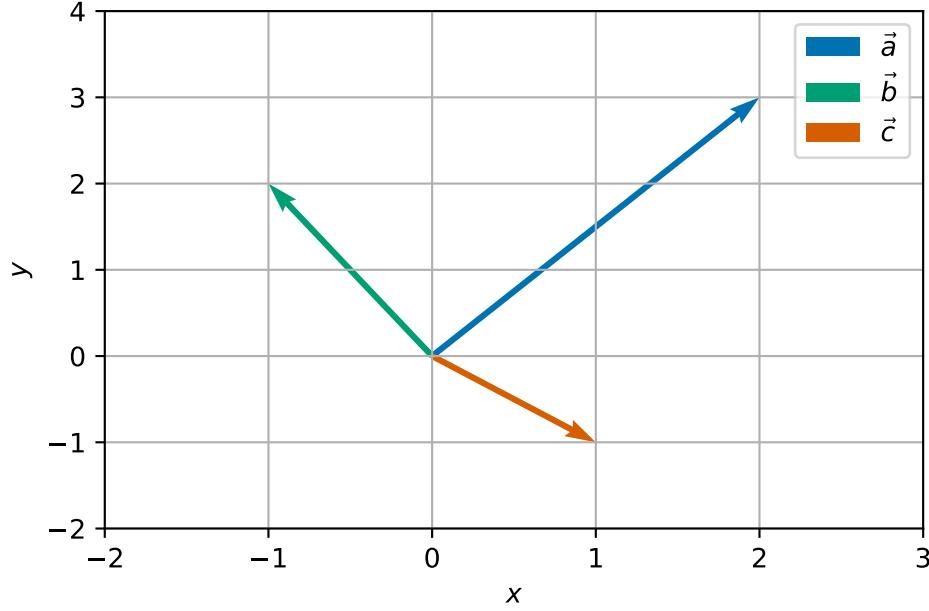


Figure 3.1: Three example vectors in a plane.

1. Let $S = \{\vec{a}\}$, then $\text{span}(S) = \{x\vec{a} : x \in \mathbb{R}\}$. Geometrically, we can think of the span of a single vector to be an infinite straight line which passes through the origin and \vec{a} .
2. Let $S = \{\vec{a}, \vec{b}\}$, then $\text{span}(S) = \mathbb{R}^2$. To see this is true, we first see that $\text{span}(S)$ is contained in \mathbb{R}^2 since any 2-vectors added together and the scalar multiplication of a 2-vector also form a 2-vector. For the opposite inclusion, consider an arbitrary point $\vec{y} = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} \in \mathbb{R}^2$ then

$$\begin{aligned} \frac{2y_1 + y_2}{7} \vec{a} + \frac{-3y_1 + 2y_2}{7} \vec{b} &= \frac{2y_1 + y_2}{7} \begin{pmatrix} 2 \\ 3 \end{pmatrix} + \frac{-3y_1 + 2y_2}{7} \begin{pmatrix} -1 \\ 2 \end{pmatrix} \\ &= \left(\frac{4y_1 + 2y_2}{7} + \frac{3y_1 - 2y_2}{7} \right) \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = \vec{y}. \end{aligned} \quad (3.6)$$

This calculation shows, that we can always form a linear combination of \vec{a} and \vec{b} which results in \vec{y} .

3. Let $S = \{\vec{a}, \vec{b}, \vec{c}\}$, then $\text{span}(S) = \mathbb{R}^2$. Since $\vec{c} \in \text{span}(\{\vec{a}, \vec{b}\})$, any linear combination of $\vec{a}, \vec{b}, \vec{c}$ has an equivalent combination of just \vec{a} and \vec{b} . In formulae, we can see that by applying the formula from (3.6), we have

$$\vec{c} = \frac{1}{7}\vec{a} - \frac{5}{7}\vec{b}.$$

So we have, if $\vec{y} \in \text{span}(S)$, then

$$\vec{y} = x_1\vec{a} + x_2\vec{b} + x_3\vec{c} \Rightarrow \vec{y} = (x_1 + \frac{1}{7}x_3)\vec{a} + (x_2 - \frac{5}{7}x_3)\vec{b},$$

so $\vec{y} \in \text{span}(\{\vec{a}, \vec{b}\})$. Conversely, if $\vec{y} \in \text{span}(\{\vec{a}, \vec{b}\})$, then

$$\vec{y} = x_1\vec{a} + x_2\vec{b} \Rightarrow \vec{y} = x_1\vec{a} + x_2\vec{b} + 0\vec{c}.$$

So the span of $S = \text{span}(\{\vec{a}, \vec{b}\}) = \mathbb{R}^2$. Notice that we this final linear combination of \vec{a}, \vec{b} and \vec{c} to form \vec{y} is not unique.

Our first statement is that (3.1) has a solution if \vec{b} is in the span of the columns of A . However, as we saw with Example 3.1, Part 3, we are not guaranteed that the linear combination is unique! For this we need a further condition.

3.2.2 Linear independence

Definition 3.2. Given a set of vectors of the same size, $S = \{\vec{v}_1, \dots, \vec{v}_k\}$, we say that S is *linearly dependent*, if there exist numbers x_1, x_2, \dots, x_k , not all zero, such that

$$\sum_{i=1}^k x_i \vec{v}_i = \vec{0}.$$

The set S is *linearly independent* if it is not linearly dependent.

Exercise 3.1. Can you write the definition of a linearly independent set of vectors explicitly?

Example 3.2. Continuing from Example 3.1.

1. Let $S = \{\vec{a}, \vec{b}\}$, then S is linearly independent. Indeed, let x_1, x_2 be real numbers such that

$$x_1\vec{a} + x_2\vec{b} = \vec{0},$$

then,

$$2x_1 - x_2 = 0 \quad 3x_1 + 2x_2 = 0$$

The first equation says that $x_2 = 2x_1$, which when substituted into the second equation gives $3x_1 + 4x_1 = 7x_1 = 0$. Together this implies that $x_1 = x_2 = 0$. Put simply this means that if we do have a linear combination of \vec{a} and \vec{b} which is equal zero, then the corresponding scalar multiples are all zero.

2. Let $S = \{\vec{a}, \vec{b}, \vec{c}\}$, then S is linearly dependent. We have previously seen that:

$$\vec{c} = \frac{1}{7}\vec{a} - \frac{5}{7}\vec{b},$$

which we can rearrange to say that

$$\frac{1}{7}\vec{a} - \frac{5}{7}\vec{b} - \vec{c} = \vec{0}.$$

We see that the definition of linear dependence is satisfied for $x_1 = \frac{1}{7}, x_2 = -\frac{5}{7}, x_3 = -1$ which are all nonzero.

So linear independence removes the multiplicity (or non-uniqueness) in how we form linear combinations! The ideas of linear independence and spanning lead us to the final definition of this section.

3.2.3 When vectors form a basis

Definition 3.3. We say that a set of n -vectors S is a *basis* of a set of n -vectors V if the span of S is V and S is linearly independent.

Example 3.3.

1. From Example 3.1, we have that $S = \{\vec{a}, \vec{b}\}$ is a basis of \mathbb{R}^2 .
2. Another (perhaps simpler) basis of \mathbb{R}^2 are the coordinate axes:

$$\vec{e}_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad \vec{e}_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

3. Later, when we work with eigenvectors and eigenvalues we will see that there are other convenient bases (plural of basis) to work with.

We phrase the idea that the existence and uniqueness of linear combinations together depend on the underlying set being a basis mathematically in the following Theorem:

Theorem 3.1. *Let S be a basis of V . Then any vector in V can be written uniquely as a linear combination of entries in S .*

Example 3.4.

1. From the main examples (Example 3.1) in this section, we have that $S = \{\vec{a}, \vec{b}\}$ is a basis of \mathbb{R}^2 and we already know the formula for how to write \vec{y} as a unique combination of \vec{a} and \vec{b} : it is given in (3.6).

2. For the simpler example of the coordinate axes:

$$\vec{e}_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad \vec{e}_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

we have that for any $\vec{y} = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} \in \mathbb{R}^2$

$$\vec{y} = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = y_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix} + y_2 \begin{pmatrix} 0 \\ 1 \end{pmatrix} = y_1 \vec{e}_1 + y_2 \vec{e}_2.$$

Proof of Theorem 3.1. Let \vec{y} be a vector in V and label $S = \{\vec{v}_1, \dots, \vec{v}_k\}$. Since S forms a basis of V , $\vec{y} \in \text{span}(S)$ so there exists numbers x_1, \dots, x_k such that

$$\vec{y} = \sum_{i=1}^k x_i \vec{v}_i. \tag{3.7}$$

Suppose that there exists another set of number z_1, \dots, z_k such that

$$\vec{y} = \sum_{i=1}^k z_i \vec{v}_i. \tag{3.8}$$

Taking the difference of (3.7) and (3.8), we see that

$$\vec{0} = \sum_{i=1}^k (x_i - z_i) \vec{v}_i. \tag{3.9}$$

Since S is linearly independent, this implies $x_i = z_i$ for $i = 1, \dots, k$, and we have shown that there is only one linear combination of the vectors $\{\vec{v}_i\}$ to form \vec{y} . \square

There is a theorem that says that the number of vectors in any basis of a given ‘nice’ set of vectors V is the same, but is beyond the scope of this module!

Theorem 3.2. *Let A be a $n \times n$ -matrix. If the columns of A form a basis of \mathbb{R}^n , then there exists a unique n -vector \vec{x} which satisfies $A\vec{x} = \vec{b}$.*

We do not give full details of the proof here since all the key ideas are already given above.

3.2.4 Another characterisation: the determinant

Let \vec{e}_j be the (column) vector in \mathbb{R}^n which has 0 for all coefficients apart from the j th place:

$$\vec{e}_j = (0, \dots, 0, \underset{j\text{th place}}{\underbrace{1}}, 0, \dots, 0).$$

Then, we can compute that for any $n \times n$ matrix A that we have the i th component of $A\vec{e}_j$ is given by

$$(A\vec{e}_j)_i = \sum_{k=1}^n A_{ik}(\vec{e}_j)_k = A_{ij}.$$

That is that $A\vec{e}_j$ gives the j th column of the matrix A .

One geometric way to see that the columns of A form a basis is to explore the shape of polytope with edges away from the origin given by the columns of A (hyper-parallelopiped).

Example 3.5. For A given by

$$A = \begin{pmatrix} 3 & 1 \\ 0 & 3 \end{pmatrix}$$

the shape is a parallelogram that looks like this:



For A given by

$$A = \begin{pmatrix} 3 & 1 & 1 \\ 0 & 3 & 1 \\ 0 & 0 & 3 \end{pmatrix},$$

the shape is a parallelopiped given that looks like this:



If we are given an $n \times n$ matrix A , its n columns form a basis of \mathbb{R}^n if, and only if, the area/volume/hyper-volume of the associated hyper-parallelepiped is nonzero. Roughly speaking this follows since if the area/volume/hyper-volume is zero then two of the column vectors must point in the same direction. This property is so important that the area/volume/hyper-volume of the hyper-parallelepiped associated with the matrix A has a special name: the *determinant* of A and we write $\det A$.

Definition 3.4. Let A be a square $n \times n$ matrix.

If $n = 2$,

$$\det A = \det \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} = a_{11}a_{22} - a_{21}a_{12}. \quad (3.10)$$

If $n = 3$,

$$\begin{aligned} \det A &= \det \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \\ &= a_{11}(a_{22}a_{33} - a_{23}a_{32}) - a_{12}(a_{21}a_{33} - a_{23}a_{31}) + a_{13}(a_{21}a_{32} - a_{22}a_{31}). \end{aligned}$$

For general n , the determinant can be found by, for example, Laplace expansions

$$\det A = \sum_{j=1}^n (-1)^{j+1} a_{1,j} m_{1,j},$$

where $a_{1,j}$ is the entry of the first row and j th column of A and $m_{1,j}$ is the determinant of the submatrix obtained by removing the first row and the j th column from A .

Example 3.6.

1. Let A be given by

$$A = \begin{pmatrix} 3 & 1 \\ 0 & 3 \end{pmatrix}.$$

Then we can compute that

$$\det A = 3 \times 3 - 1 \times 0 = 9 - 0 = 9.$$

2. Let A be given by

$$A = \begin{pmatrix} 3 & 1 & 1 \\ 0 & 3 & 1 \\ 0 & 0 & 3 \end{pmatrix}.$$

Then we can compute that

$$\begin{aligned} \det A &= 3 \times (1 \times 3 - 0 \times 3) - 1 \times (0 \times 3 - 3 \times 0) + 1 \times (0 \times 0 - 3 \times 0) \\ &= 3 \times 3 - 1 \times 0 + 1 \times 0 = 9. \end{aligned}$$

Exercise 3.2. Compute the determinant of

$$\begin{pmatrix} 2 & -1 & 3 \\ 3 & 2 & -4 \\ 5 & 1 & 1 \end{pmatrix}.$$

We have been inaccurate in what we have said before. Strictly speaking the determinant we have defined here is the *signed* area/volume/hyper-volume of the associated hyper-parallelepiped, and we can recover the actual volume by taking $|\det A|$.

Theorem 3.3. *Let A be an $n \times n$ matrix and \vec{b} be an n -column vector. The following are equivalent:*

1. $A\vec{x} = \vec{b}$ has a unique solution.
2. The columns of A form a basis of \mathbb{R}^n .
3. $\det A \neq 0$.

This proof is beyond the scope of this course.

We do have the following rule for manipulating determinants too:

- Let A, B be square $n \times n$ -matrices then $\det(AB) = \det A \det B$.

- Let A be a square $n \times n$ -matrix and c a real number then $\det(cA) = c^n \det A$.
- Let A be an invertible square matrix, then $\det(A^{-1}) = \frac{1}{\det A}$.

Exercise 3.3. Prove these three rules for manipulating determinants for 2×2 matrices by direct calculation.

Remark 3.2. Computing determinants numerically is an important topic in its own right but we do not focus on this in this module.

You can use `numpy` to compute determinants

```

1 A = np.array([[3.0, 1.0], [0.0, 3.0]])
2 np.linalg.det(A)

np.float64(9.000000000000002)

```

3.3 Special types of matrices

The general matrix A before the examples is known as a **full** matrix: any of its components a_{ij} might be nonzero.

Almost always, the problem being solved leads to a matrix with a particular structure of entries: Some entries may be known to be zero. If this is the case then it is often possible to use this knowledge to improve the efficiency of the algorithm (in terms of both speed and/or storage).

Example 3.7 (Triangular matrix). One common (and important) structure takes the form

$$A = \begin{pmatrix} a_{11} & 0 & 0 & \cdots & 0 \\ a_{21} & a_{22} & 0 & \cdots & 0 \\ a_{31} & a_{32} & a_{33} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \cdots & a_{nn} \end{pmatrix}.$$

- A is a **lower triangular** matrix. Every entry above the leading diagonal is zero:

$$a_{ij} = 0 \quad \text{for} \quad j > i.$$

- The *transpose* of this matrix is an **upper triangular** matrix and can be treated in a very similar manner.

- Note that the determinant of a triangular matrix is simply the product of diagonal coefficients:

$$\det A = a_{11}a_{22} \cdots a_{nn} = \prod_{i=1}^n a_{ii}.$$

Example 3.8 (Sparse matrices). **Sparse matrices** are prevalent in any application which relies on some form of *graph* structure (see both the temperature, Example 1.4, and traffic network examples, Example 1.5).

- The a_{ij} typically represents some form of “communication” between vertices i and j of the graph, so the element is only nonzero if the vertices are connected.
- There is no generic pattern for these entries, though there is usually one that is specific to the problem solved.
- Usually, $a_{ii} \neq 0$ - the diagonal is nonzero.
- A “large” portion of the matrix is zero.
 - A full $n \times n$ matrix has n^2 nonzero entries.
 - A sparse $n \times n$ has αn nonzero entries, where $\alpha \ll n$.
- Many special techniques exist for handling sparse matrices, some of which can be used automatically within Python ([scipy.sparse documentation](#))

What is the significance of these special examples?

- In the next section we will discuss a general numerical algorithm for the solution of linear systems of equations.
- This will involve **reducing** the problem to one involving a **triangular matrix**, which, as we show below, is relatively easy to solve.
- In subsequent lectures, we will see that, for *sparse* matrix systems, alternative solution techniques are available.

3.4 Further reading

- Gregory Gundersen [Why shouldn't I invert that matrix?](#), 2020.

4 Direct solvers for systems of linear equations

Module learning objective

Apply direct and iterative solvers to solve systems of linear equations; implement methods using floating point numbers and investigate computational cost using computer experiments.

This section deals with first method we will use to solve systems of linear equations. We will see that by using the approach of Gaussian elimination (and variations of that method), we can solve any system of linear equations that has a solution.

Gaussian elimination should look very familiar to you – this looks a lot like solving simultaneous equations in high school. Here, we are trying to codify this approach into an algorithm that a computer can apply without any further human input in a way that always ‘works’ (or at least works when it should!).

4.1 Reminder of the problem

Recall the problem is to solve a set of n **linear** equations for n unknown values x_j , for $j = 1, 2, \dots, n$.

Notation:

$$\begin{array}{ll} \text{Equation 1 :} & a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \cdots + a_{1n}x_n = b_1 \\ \text{Equation 2 :} & a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + \cdots + a_{2n}x_n = b_2 \\ \vdots & \\ \text{Equation } i : & a_{i1}x_1 + a_{i2}x_2 + a_{i3}x_3 + \cdots + a_{in}x_n = b_i \\ \vdots & \\ \text{Equation } n : & a_{n1}x_1 + a_{n2}x_2 + a_{n3}x_3 + \cdots + a_{nn}x_n = b_n. \end{array}$$

We can also write the system of linear equations in *general matrix-vector* form:

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2n} \\ a_{31} & a_{32} & a_{33} & \cdots & a_{3n} \\ \vdots & \vdots & \vdots & & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \cdots & a_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_n \end{pmatrix}.$$

Recall that the $n \times n$ matrix A represents the coefficients that multiply the unknowns in each equation (row), while the n -vector \vec{b} represents the right-hand-side values.

Our strategy will be to reduce the system to a triangular system of matrices, which is then easy to solve!

4.2 Elementary row operations

Consider equation p of the above system:

$$a_{p1}x_1 + a_{p2}x_2 + a_{p3}x_3 + \cdots + a_{pn}x_n = b_p,$$

and equation q :

$$a_{q1}x_1 + a_{q2}x_2 + a_{q3}x_3 + \cdots + a_{qn}x_n = b_q.$$

Note three things...

- The order in which we choose to write the n equations is irrelevant
- We can multiply any equation by an arbitrary real number ($k \neq 0$ say):

$$ka_{p1}x_1 + ka_{p2}x_2 + ka_{p3}x_3 + \cdots + ka_{pn}x_n = kb_p.$$

- We can add any two equations:

$$ka_{p1}x_1 + ka_{p2}x_2 + ka_{p3}x_3 + \cdots + ka_{pn}x_n = kb_p$$

added to

$$a_{q1}x_1 + a_{q2}x_2 + a_{q3}x_3 + \cdots + a_{qn}x_n = b_q$$

yields

$$(ka_{p1} + a_{q1})x_1 + (ka_{p2} + a_{q2})x_2 + \cdots + (ka_{pn} + a_{qn})x_n = kb_p + b_q.$$

Example 4.1. Consider the system

$$2x_1 + 3x_2 = 4 \quad (4.1)$$

$$-3x_1 + 2x_2 = 7. \quad (4.2)$$

Then we have:

$$\begin{array}{ll} 4 \times (4.1) \rightarrow & 8x_1 + 12x_2 = 16 \\ -15 \times (4.2) \rightarrow & 4.5x_2 - 3x_2 = -10.5 \\ (4.1) + (4.2) \rightarrow & -x_1 + 5x_2 = 11 \\ (4.2) + 1.5 \times (4.1) \rightarrow & 0 + 6.5x_2 = 13. \end{array}$$

Exercise 4.1. Consider the system

$$x_1 + 2x_2 = 1 \quad (4.3)$$

$$4x_1 + x_2 = -3. \quad (4.4)$$

Work out the result of these elementary row operations:

$$\begin{array}{l} 2 \times (4.3) \rightarrow \\ 0.25 \times (4.4) \rightarrow \\ (4.4) + (-1) \times (4.3) \rightarrow \\ (4.4) + (-4) \times (4.3) \rightarrow \end{array}$$

For a system written in matrix form our three observations mean the following:

- We can swap any two rows of the matrix (and corresponding right-hand side entries). For example:

$$\begin{pmatrix} 2 & 3 \\ -3 & 2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 4 \\ 7 \end{pmatrix} \Rightarrow \begin{pmatrix} -3 & 2 \\ 2 & 3 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 7 \\ 4 \end{pmatrix}$$

- We can multiply any row of the matrix (and corresponding right-hand side entry) by a scalar. For example:

$$\begin{pmatrix} 2 & 3 \\ -3 & 2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 4 \\ 7 \end{pmatrix} \Rightarrow \begin{pmatrix} 1 & \frac{3}{2} \\ -3 & 2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 2 \\ 7 \end{pmatrix}$$

- We can replace row q by row $q + k \times$ row p . For example:

$$\begin{pmatrix} 2 & 3 \\ -3 & 2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 4 \\ 7 \end{pmatrix} \Rightarrow \begin{pmatrix} 2 & 3 \\ 0 & 6.5 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 4 \\ 13 \end{pmatrix}$$

(here we replaced row w by row $2 + 1.5 \times$ row 1)

$$\begin{pmatrix} 1 & 2 \\ 4 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 1 \\ -3 \end{pmatrix} \Rightarrow \begin{pmatrix} 1 & 2 \\ 0 & -7 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 1 \\ -7 \end{pmatrix}$$

(here we replaced row 2 by row $2 + (-4) \times$ row 1)

Our strategy for solving systems of linear equations using Gaussian elimination is based on the following ideas:

- The three types of operation described above are called **elementary row operations** (ERO).
- We will apply a sequence of ERO to reduce an arbitrary system to a triangular form, which, we will see, can be easily solved.
- The algorithm for reducing a general matrix to upper triangular form is known as **forward elimination** or (more commonly) as **Gaussian elimination**.

4.3 Gaussian elimination

The algorithm of Gaussian elimination is an ancient method that you may have already met at school – perhaps by a different name. The details of the method may seem confusing at first. We are following the ideas of elimination from systems of simultaneous equations, but in a way that a computer understands. Thinking like a computer is an important point in this section. You will have seen different ideas of how to solve systems of simultaneous equations where the first step is to “look at the equations to decide the easiest first step”. When there are 10^9 equations, it is not effective for a computer to try to find an easy way through the problem. The computer must be given a simple set of instructions to follow: this will be our algorithm.

The method is so old, in fact we have evidence of Chinese mathematicians using Gaussian elimination in 179CE (From [Wikipedia](#)):

The method of Gaussian elimination appears in the Chinese mathematical text Chapter Eight: Rectangular Arrays of The Nine Chapters on the Mathematical Art. Its use is illustrated in eighteen problems, with two to five equations. The first reference to the book by this title is dated to 179 CE, but parts of it were written

as early as approximately 150 BCE. It was commented on by Liu Hui in the 3rd century.

The method in Europe stems from the notes of Isaac Newton. In 1670, he wrote that all the algebra books known to him lacked a lesson for solving simultaneous equations, which Newton then supplied. Carl Friedrich Gauss in 1810 devised a notation for symmetric elimination that was adopted in the 19th century by professional hand computers to solve the normal equations of least-squares problems. The algorithm that is taught in high school was named for Gauss only in the 1950s as a result of confusion over the history of the subject.

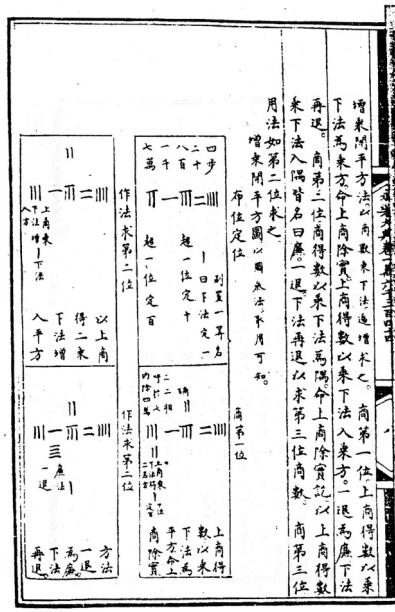


Figure 4.1: Image from Nine Chapter of the Mathematical art. By Yang Hui(1238-1298) - mybook, Public Domain, <https://commons.wikimedia.org/w/index.php?curid=10317744>

4.3.1 The algorithm

The following algorithm systematically introduces zeros into the system of equations, below the diagonal.

1. Subtract multiples of row 1 from the rows below it to eliminate (make zero) non-zero entries in column 1.
2. Subtract multiples of the new row 2 from the rows below it to eliminate non-zero entries in column 2.

3. Repeat for row $3, 4, \dots, n - 1$.

After row $n - 1$ all entities below the diagonal have been eliminated, so A is now upper triangular and the resulting system can be solved by backward substitution.

Example 4.2. Use Gaussian elimination to reduce the following system of equations to upper triangular form:

$$\begin{pmatrix} 2 & 1 & 4 \\ 1 & 2 & 2 \\ 2 & 4 & 6 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 12 \\ 9 \\ 22 \end{pmatrix}.$$

First, use the first row to eliminate the first column below the diagonal:

- (row 2) $-0.5 \times$ (row 1) gives

$$\begin{pmatrix} 2 & 1 & 4 \\ \mathbf{0} & 1.5 & 0 \\ 2 & 4 & 6 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 12 \\ 3 \\ 22 \end{pmatrix}$$

- (row 3) $- (row 1)$ then gives

$$\begin{pmatrix} 2 & 1 & 4 \\ \mathbf{0} & 1.5 & 0 \\ \mathbf{0} & 3 & 2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 12 \\ 3 \\ 10 \end{pmatrix}$$

Now use the second row to eliminate the second column below the diagonal.

- (row 3) $-2 \times$ (row 2) gives

$$\begin{pmatrix} 2 & 1 & 4 \\ \mathbf{0} & 1.5 & 0 \\ \mathbf{0} & \mathbf{0} & 2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 12 \\ 3 \\ 4 \end{pmatrix}$$

Exercise 4.2. Use Gaussian elimination to reduce the following system of linear equations to upper triangular form.

$$\begin{pmatrix} 4 & -1 & -1 \\ 2 & 4 & 2 \\ 1 & 2 & 4 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 9 \\ -6 \\ 3 \end{pmatrix}.$$

The key idea is that:

- Each row i is used to eliminate the entries in column i below a_{ii} , i.e. it forces $a_{ji} = 0$ for $j > i$.
- The elimination is done by subtracting a multiple of row i from row j :

$$(\text{row } j) \leftarrow (\text{row } j) - \frac{a_{ji}}{a_{ii}} (\text{row } i).$$

- Our update formula guarantees that a_{ji} becomes zero because

$$a_{ji} \leftarrow a_{ji} - \frac{a_{ji}}{a_{ii}} a_{ii} = a_{ji} - a_{ji} = 0.$$

4.3.2 Python version

We start with some helper code which determines the size of the system we are working with:

```

1 def system_size(A, b):
2     """
3         Validate the dimensions of a linear system and return its size.
4
5         This function checks whether the given coefficient matrix `A` is square
6         and whether its dimensions are compatible with the right-hand side vector
7         `b`. If the dimensions are valid, it returns the size of the system.
8
9     Parameters
10    -----
11     A : numpy.ndarray
12         A 2D array of shape ``(n, n)`` representing the coefficient matrix of
13         the linear system.
14     b : numpy.ndarray
15         A array of shape ``(n, o)`` representing the right-hand side vector.
16
17     Returns
18    -----
19     int
20         The size of the system, i.e., the number of variables `n`.
21
22     Raises
23    -----
24     ValueError
25         If `A` is not square or if the size of `b` does not match the number of

```

```

26         rows in `A`.
27 """
28
29 # Validate that A is a 2D square matrix
30 if A.ndim != 2:
31     raise ValueError(f"Matrix A must be 2D, but got {A.ndim}D array")
32
33 n, m = A.shape
34 if n != m:
35     raise ValueError(f"Matrix A must be square, but got A.shape={A.shape}")
36
37 if b.shape[0] != n:
38     raise ValueError(
39         f"System shapes are not compatible: A.shape={A.shape}, "
40         f"b.shape={b.shape}"
41     )
42
43 return n

```

Then we can implement the elementary row operations

```

1 def row_swap(A, b, p, q):
2 """
3     Swap two rows in a linear system of equations in place.
4
5     This function swaps the rows `p` and `q` of the coefficient matrix `A`
6     and the right-hand side vector `b` for a linear system of equations
7     of the form ``Ax = b``. The operation is performed **in place**, modifying
8     the input arrays directly.
9
10    Parameters
11    -----
12    A : numpy.ndarray
13        A 2D NumPy array of shape ``n, n`` representing the coefficient matrix
14        of the linear system.
15    b : numpy.ndarray
16        A 2D NumPy array of shape ``n, 1`` representing the right-hand side
17        vector of the system.
18    p : int
19        The index of the first row to swap. Must satisfy ``0 <= p < n``.
20    q : int
21        The index of the second row to swap. Must satisfy ``0 <= q < n``.

```

```

22
23     Returns
24     -----
25     None
26         This function modifies `A` and `b` directly and does not return
27         anything.
28     """
29
30     # get system size
31     n = system_size(A, b)
32     # swap rows of A
33     for j in range(n):
34         A[p, j], A[q, j] = A[q, j], A[p, j]
35     # swap rows of b
36     b[p, 0], b[q, 0] = b[q, 0], b[p, 0]
37
38 def row_scale(A, b, p, k):
39     """
40     Scale a row of a linear system by a constant factor in place.
41
42     This function multiplies all entries in row `p` of the coefficient matrix
43     `A` and the corresponding entry in the right-hand side vector `b` by a
44     scalar `k`. The operation is performed **in place**, modifying the input
45     arrays directly.
46
47     Parameters
48     -----
49     A : numpy.ndarray
50         A 2D NumPy array of shape ``(n, n)`` representing the coefficient matrix
51         of the linear system.
52     b : numpy.ndarray
53         A 2D NumPy array of shape ``(n, 1)`` representing the right-hand side
54         vector of the system.
55     p : int
56         The index of the row to scale. Must satisfy ``0 <= p < n``.
57     k : float
58         The scalar multiplier applied to the entire row.
59
60     Returns
61     -----
62     None
63         This function modifies `A` and `b` directly and does not return

```

```

64         anything.
65 """
66 n = system_size(A, b)
67
68 # scale row p of A
69 for j in range(n):
70     A[p, j] = k * A[p, j]
71 # scale row p of b
72 b[p, 0] = b[p, 0] * k
73
74
75 def row_add(A, b, p, k, q):
76 """
77 Perform an in-place row addition operation on a linear system.
78
79 This function applies the elementary row operation:
80
81 ``row_p ← row_p + k * row_q``
82
83 where `row_p` and `row_q` are rows in the coefficient matrix `A` and the
84 right-hand side vector `b`. It updates the entries of `A` and `b`
85 **in place**, directly modifying the original data.
86
87 Parameters
88 -----
89 A : numpy.ndarray
90     A 2D NumPy array of shape `` $(n, n)$ `` representing the coefficient matrix
91     of the linear system.
92 b : numpy.ndarray
93     A 2D NumPy array of shape `` $(n, 1)$ `` representing the right-hand side
94     vector of the system.
95 p : int
96     The index of the row to be updated (destination row). Must satisfy
97     `` $0 \leq p < n$ ``.
98 k : float
99     The scalar multiplier applied to `row_q` before adding it to `row_p`.
100 q : int
101    The index of the source row to be scaled and added. Must satisfy
102    `` $0 \leq q < n$ ``.
103 """
104 n = system_size(A, b)
105

```

```

106     # Perform the row operation
107     for j in range(n):
108         A[p, j] = A[p, j] + k * A[q, j]
109
110     # Update the corresponding value in b
111     b[p, 0] = b[p, 0] + k * b[q, 0]

```

Let's test we are ok so far:

Test 1: swapping rows

```

1 A = np.array([[2.0, 3.0], [-3.0, 2.0]])
2 b = np.array([[4.0], [7.0]])
3
4 print("starting arrays:")
5 print_array(A)
6 print_array(b)
7 print()
8
9 print("swapping rows 0 and 1")
10 row_swap(A, b, 0, 1) # remember numpy arrays are indexed starting from zero!
11 print()
12
13 print("new arrays:")
14 print_array(A)
15 print_array(b)
16 print()

```

```

starting arrays:
A = [ 2.0,  3.0 ]
    [ -3.0,  2.0 ]
b = [ 4.0 ]
    [ 7.0 ]

swapping rows 0 and 1

new arrays:
A = [ -3.0,  2.0 ]
    [ 2.0,  3.0 ]
b = [ 7.0 ]
    [ 4.0 ]

```

Test 2: scaling one row

```
1 A = np.array([[2.0, 3.0], [-3.0, 2.0]])
2 b = np.array([[4.0], [7.0]])
3
4 print("starting arrays:")
5 print_array(A)
6 print_array(b)
7 print()
8
9 print("row 0 |-> 0.5 * row 0")
10 row_scale(A, b, 0, 0.5) # remember numpy arrays are indexed started from zero!
11 print()
12
13 print("new arrays:")
14 print_array(A)
15 print_array(b)
16 print()
```

```
starting arrays:
A = [ 2.0,  3.0 ]
[ -3.0,  2.0 ]
b = [ 4.0 ]
[ 7.0 ]

row 0 |-> 0.5 * row 0

new arrays:
A = [ 1.0,  1.5 ]
[ -3.0,  2.0 ]
b = [ 2.0 ]
[ 7.0 ]
```

Test 3: replacing a row by that adding a multiple of another row

```
1 A = np.array([[2.0, 3.0], [-3.0, 2.0]])
2 b = np.array([[4.0], [7.0]])
3
4 print("starting arrays:")
5 print_array(A)
6 print_array(b)
7 print()
```

```

8
9 print("row 1 |-> row 1 + 1.5 * row 0")
10 row_add(A, b, 1, 1.5, 0) # remember numpy arrays are indexed started from zero!
11 print()
12
13 print("new arrays:")
14 print_array(A)
15 print_array(b)
16 print()

```

```

starting arrays:
A = [ 2.0,  3.0 ]
      [ -3.0,  2.0 ]
b = [ 4.0 ]
      [ 7.0 ]

row 1 |-> row 1 + 1.5 * row 0

new arrays:
A = [ 2.0,  3.0 ]
      [ 0.0,  6.5 ]
b = [ 4.0 ]
      [ 13.0 ]

```

Now we can define our Gaussian elimination function. We update the values in-place to avoid extra memory allocations.

```

1 def gaussian_elimination(A, b, verbose=False):
2     """
3         Perform Gaussian elimination to reduce a linear system to upper triangular
4         form.
5
6         This function performs **forward elimination** to transform the coefficient
7         matrix `A` into an upper triangular matrix, while applying the same
8         operations to the right-hand side vector `b`. This is the first step in
9         solving a linear system of equations of the form ``Ax = b`` using Gaussian
10        elimination.
11
12    Parameters
13    -----
14    A : numpy.ndarray

```

```

15      A 2D NumPy array of shape ``(n, n)`` representing the coefficient matrix
16      of the system.
17  b : numpy.ndarray
18      A 2D NumPy array of shape ``(n, 1)`` representing the right-hand side
19      vector.
20  verbose : bool, optional
21      If ``True``, prints detailed information about each elimination step,
22      including the row operations performed and the intermediate forms of
23      `A` and `b`. Default is ``False``.
24
25  Returns
26  -----
27  None
28      This function modifies `A` and `b` **in place** and does not return
29      anything.
30  """
31  # find shape of system
32  n = system_size(A, b)
33
34  # perform forwards elimination
35  for i in range(n - 1):
36      # eliminate column i
37      if verbose:
38          print(f"eliminating column {i}")
39      for j in range(i + 1, n):
40          # row j
41          factor = A[j, i] / A[i, i]
42          if verbose:
43              print(f"  row {j} |-> row {j} - {factor} * row {i}")
44          row_add(A, b, j, -factor, i)
45
46      if verbose:
47          print()
48          print("new system")
49          print_array(A)
50          print_array(b)
51          print()

```

We can try our code on Example 1:

```

1 A = np.array([[2.0, 1.0, 4.0], [1.0, 2.0, 2.0], [2.0, 4.0, 6.0]])
2 b = np.array([[12.0], [9.0], [22.0]])
3
4 print("starting system:")
5 print_array(A)
6 print_array(b)
7 print()
8
9 print("performing Gaussian Elimination")
10 gaussian_elimination(A, b, verbose=True)
11 print()
12
13 print("final system:")
14 print_array(A)
15 print_array(b)
16 print()
17
18 # test that A is really upper triangular
19 print("Is A really upper triangular?", np.allclose(A, np.triu(A)))

```

```

starting system:
A = [ 2.0, 1.0, 4.0 ]
[ 1.0, 2.0, 2.0 ]
[ 2.0, 4.0, 6.0 ]
b = [ 12.0 ]
[ 9.0 ]
[ 22.0 ]

performing Gaussian Elimination
eliminating column 0
row 1 |-> row 1 - 0.5 * row 0
row 2 |-> row 2 - 1.0 * row 0

new system
A = [ 2.0, 1.0, 4.0 ]
[ 0.0, 1.5, 0.0 ]
[ 0.0, 3.0, 2.0 ]
b = [ 12.0 ]
[ 3.0 ]
[ 10.0 ]

eliminating column 1

```

```
row 2 |-> row 2 - 2.0 * row 1
```

```
new system
A = [ 2.0,  1.0,  4.0 ]
     [ 0.0,  1.5,  0.0 ]
     [ 0.0,  0.0,  2.0 ]
b = [ 12.0 ]
     [ 3.0 ]
     [ 4.0 ]
```

```
final system:
A = [ 2.0,  1.0,  4.0 ]
     [ 0.0,  1.5,  0.0 ]
     [ 0.0,  0.0,  2.0 ]
b = [ 12.0 ]
     [ 3.0 ]
     [ 4.0 ]
```

```
Is A really upper triangular? True
```

4.4 Solving triangular systems of equations

A general *lower triangular* system of equations has $a_{ij} = 0$ for $j > i$ and takes the form:

$$\begin{pmatrix} a_{11} & 0 & 0 & \cdots & 0 \\ a_{21} & a_{22} & 0 & \cdots & 0 \\ a_{31} & a_{32} & a_{33} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \cdots & a_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_n \end{pmatrix}.$$

Note that first equation is

$$a_{11}x_1 = b_1.$$

Then x_i can be found by calculating

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

for each row $i = 1, 2, \dots, n$ in turn.

- Each calculation requires only previously computed values x_j (and the sum gives a loop for $j < i$).
- The matrix A **must** have non-zero diagonal entries
i.e. $a_{ii} \neq 0$ for $i = 1, 2, \dots, n$.
- **Upper triangular** systems of equations can be solved in similarly.

Example 4.3. Solve the lower triangular system of equations given by

$$\begin{array}{rcl} 2x_1 & = 2 \\ x_1 + 2x_2 & = 7 \\ 2x_1 + 4x_2 + 6x_3 & = 26 \end{array}$$

or, equivalently,

$$\begin{pmatrix} 2 & 0 & 0 \\ 1 & 2 & 0 \\ 2 & 4 & 6 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 2 \\ 7 \\ 26 \end{pmatrix}.$$

The solution can be calculated systematically from

$$\begin{aligned} x_1 &= \frac{b_1}{a_{11}} = \frac{2}{2} = 1 \\ x_2 &= \frac{b_2 - a_{21}x_1}{a_{22}} = \frac{7 - 1 \times 1}{2} = \frac{6}{2} = 3 \\ x_3 &= \frac{b_3 - a_{31}x_1 - a_{32}x_2}{a_{33}} = \frac{26 - 2 \times 1 - 4 \times 3}{6} = \frac{12}{6} = 2 \end{aligned}$$

which gives the solution $\vec{x} = (1, 3, 2)^T$.

Exercise 4.3. Solve the upper triangular linear system given by

$$\begin{array}{rcl} 2x_1 + x_2 + 4x_3 & = & 12 \\ 1.5x_2 & = & 3 \\ 2x_3 & = & 4 \end{array}$$

Remark 4.1.

- It is simple to solve a lower (upper) triangular system of equations (provided the diagonal is non-zero).

- This process is often referred to as **forward (backwards) substitution**.
- A general system of equations (i.e. a full matrix A) can be solved rapidly once it has been reduced to upper triangular form. The entire process is called Gaussian elimination with backward substitution.

We can define functions to solve both upper and lower triangular form systems of linear equations:

```

1 def forward_substitution(A, b):
2     """
3         Solve a lower triangular system of linear equations using forward
4         substitution.
5
6         This function solves the system of equations:
7
8         .. math::
9             A \ x = b
10
11        where `A` is a **lower triangular matrix** (all elements above the main
12        diagonal are zero). The solution vector `x` is computed sequentially by
13        solving each equation starting from the first row.
14
15        Parameters
16        -----
17        A : numpy.ndarray
18            A 2D NumPy array of shape ``(n, n)`` representing the lower triangular
19            coefficient matrix of the system.
20        b : numpy.ndarray
21            A 1D NumPy array of shape ``(n,)`` or a 2D NumPy array of shape
22            ``(n, 1)`` representing the right-hand side vector.
23
24        Returns
25        -----
26        x : numpy.ndarray
27            A NumPy array of shape ``(n,)`` containing the solution vector.
28        """
29
30        solves the system of linear equations  $Ax = b$  assuming that  $A$  is lower
31        triangular. returns the solution  $x$ 
32
33        # get size of system
34        n = system_size(A, b)

```

```

35
36     # check is lower triangular
37     if not np.allclose(A, np.tril(A)):
38         raise ValueError("Matrix A is not lower triangular")
39
40     # create solution variable
41     x = np.empty_like(b)
42
43     # perform forwards solve
44     for i in range(n):
45         partial_sum = 0.0
46         for j in range(0, i):
47             partial_sum += A[i, j] * x[j]
48         x[i] = 1.0 / A[i, i] * (b[i] - partial_sum)
49
50     return x
51
52
53 def backward_substitution(A, b):
54     """
55     Solve an upper triangular system of linear equations using backward
56     substitution.
57
58     This function solves the system of equations:
59
60     .. math::
61         A \ x = b
62
63     where `A` is an **upper triangular matrix** (all elements below the main
64     diagonal are zero). The solution vector `x` is computed starting from the
65     last equation and proceeding backward.
66
67     Parameters
68     -----
69     A : numpy.ndarray
70         A 2D NumPy array of shape ``(n, n)`` representing the upper triangular
71         coefficient matrix of the system.
72     b : numpy.ndarray
73         A 1D NumPy array of shape ``(n,)`` or a 2D NumPy array of shape
74         ``(n, 1)`` representing the right-hand side vector.
75
76     Returns

```

```

77     -----
78     x : numpy.ndarray
79         A NumPy array of shape ``n,`` containing the solution vector.
80     """
81
82     # get size of system
83     n = system_size(A, b)
84
85     # check is upper triangular
86     assert np.allclose(A, np.triu(A))
87
88     # create solution variable
89     x = np.empty_like(b)
90
91     # perform backwards solve
92     for i in range(n - 1, -1, -1): # iterate over rows backwards
93         partial_sum = 0.0
94         for j in range(i + 1, n):
95             partial_sum += A[i, j] * x[j]
96         x[i] = 1.0 / A[i, i] * (b[i] - partial_sum)
97
98     return x

```

And we can then test it out!

```

1 A = np.array([[2.0, 0.0, 0.0], [1.0, 2.0, 0.0], [2.0, 4.0, 6.0]])
2 b = np.array([[2.0], [7.0], [26.0]])
3
4 print("The system is given by:")
5 print_array(A)
6 print_array(b)
7 print()
8
9 print("Solving the system using forward substitution")
10 x = forward_substitution(A, b)
11 print()
12
13 print("The solution using forward substitution is:")
14 print_array(x)
15 print()
16
17 print("Does x really solve the system?", np.allclose(A @ x, b))

```

```
The system is given by:  
A = [ 2.0,  0.0,  0.0 ]  
    [ 1.0,  2.0,  0.0 ]  
    [ 2.0,  4.0,  6.0 ]  
b = [ 2.0 ]  
    [ 7.0 ]  
    [ 26.0 ]
```

Solving the system using forward substitution

The solution using forward substitution is:

```
x = [ 1.0 ]  
    [ 3.0 ]  
    [ 2.0 ]
```

Does x really solve the system? True

We can also do a backward substitution test:

```
1 A = np.array([[2.0, 1.0, 4.0], [0.0, 1.5, 0.0], [0.0, 0.0, 2.0]])  
2 b = np.array([[12.0], [3.0], [4.0]])  
3  
4 print("The system is given by:")  
5 print_array(A)  
6 print_array(b)  
7 print()  
8  
9 print("Solving the system using backward substitution")  
10 x = backward_substitution(A, b)  
11 print()  
12  
13 print("The solution using backward substitution is:")  
14 print_array(x)  
15 print()  
16  
17 print("Does x really solve the system?", np.allclose(A @ x, b))
```

```
The system is given by:  
A = [ 2.0,  1.0,  4.0 ]  
    [ 0.0,  1.5,  0.0 ]  
    [ 0.0,  0.0,  2.0 ]  
b = [ 12.0 ]
```

```
[ 3.0 ]  
[ 4.0 ]
```

Solving the system using backward substitution

The solution using backward substitution is:

```
x = [ 1.0 ]  
[ 2.0 ]  
[ 2.0 ]
```

Does x really solve the system? True

4.5 Combining Gaussian elimination and backward substitution

Our grand strategy can now come together so we have a method to solve systems of linear equations:

Given a system of linear equations $A\vec{x} = \vec{b}$;

- First perform Gaussian elimination to give an equivalent system of equations in upper triangular form;
- Then use backward substitution to produce a solution \vec{x}

We can use our code to test this:

```
1 A = np.array([[2.0, 1.0, 4.0], [1.0, 2.0, 2.0], [2.0, 4.0, 6.0]])  
2 b = np.array([[12.0], [9.0], [22.0]])  
3  
4 print("starting system:")  
5 print_array(A)  
6 print_array(b)  
7 print()  
8  
9 print("performing Gaussian Elimination")  
10 gaussian_elimination(A, b, verbose=True)  
11 print()  
12  
13 print("upper triangular system:")  
14 print_array(A)  
15 print_array(b)  
16 print()  
17
```

```

18 print("Solving the system using backward substitution")
19 x = backward_substitution(A, b)
20 print()
21
22 print("solution using backward substitution:")
23 print_array(x)
24 print()
25
26 A = np.array([[2.0, 1.0, 4.0], [1.0, 2.0, 2.0], [2.0, 4.0, 6.0]])
27 b = np.array([[12.0], [9.0], [22.0]])
28 print("Does x really solve the original system?", np.allclose(A @ x, b))

```

```

starting system:
A = [ 2.0,  1.0,  4.0 ]
    [ 1.0,  2.0,  2.0 ]
    [ 2.0,  4.0,  6.0 ]
b = [ 12.0 ]
    [ 9.0 ]
    [ 22.0 ]

performing Gaussian Elimination
eliminating column 0
row 1 |-> row 1 - 0.5 * row 0
row 2 |-> row 2 - 1.0 * row 0

new system
A = [ 2.0,  1.0,  4.0 ]
    [ 0.0,  1.5,  0.0 ]
    [ 0.0,  3.0,  2.0 ]
b = [ 12.0 ]
    [ 3.0 ]
    [ 10.0 ]

eliminating column 1
row 2 |-> row 2 - 2.0 * row 1

new system
A = [ 2.0,  1.0,  4.0 ]
    [ 0.0,  1.5,  0.0 ]
    [ 0.0,  0.0,  2.0 ]
b = [ 12.0 ]
    [ 3.0 ]

```

```
[ 4.0 ]
```

```
upper triangular system:  
A = [ 2.0, 1.0, 4.0 ]  
    [ 0.0, 1.5, 0.0 ]  
    [ 0.0, 0.0, 2.0 ]  
b = [ 12.0 ]  
    [ 3.0 ]  
    [ 4.0 ]
```

Solving the system using backward substitution

```
solution using backward substitution:
```

```
x = [ 1.0 ]  
    [ 2.0 ]  
    [ 2.0 ]
```

Does x really solve the original system? True

Exercise 4.4. Use Gaussian elimination followed by backwards elimination to solve the system:

$$\begin{pmatrix} 2 & 1 & -1 \\ 4 & 5 & 7 \\ -8 & -3 & 3 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 6 \\ 30 \\ -22 \end{pmatrix}.$$

. \$\$

4.6 The cost of Gaussian Elimination

Gaussian elimination (GE) is unnecessarily expensive when it is applied to many systems of equations with the same matrix A but different right-hand sides \vec{b} .

- The forward elimination process is the most computationally expensive part at $O(n^3)$ but is exactly the same for any choice of \vec{b} .
- In contrast, the solution of the resulting upper triangular system only requires $O(n^2)$ operations.

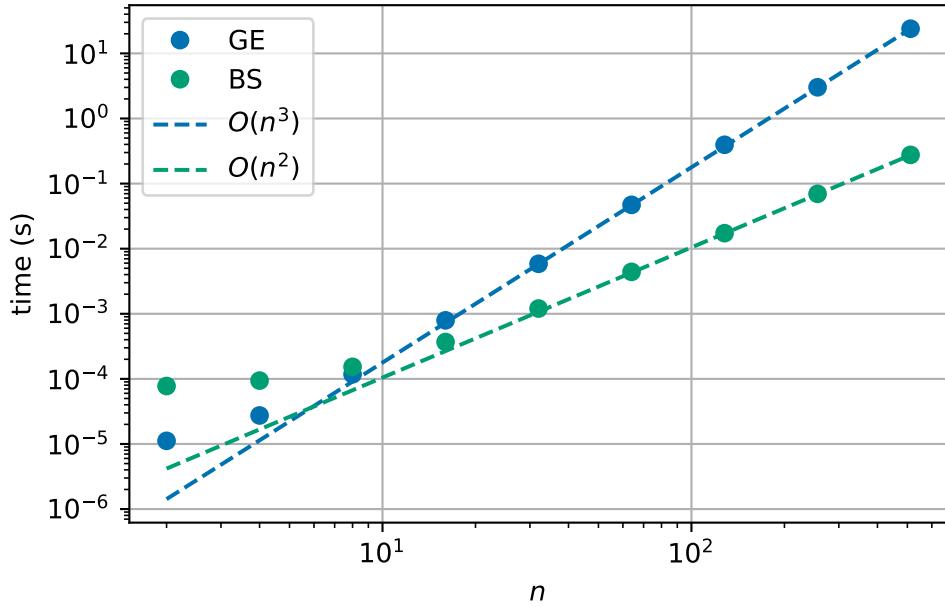


Figure 4.2: Runtime cost of applying Gaussian elimination (GE) and backwards solution (BS).

We can use this information to improve the way in which we solve multiple systems of equations with the same matrix A but different right-hand sides \vec{b} .

4.7 LU factorisation

Our next algorithm, called LU factorisation, is a way to try to speed up Gaussian elimination by reusing information. This can be used when we solve systems of equations with the same matrix A but different right hand sides \vec{b} - this is more common than you would think!

Recall the elementary row operations (EROs) from above. Note that the EROs can be produced by left multiplication with a suitable matrix:

- Row swap:

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} a & b & c \\ d & e & f \\ g & h & i \end{pmatrix} = \begin{pmatrix} a & b & c \\ g & h & i \\ d & e & f \end{pmatrix}$$

- Row swap:

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} a & b & c & d \\ e & f & g & h \\ i & j & k & l \\ m & n & o & p \end{pmatrix} = \begin{pmatrix} a & b & c & d \\ i & j & k & l \\ e & f & g & h \\ m & n & o & p \end{pmatrix}$$

- Multiply row by α :

$$\begin{pmatrix} \alpha & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} a & b & c \\ d & e & f \\ g & h & i \end{pmatrix} = \begin{pmatrix} \alpha a & \alpha b & \alpha c \\ d & e & f \\ g & h & i \end{pmatrix}$$

- $\alpha \times \text{row } p + \text{row } q$:

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \alpha & 0 & 1 \end{pmatrix} \begin{pmatrix} a & b & c \\ d & e & f \\ g & h & i \end{pmatrix} = \begin{pmatrix} a & b & c \\ d & e & f \\ \alpha a + g & \alpha b + h & \alpha c + i \end{pmatrix}$$

Since Gaussian elimination (GE) is just a sequence of EROs and each ERO is just multiplication by a suitable matrix, say E_k , forward elimination applied to the system $A\vec{x} = \vec{b}$ can be expressed as

$$(E_m \cdots E_1)A\vec{x} = (E_m \cdots E_1)\vec{b},$$

here m is the number of EROs required to reduce the upper triangular form.

Let $U = (E_m \cdots E_1)A$ and $L = (E_m \cdots E_1)^{-1}$. Now the original system $A\vec{x} = \vec{b}$ is equivalent to

$$LU\vec{x} = \vec{b} \tag{4.5}$$

where U is *upper triangular* (by construction) and L may be shown to be lower triangular (provided the EROs do not include any row swaps).

Once L and U are known it is easy to solve (4.5)

- Solve $L\vec{z} = \vec{b}$ in $O(n^2)$ operations.
- Solve $U\vec{x} = \vec{z}$ in $O(n^2)$ operations.

L and U may be found in $O(n^3)$ operations by performing GE and saving the E_i matrices; however, it is more convenient to find them directly (also $O(n^3)$ operations).

4.7.1 Computing L and U

Consider a general 4×4 matrix A and its factorisation LU :

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ l_{21} & 1 & 0 & 0 \\ l_{31} & l_{32} & 1 & 0 \\ l_{41} & l_{42} & l_{43} & 1 \end{pmatrix} \begin{pmatrix} u_{11} & u_{12} & u_{13} & u_{14} \\ 0 & u_{22} & u_{23} & u_{24} \\ 0 & 0 & u_{33} & u_{34} \\ 0 & 0 & 0 & u_{44} \end{pmatrix}$$

For the first column,

$$\begin{aligned} a_{11} &= (1, 0, 0, 0)(u_{11}, 0, 0, 0)^T &= u_{11} &\rightarrow u_{11} = a_{11} \\ a_{21} &= (l_{21}, 1, 0, 0)(u_{11}, 0, 0, 0)^T &= l_{21}u_{11} &\rightarrow l_{21} = a_{21}/u_{11} \\ a_{31} &= (l_{31}, l_{32}, 1, 0)(u_{11}, 0, 0, 0)^T &= l_{31}u_{11} &\rightarrow l_{31} = a_{31}/u_{11} \\ a_{41} &= (l_{41}, l_{42}, l_{43}, 1)(u_{11}, 0, 0, 0)^T &= l_{41}u_{11} &\rightarrow l_{41} = a_{41}/u_{11} \end{aligned}$$

The second, third and fourth columns follow in a similar manner, giving all the entries in L and U .

Remark 4.2.

- L is assumed to have 1's on the diagonal, to ensure that the factorisation is unique.
- The process involves division by the diagonal entries u_{11}, u_{22} , etc., so they **must** be non-zero.
- In general the factors l_{ij} and u_{ij} are calculated for each column j in turn, i.e.,

```

1  for j in range(n):
2      for i in range(j+1):
3          # Compute factors u_{ij}
4          ...
5      for i in range(j+1, n):
6          # Compute factors l_{ij}
7          ...

```

Example 4.4. Use LU factorisation to solve the linear system of equations given by

$$\begin{pmatrix} 2 & 1 & 4 \\ 1 & 2 & 2 \\ 2 & 4 & 6 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 12 \\ 9 \\ 22 \end{pmatrix}.$$

This can be rewritten in the form $A = LU$ where

$$\begin{pmatrix} 2 & 1 & 4 \\ 1 & 2 & 2 \\ 2 & 4 & 6 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ l_{21} & 1 & 0 \\ l_{31} & l_{32} & 1 \end{pmatrix} \begin{pmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{pmatrix}.$$

Column 1 of A gives

$$\begin{aligned} 2 &= u_{11} & \rightarrow u_{11} &= 2 \\ 1 &= l_{21}u_{11} & \rightarrow l_{21} &= 0.5 \\ 2 &= l_{31}u_{11} & \rightarrow l_{31} &= 1. \end{aligned}$$

Column 2 of A gives

$$\begin{aligned} 1 &= u_{12} & \rightarrow u_{12} &= 1 \\ 2 &= l_{21}u_{12} + u_{22} & \rightarrow u_{22} &= 1.5 \\ 4 &= l_{31}u_{12} + l_{32}u_{22} & \rightarrow l_{32} &= 2. \end{aligned}$$

Column 3 of A gives

$$\begin{aligned} 4 &= u_{13} & \rightarrow u_{13} &= 4 \\ 2 &= l_{21}u_{13} + u_{23} & \rightarrow u_{23} &= 0 \\ 6 &= l_{31}u_{13} + l_{32}u_{23} + u_{33} & \rightarrow u_{33} &= 2. \end{aligned}$$

Solve the lower triangular system $L\vec{z} = \vec{b}$:

$$\begin{pmatrix} 1 & 0 & 0 \\ 0.5 & 1 & 0 \\ 1 & 2 & 1 \end{pmatrix} \begin{pmatrix} z_1 \\ z_2 \\ z_3 \end{pmatrix} = \begin{pmatrix} 12 \\ 9 \\ 22 \end{pmatrix} \rightarrow \begin{pmatrix} z_1 \\ z_2 \\ z_3 \end{pmatrix} = \begin{pmatrix} 12 \\ 3 \\ 4 \end{pmatrix}$$

Solve the upper triangular system $U\vec{x} = \vec{z}$:

$$\begin{pmatrix} 2 & 1 & 4 \\ 0 & 1.5 & 0 \\ 0 & 0 & 2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \begin{pmatrix} 12 \\ 3 \\ 4 \end{pmatrix} \rightarrow \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 1 \\ 2 \\ 2 \end{pmatrix}.$$

Exercise 4.5. Rewrite the matrix A as the product of lower and upper triangular matrices where

$$A = \begin{pmatrix} 4 & 2 & 0 \\ 2 & 3 & 1 \\ 0 & 1 & 2.5 \end{pmatrix}.$$

Remark. The first example gives

$$\begin{pmatrix} 2 & 1 & 4 \\ 1 & 2 & 2 \\ 2 & 4 & 6 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0.5 & 1 & 0 \\ 1 & 2 & 1 \end{pmatrix} \begin{pmatrix} 2 & 1 & 4 \\ 0 & 1.5 & 0 \\ 0 & 0 & 2 \end{pmatrix}$$

Note that

- the matrix U is the same as the fully eliminated upper triangular form produced by Gaussian elimination;
- L contains the multipliers that were used at each stage to eliminate the rows.

4.8 Effects of finite precision arithmetic

Example 4.5. Consider the following linear system of equations

$$\begin{pmatrix} 0 & 2 & 1 \\ 2 & 1 & 0 \\ 1 & 2 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 7 \\ 4 \\ 5 \end{pmatrix}$$

Problem. We cannot eliminate the first column by the diagonal by adding multiples of row 1 to rows 2 and 3, respectively.

Solution. Swap the order of the equations!

- Swap rows 1 and 2:

$$\begin{pmatrix} 2 & 1 & 0 \\ 0 & 2 & 1 \\ 1 & 2 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 4 \\ 7 \\ 5 \end{pmatrix}$$

- Now apply Gaussian elimination

$$\begin{pmatrix} 2 & 1 & 0 \\ 0 & 2 & 1 \\ 0 & 1.5 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 4 \\ 7 \\ 3 \end{pmatrix}$$

$$\begin{pmatrix} 2 & 1 & 0 \\ 0 & 2 & 1 \\ 0 & 0 & -0.75 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 4 \\ 7 \\ -2.25 \end{pmatrix}.$$

Example 4.6. Consider another system of equations

$$\begin{pmatrix} 2 & 1 & 1 \\ 4 & 2 & 1 \\ 2 & 2 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 3 \\ 5 \\ 2 \end{pmatrix}$$

- Apply Gaussian elimination as usual:

$$\begin{pmatrix} 2 & 1 & 1 \\ 0 & 0 & -1 \\ 2 & 2 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 3 \\ -1 \\ 2 \end{pmatrix}$$

$$\begin{pmatrix} 2 & 1 & 1 \\ 0 & 0 & -1 \\ 0 & 1 & -1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 3 \\ -1 \\ -1 \end{pmatrix}$$

- *Problem.* We cannot eliminate the second column below the diagonal by adding a multiple of row 2 to row 3.
- Again, this problem may be overcome simply by swapping the order of the equations – this time, swapping rows 2 and 3:

$$\begin{pmatrix} 2 & 1 & 1 \\ 0 & 1 & -1 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 3 \\ -1 \\ -1 \end{pmatrix}$$

- We can now continue the Gaussian elimination process as usual.

In general. Gaussian elimination requires row swaps to avoid breaking down when there is a zero in the “pivot” position. Avoiding zero-division might be a familiar aspect of Gaussian elimination, but there is an additional reason to apply pivoting when working with floating point numbers:

Example 4.7. Consider using Gaussian elimination to solve the linear system of equations given by

$$\begin{pmatrix} \varepsilon & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 2 + \varepsilon \\ 3 \end{pmatrix}$$

where $\varepsilon \neq 1$.

- The true, unique solution is $(x_1, x_2)^T = (1, 2)^T$.

- If $\varepsilon \neq 0$, Gaussian elimination gives

$$\begin{pmatrix} \varepsilon & 1 \\ 0 & 1 - \frac{1}{\varepsilon} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 2 + \varepsilon \\ 3 - \frac{2+\varepsilon}{\varepsilon} \end{pmatrix}$$

- Problems occur not only when $\varepsilon = 0$ but also when it is very small, i.e. when $\frac{1}{\varepsilon}$ is very large, which will introduce very significant rounding errors into the computation.

Use Gaussian elimination to solve the linear system of equations given by

$$\begin{pmatrix} 1 & 1 \\ \varepsilon & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 3 \\ 2 + \varepsilon \end{pmatrix}$$

where $\varepsilon \neq 1$.

- The true solution is still $(x_1, x_2)^T = (1, 2)^T$.
- Gaussian elimination now gives

$$\begin{pmatrix} 1 & 1 \\ 0 & 1 - \varepsilon \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 3 \\ 2 - 2\varepsilon \end{pmatrix}$$

- The problems due to small values of ε have disappeared.

This is a genuine problem we see in the code versions too!

```

1 print("without row swapping:")
2 for eps in [1.0e-2, 1.0e-4, 1.0e-6, 1.0e-8, 1.0e-10, 1.0e-12, 1.0e-14]:
3     A = np.array([[eps, 1.0], [1.0, 1.0]])
4     b = np.array([[2.0 + eps], [3.0]])
5
6     gaussian_elimination(A, b)
7     x = backward_substitution(A, b)
8     print(f"\{eps=:.1e}\", end=\" ", ")
9     print_array(x.T, "x.T", end=" ", ")
10
11    A = np.array([[eps, 1.0], [1.0, 1.0]])
12    b = np.array([[2.0 + eps], [3.0]])
13    print("Solution?", np.allclose(A @ x, b))
14    print()
15
16 print("with row swapping:")
17 for eps in [1.0e-2, 1.0e-4, 1.0e-6, 1.0e-8, 1.0e-10, 1.0e-12, 1.0e-14]:
```

```

18     A = np.array([[1.0, 1.0], [eps, 1.0]])
19     b = np.array([[3.0], [2.0 + eps]])
20
21     gaussian_elimination(A, b)
22     x = backward_substitution(A, b)
23     print(f"{{eps=:.1e}}", end=", ")
24     print_array(x.T, "x.T", end=", ")
25
26     A = np.array([[1.0, 1.0], [eps, 1.0]])
27     b = np.array([[3.0], [2.0 + eps]])
28     print("Solution?", np.allclose(A @ x, b))
29     print()

```

without row swapping:

```

eps=1.0e-02, x.T = [ 1.0, 2.0 ], Solution? True
eps=1.0e-04, x.T = [ 1.0, 2.0 ], Solution? True
eps=1.0e-06, x.T = [ 1.0, 2.0 ], Solution? True
eps=1.0e-08, x.T = [ 1.0, 2.0 ], Solution? True
eps=1.0e-10, x.T = [ 1.0, 2.0 ], Solution? True
eps=1.0e-12, x.T = [ 1.00009, 2.00000 ], Solution? False
eps=1.0e-14, x.T = [ 1.0214, 2.0000 ], Solution? False

```

with row swapping:

```

eps=1.0e-02, x.T = [ 1.0, 2.0 ], Solution? True
eps=1.0e-04, x.T = [ 1.0, 2.0 ], Solution? True
eps=1.0e-06, x.T = [ 1.0, 2.0 ], Solution? True
eps=1.0e-08, x.T = [ 1.0, 2.0 ], Solution? True
eps=1.0e-10, x.T = [ 1.0, 2.0 ], Solution? True
eps=1.0e-12, x.T = [ 1.0, 2.0 ], Solution? True
eps=1.0e-14, x.T = [ 1.0, 2.0 ], Solution? True

```

Remark 4.3.

- Writing the equations in a different order has removed the previous problem.
- The diagonal entries are now always *relatively* larger.
- The interchange of the order of equations is a simple example of **row pivoting**. This strategy avoids excessive rounding errors in the computations.

4.8.1 Gaussian elimination with pivoting

Key idea:

- Before eliminating entries in column j :
 - find the entry in column j , below the diagonal, of maximum magnitude;
 - if that entry is larger in magnitude than the diagonal entry then swap its row with row j .
- Then eliminate column j as before.

This algorithm will always work when the matrix A is non-singular. Conversely, if all of the possible pivot values are zero this implies that the matrix is singular and a unique solution does not exist. At each elimination step the row multipliers used are guaranteed to be at most one in magnitude so any errors in the representation of the system cannot be amplified by the elimination process. As always, solving $A\vec{x} = \vec{b}$ requires that the entries in \vec{b} are also swapped in the appropriate way.

Pivoting can be applied in an equivalent way to LU factorisation. The sequence of pivots is independent of the vector \vec{b} and can be recorded and reused. The constraint imposed on the row multipliers means that for LU factorisation every entry in L satisfies $|l_{ij}| \leq 1$.

Example 4.8. Consider the linear system of equations given by

$$\begin{pmatrix} 10 & -7 & 0 \\ -3 & 2.1 - \varepsilon & 6 \\ 5 & -1 & 5 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 7 \\ 9.9 + \varepsilon \\ 11 \end{pmatrix}$$

where $0 \leq \varepsilon \ll 1$, and solve it using

1. Gaussian elimination without pivoting
2. Gaussian elimination with pivoting.

The exact solution is $\vec{x} = (0, -1, 2)^T$ for any ε in the given range.

1. Solve the system using Gaussian elimination with no pivoting.

Eliminating the first column gives

$$\begin{pmatrix} 10 & -7 & 0 \\ 0 & -\varepsilon & 6 \\ 0 & 2.5 & 5 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 7 \\ 12 + \varepsilon \\ 7.5 \end{pmatrix}$$

and then the second column gives

$$\begin{pmatrix} 10 & -7 & 0 \\ 0 & -\varepsilon & 6 \\ 0 & 0 & 5 + 15/\varepsilon \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 7 \\ 12 + \varepsilon \\ 7.5 + 2.5(12 + \varepsilon)/\varepsilon \end{pmatrix}$$

which leads to

$$x_3 = \frac{3 + \frac{12+\varepsilon}{\varepsilon}}{2 + \frac{6}{\varepsilon}} \quad x_2 = \frac{(12 + \varepsilon) - 6x_3}{-\varepsilon} \quad x_1 = \frac{7 + 7x_2}{10}.$$

There are many divisions by ε , so we will have problems if ε is (very) small.

2. Solve the system using Gaussian elimination with pivoting.

The first stage is identical (because $a_{11} = 10$ is largest).

$$\begin{pmatrix} 10 & -7 & 0 \\ 0 & -\varepsilon & 6 \\ 0 & 2.5 & 5 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 7 \\ 12 + \varepsilon \\ 7.5 \end{pmatrix}$$

but now $|a_{22}| = \varepsilon$ and $|a_{32}| = 2.5$ so we swap rows 2 and 3 to give

$$\begin{pmatrix} 10 & -7 & 0 \\ 0 & 2.5 & 5 \\ 0 & -\varepsilon & 6 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 7 \\ 7.5 \\ 12 + \varepsilon \end{pmatrix}$$

Now we may eliminate column 2:

$$\begin{pmatrix} 10 & -7 & 0 \\ 0 & 2.5 & 5 \\ 0 & 0 & 6 + 2\varepsilon \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 7 \\ 7.5 \\ 12 + 4\varepsilon \end{pmatrix}$$

which leads to the exact answer:

$$x_3 = \frac{12 + 4\varepsilon}{6 + 2\varepsilon} = 2 \quad x_2 = \frac{7.5 - 5x_3}{2.5} = -1 \quad x_1 = \frac{7 + 7x_2}{10} = 0.$$

4.8.2 Python code for Gaussian elimination with pivoting

```

1 def gaussian_elimination_with_pivoting(A, b, verbose=False):
2     """
3         perform Gaussian elimination with pivoting to reduce the system of linear
4         equations Ax=b to upper triangular form.
5         use verbose to print out intermediate representations
6     """
7     # find shape of system
8     n = system_size(A, b)
9
10    # perform forwards elimination
11    for i in range(n - 1):
12        # eliminate column i
13        if verbose:
14            print(f"eliminating column {i}")
15
16        # find largest entry in column i
17        largest = abs(A[i, i])
18        j_max = i
19        for j in range(i + 1, n):
20            if abs(A[j, i]) > largest:
21                largest, j_max = abs(A[j, i]), j
22
23        # swap rows j_max and i
24        row_swap(A, b, i, j_max)
25        if verbose:
26            print(f"swapped system ({i} <-> {j_max})")
27            print_array(A)
28            print_array(b)
29            print()
30
31        for j in range(i + 1, n):
32            # row j
33            factor = A[j, i] / A[i, i]
34            if verbose:
35                print(f"row {j} |-> row {j} - {factor} * row {i}")
36            row_add(A, b, j, -factor, i)
37
38        if verbose:
39            print("new system")
40            print_array(A)
41            print_array(b)
42            print()

```

Gaussian elimination without pivoting following by back substitution:

```
1  eps = 1.0e-14
2  A = np.array([[10.0, -7.0, 0.0], [-3.0, 2.1 - eps, 6.0], [5.0, -1.0, 5.0]])
3  b = np.array([[7.0], [9.9 + eps], [11.0]])
4
5  print("starting system:")
6  print_array(A)
7  print_array(b)
8  print()
9
10 print("performing Gaussian elimination without pivoting")
11 gaussian_elimination(A, b, verbose=True)
12 print()
13
14 print("upper triangular system:")
15 print_array(A)
16 print_array(b)
17 print()
18
19 print("performing backward substitution")
20 x = backward_substitution(A, b)
21 print()
22
23 print("solution using backward substitution:")
24 print_array(x)
25 print()
26
27 A = np.array([[10.0, -7.0, 0.0], [-3.0, 2.1 - eps, 6.0], [5.0, -1.0, 5.0]])
28 b = np.array([[7.0], [9.9 + eps], [11.0]])
29 print("Does x solve the original system?", np.allclose(A @ x, b))
```

```
starting system:
A = [ 10.0, -7.0,  0.0 ]
      [ -3.0,   2.1,   6.0 ]
      [  5.0,  -1.0,   5.0 ]
b = [  7.0 ]
      [  9.9 ]
      [ 11.0 ]

performing Gaussian elimination without pivoting
eliminating column 0
```

```

row 1 |-> row 1 - -0.3 * row 0
row 2 |-> row 2 - 0.5 * row 0

new system
A = [ 10.0, -7.0,  0.0 ]
     [ 0.0, -0.0,  6.0 ]
     [ 0.0,  2.5,  5.0 ]
b = [ 7.0 ]
     [ 12.0 ]
     [ 7.5 ]

eliminating column 1
row 2 |-> row 2 - -244760849313613.9 * row 1

new system
A = [ 10.0, -7.0,  0.0 ]
     [ 0.0, -0.0,  6.0 ]
     [ 0.0,  0.0, 1468565095881688.5 ]
b = [ 7.0 ]
     [ 12.0 ]
     [ 2937130191763377.0 ]

upper triangular system:
A = [ 10.0, -7.0,  0.0 ]
     [ 0.0, -0.0,  6.0 ]
     [ 0.0,  0.0, 1468565095881688.5 ]
b = [ 7.0 ]
     [ 12.0 ]
     [ 2937130191763377.0 ]

performing backward substitution

solution using backward substitution:
x = [ -0.030435 ]
     [ -1.043478 ]
     [  2.000000 ]

```

Does x solve the original system? False

Gaussian elimination with pivoting following by back substitution:

```

1  eps = 1.0e-14
2  A = np.array([[10.0, -7.0, 0.0], [-3.0, 2.1 - eps, 6.0], [5.0, -1.0, 5.0]])
3  b = np.array([[7.0], [9.9 + eps], [11.0]])
4
5  print("starting system:")
6  print_array(A)
7  print_array(b)
8  print()
9
10 print("performing Gaussian elimination with pivoting")
11 gaussian_elimination_with_pivoting(A, b, verbose=True)
12 print()
13
14 print("upper triangular system:")
15 print_array(A)
16 print_array(b)
17 print()
18
19 print("performing backward substitution")
20 x = backward_substitution(A, b)
21 print()
22
23 print("solution using backward substitution:")
24 print_array(x)
25 print()
26
27 A = np.array([[10.0, -7.0, 0.0], [-3.0, 2.1 - eps, 6.0], [5.0, -1.0, 5.0]])
28 b = np.array([[7.0], [9.9 + eps], [11.0]])
29 print("Does x solve the original system?", np.allclose(A @ x, b))

```

```

starting system:
A = [ 10.0, -7.0,  0.0 ]
      [ -3.0,  2.1,   6.0 ]
      [  5.0, -1.0,   5.0 ]
b = [  7.0 ]
      [  9.9 ]
      [ 11.0 ]

performing Gaussian elimination with pivoting
eliminating column 0
swapped system (0 <-> 0)
A = [ 10.0, -7.0,  0.0 ]

```

```

[ -3.0,  2.1,  6.0 ]
[  5.0, -1.0,  5.0 ]
b = [  7.0 ]
[  9.9 ]
[ 11.0 ]

row 1 |-> row 1 - -0.3 * row 0
row 2 |-> row 2 - 0.5 * row 0
new system
A = [ 10.0, -7.0,  0.0 ]
[  0.0, -0.0,  6.0 ]
[  0.0,  2.5,  5.0 ]
b = [  7.0 ]
[ 12.0 ]
[  7.5 ]

eliminating column 1
swapped system (1 <-> 2)
A = [ 10.0, -7.0,  0.0 ]
[  0.0,  2.5,  5.0 ]
[  0.0, -0.0,  6.0 ]
b = [  7.0 ]
[  7.5 ]
[ 12.0 ]

row 2 |-> row 2 - -4.085620730620576e-15 * row 1
new system
A = [ 10.0, -7.0,  0.0 ]
[  0.0,  2.5,  5.0 ]
[  0.0,  0.0,  6.0 ]
b = [  7.0 ]
[  7.5 ]
[ 12.0 ]

upper triangular system:
A = [ 10.0, -7.0,  0.0 ]
[  0.0,  2.5,  5.0 ]
[  0.0,  0.0,  6.0 ]
b = [  7.0 ]
[  7.5 ]
[ 12.0 ]

```

```
performing backward substitution

solution using backward substitution:
x = [ 0.0 ]
    [ -1.0 ]
    [  2.0 ]

Does x solve the original system? True
```

4.9 Further reading

Some basic reading:

- Joseph F. Grcar. [How ordinary elimination became Gaussian elimination](#). Historia Mathematica. Volume 38, Issue 2, May 2011. (More history)

Some implementations:

- Numpy [numpy.linalg.solve](#)
- Scipy [scipy.linalg.lu](#)
- LAPACK Gaussian elimination (uses LU factorisation): [dgesv\(\)](#)
- LAPACK LU Factorisation: [dgetrf\(\)](#).

5 Iterative solutions of linear equations

Module learning objective

Apply direct and iterative solvers to solve systems of linear equations; implement methods using floating point numbers and investigate computational cost using computer experiments.

5.1 Iterative methods

In the previous section we looked at what are known as *direct* methods for solving systems of linear equations. They are guaranteed to solve with a fixed amount of work (we can even prove this in exact arithmetic!), but this fixed amount of work may be **very** large.

For a general $n \times n$ system of linear equations $A\vec{x} = \vec{b}$, the computation expense of all direct methods is $O(n^3)$. The amount of storage required for these approaches is $O(n^2)$ which is dominated by the cost of storing the matrix A . As n becomes larger the storage and computation work required limit the practicality of direct approaches.

As an alternative, we will propose some **iterative methods**. Iterative methods produce a sequence $(\vec{x}^{(k)})$ of approximations to the solution of the linear system of equations $A\vec{x} = \vec{b}$. The iteration is defined recursively and is typically of the form:

$$\vec{x}^{(k+1)} = \vec{F}(\vec{x}^{(k)}),$$

where $\vec{x}^{(k)}$ is now a vector of values and \vec{F} is some vector function (which needs to be defined to define the method). We will need to choose a starting value $\vec{x}^{(0)}$ but there is often a reasonable approximation which can be used. Once all this is defined, we still need to decide when we need to stop!

Remark 5.1. We use a value in brackets in the superscript to denote the iteration number to avoid confusion between the iteration number and the component of the vector:

$$\vec{x}^{(k)} = (\vec{x}_1^{(k)}, \vec{x}_2^{(k)}, \dots, \vec{x}_n^{(k)}).$$

Example 5.1 (Some terrible examples). These are examples of potential iterative methods which would not work very well!

1. Consider

$$\vec{F}(\vec{x}^{(k)}) = \vec{x}^{(k)}.$$

Each iteration is very cheap to compute but very inaccurate - it never converges!

2. Consider

$$\vec{F}(\vec{x}^{(k)}) = \vec{x}^{(k)} + A^{-1}(\vec{b} - A\vec{x}^{(k)}).$$

Each iteration is very expensive to compute - you have to invert A ! - but it converges in just one step since

$$\begin{aligned} A\vec{x}^{(k+1)} &= A\vec{x}^{(k)} + AA^{-1}(\vec{b} - A\vec{x}^{(k)}) \\ &= A\vec{x}^{(k)} + \vec{b} - A\vec{x}^{(k)} \\ &= \vec{b}. \end{aligned}$$

The key point here is that we want a method that is both computationally cheap and converges quickly to the solution. One way to do this is to construct an iteration given by

$$\vec{F}(\vec{x}^{(k)}) = \vec{x}^{(k)} + P(\vec{b} - A\vec{x}^{(k)}). \quad (5.1)$$

for some matrix P such that

- P is easy to compute, or the matrix-vector product $\vec{r} \mapsto P\vec{r}$ is easy to compute,
- P approximates A^{-1} well enough that the algorithm converges in few iterations.

We call $\vec{b} - A\vec{x}^{(k)} = \vec{r}$ the **residual**. Note that the above bad examples could be written in the form of (5.1) with $P = O$ (the zero matrix) or $P = A^{-1}$.

5.2 Jacobi iteration

One straightforward choice for P in (5.1) is given by the Jacobi method where we take $P = D^{-1}$ where D is the diagonal of A :

$$D_{ii} = A_{ii} \quad \text{and} \quad D_{ij} = 0 \text{ for } i \neq j.$$

The **Jacobi iteration** is given by

$$\vec{x}^{(k+1)} = \vec{x}^{(k)} + D^{-1}(\vec{b} - A\vec{x}^{(k)})$$

D is a *diagonal matrix*, so D^{-1} is trivial to form (as long as the diagonal entries are all non-zero):

$$(D^{-1})_{ii} = \frac{1}{D_{ii}} \quad \text{and} \quad (D^{-1})_{ij} = 0 \text{ for } i \neq j.$$

Remark.

- The cost of one iteration is $O(n^2)$ for a full matrix, and this is dominated by the matrix-vector product $A\vec{x}^{(k)}$.
- This cost can be reduced to $O(n)$ if the matrix A is sparse - this is when iterative methods are especially attractive (Example 3.8).
- The amount of work also depends on the number of iterations required to get a “satisfactory” solution.
 - The number of iterations depends on the matrix;
 - * Fewer iterations are needed for a less accurate solution;
 - A good initial estimate $\vec{x}^{(0)}$ reduces the required number of iterations.
- Unfortunately, the iteration might not converge!

The Jacobi iteration updates all elements of $\vec{x}^{(k)}$ *simultaneously* to get $\vec{x}^{(k+1)}$. Writing the method out component by component gives

$$\begin{aligned}
x_1^{(k+1)} &= x_1^{(k)} + \frac{1}{A_{11}} \left(b_1 - \sum_{j=1}^n A_{1j} x_j^{(k)} \right) \\
x_2^{(k+1)} &= x_2^{(k)} + \frac{1}{A_{22}} \left(b_2 - \sum_{j=1}^n A_{2j} x_j^{(k)} \right) \\
&\vdots \quad \vdots \\
x_n^{(k+1)} &= x_n^{(k)} + \frac{1}{A_{nn}} \left(b_n - \sum_{j=1}^n A_{nj} x_j^{(k)} \right).
\end{aligned}$$

Note that once the first step has been taken, $x_1^{(k+1)}$ is already known, but the Jacobi iteration does not make use of this information!

Example 5.2. Take two iterations of Jacobi iteration to approximate the solution of the following system using the initial guess $\vec{x}^{(0)} = (1, 1)^T$:

$$\begin{pmatrix} 2 & 1 \\ -1 & 4 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 3.5 \\ 0.5 \end{pmatrix}$$

Starting from $\vec{x}^{(0)} = (1, 1)^T$, the first iteration is

$$\begin{aligned}
x_1^{(1)} &= x_1^{(0)} + \frac{1}{A_{11}} (b_1 - A_{11}x_1^{(0)} - A_{12}x_2^{(0)}) \\
&= 1 + \frac{1}{2}(3.5 - 2 \times 1 - 1 \times 1) = 1.25 \\
x_2^{(1)} &= x_2^{(0)} + \frac{1}{A_{22}} (b_2 - A_{21}x_1^{(0)} - A_{22}x_2^{(0)}) \\
&= 1 + \frac{1}{4}(0.5 - (-1) \times 1 - 4 \times 1) = 0.375.
\end{aligned}$$

So we have $\vec{x}^{(1)} = (1.25, 0.375)^T$. Then the second iteration is

$$\begin{aligned}
x_1^{(2)} &= x_1^{(1)} + \frac{1}{A_{11}} (b_1 - A_{11}x_1^{(1)} - A_{12}x_2^{(1)}) \\
&= 1.25 + \frac{1}{2}(3.5 - 2 \times 1.25 - 1 \times 0.375) = 1.5625 \\
x_2^{(2)} &= x_2^{(1)} + \frac{1}{A_{22}} (b_2 - A_{21}x_1^{(1)} - A_{22}x_2^{(1)}) \\
&= 0.375 + \frac{1}{4}(0.5 - (-1) \times 1.25 - 4 \times 0.375) = 0.4375.
\end{aligned}$$

So we have $\vec{x}^{(2)} = (1.5625, 0.4375)$.

Note the only difference between the formulae for Iteration 1 and 2 is the iteration number, the superscript in brackets. The exact solution is given by $\vec{x} = (1.5, 0.5)^T$.

We note that we can also slightly simplify the way the Jacobi iteration is written. We can expand A into $A = L + D + U$, where L and U are the parts of the matrix from below and above the diagonal respectively:

$$L_{ij} = \begin{cases} A_{ij} & \text{if } i < j \\ 0 & \text{if } i \geq j, \end{cases} \quad U_{ij} = \begin{cases} A_{ij} & \text{if } i > j \\ 0 & \text{if } i \leq j. \end{cases}$$

Then we can calculate that:

$$\begin{aligned} \vec{x}^{(k+1)} &= \vec{x}^{(k)} + D^{-1}(\vec{b} - A\vec{x}^{(k)}) \\ &= \vec{x}^{(k)} + D^{-1}(\vec{b} - (L + D + U)\vec{x}^{(k)}) \\ &= \vec{x}^{(k)} - D^{-1}D\vec{x}^{(k)} + D^{-1}(\vec{b} - (L + U)\vec{x}^{(k)}) \\ &= \vec{x}^{(k)} - \vec{x}^{(k)} + D^{-1}(\vec{b} - (L + U)\vec{x}^{(k)}) \\ &= D^{-1}(\vec{b} - (L + U)\vec{x}^{(k)}). \end{aligned}$$

In this formulation, we do not explicitly form the residual as part of the computations. In practical situations, this may be a simpler formulation we can use if we have knowledge of the coefficients of A , rather than just the matrix-vector product.

5.3 Gauss-Seidel iteration

As an alternative to Jacobi iteration, the iteration might use $x_i^{(k+1)}$ as soon as it is calculated (rather than using the previous iteration), giving

$$\begin{aligned} x_1^{(k+1)} &= x_1^{(k)} + \frac{1}{A_{11}} \left(b_1 - \sum_{j=1}^n A_{1j}x_j^{(k)} \right) \\ x_2^{(k+1)} &= x_2^{(k)} + \frac{1}{A_{22}} \left(b_2 - A_{21}x_1^{(k+1)} - \sum_{j=2}^n A_{2j}x_j^{(k)} \right) \\ x_3^{(k+1)} &= x_3^{(k)} + \frac{1}{A_{33}} \left(b_3 - \sum_{j=1}^2 A_{3j}x_j^{(k+1)} - \sum_{j=3}^n A_{3j}x_j^{(k)} \right) \\ &\vdots \quad \vdots \\ x_i^{(k+1)} &= x_i^{(k)} + \frac{1}{A_{ii}} \left(b_i - \sum_{j=1}^{i-1} A_{ij}x_j^{(k+1)} - \sum_{j=i}^n A_{ij}x_j^{(k)} \right) \\ &\vdots \quad \vdots \\ x_n^{(k+1)} &= x_n^{(k)} + \frac{1}{A_{nn}} \left(b_n - \sum_{j=1}^{n-1} A_{nj}x_j^{(k+1)} - A_{nn}x_n^{(k)} \right). \end{aligned}$$

Consider the system $A\vec{x} = b$ with the matrix A split as $A = L + D + U$, where D is the diagonal of A , L contains the elements below the diagonal, and U contains the elements above the diagonal. The componentwise iteration above can be written in matrix form as

$$\begin{aligned}
 \vec{x}^{(k+1)} &= \vec{x}^{(k)} + D^{-1}(\vec{b} - L\vec{x}^{(k+1)} - (D + U)\vec{x}^{(k)}) \\
 &= \vec{x}^{(k)} - D^{-1}L\vec{x}^{(k+1)} + D^{-1}(\vec{b} - (D + U)\vec{x}^{(k)}) \\
 &= \vec{x}^{(k)} - D^{-1}L\vec{x}^{(k+1)} + D^{-1}L\vec{x}^{(k)} + D^{-1}(\vec{b} - (L + D + U)\vec{x}^{(k)}) \\
 \vec{x}^{(k+1)} + D^{-1}L\vec{x}^{(k+1)} &= \vec{x}^{(k)} + D^{-1}L\vec{x}^{(k)} + D^{-1}(\vec{b} - (L + D + U)\vec{x}^{(k)}) \\
 D^{-1}(D + L)\vec{x}^{(k+1)} &= D^{-1}(D + L)\vec{x}^{(k)} + D^{-1}(\vec{b} - A\vec{x}^{(k)}) \\
 (D + L)\vec{x}^{(k+1)} &= DD^{-1}(D + L)\vec{x}^{(k)} + DD^{-1}(\vec{b} - A\vec{x}^{(k)}) \\
 &= (D + L)\vec{x}^{(k)} + (\vec{b} - A\vec{x}^{(k)}) \\
 \vec{x}^{(k+1)} &= (D + L)^{-1}(D + L)\vec{x}^{(k)} + (D + L)^{-1}(\vec{b} - A\vec{x}^{(k)}) \\
 &= \vec{x}^{(k)} + (D + L)^{-1}(\vec{b} - A\vec{x}^{(k)}).
 \end{aligned}$$

...and hence the **Gauss-Seidel** iteration

$$\vec{x}^{(k+1)} = \vec{x}^{(k)} + (D + L)^{-1}(\vec{b} - A\vec{x}^{(k)}).$$

That is, we use $P = (D + L)^{-1}$ in (5.1).

In general, we do not form the inverse of $D + L$ explicitly here since it is more complicated to do so than simply computing the inverse of D .

Example 5.3. Take two iterations of Gauss-Seidel iteration to approximate the solution of the following system using the initial guess $\vec{x}^{(0)} = (1, 1)^T$:

$$\begin{pmatrix} 2 & 1 \\ -1 & 4 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 3.5 \\ 0.5 \end{pmatrix}$$

Starting from $\vec{x}^{(0)} = (1, 1)^T$ we have

Iteration 1:

$$\begin{aligned}
 x_1^{(1)} &= x_1^{(0)} + \frac{1}{A_{11}}(b_1 - A_{11}x_1^{(0)} - A_{12}x_2^{(0)}) \\
 &= 2 + \frac{1}{2}(3.5 - 1 \times 2 - 1 \times 1) = 2.25 \\
 x_2^{(1)} &= x_2^{(0)} + \frac{1}{A_{22}}(b_2 - A_{21}x_1^{(1)} - A_{22}x_2^{(0)}) \\
 &= 1 + \frac{1}{4}(0.5 - (-1) \times 2.25 - 4 \times 1) = 0.6875.
 \end{aligned}$$

Iteration 2:

$$\begin{aligned}
x_1^{(2)} &= x_1^{(1)} + \frac{1}{A_{11}}(b_1 - A_{11}x_1^{(1)}a - A_{12}x_2^{(1)}) \\
&= 1.25 + \frac{1}{2}(3.5 - 2 \times 1.25 - 1 \times 0.4375) = 1.53125 \\
x_2^{(2)} &= x_2^{(1)} + \frac{1}{A_{22}}(b_2 - A_{21}x_1^{(2)} - A_{22}x_2^{(1)}) \\
&= 0.4375 + \frac{1}{4}(0.5 - (-1) \times 1.53125 - 4 \times 0.4375) = 0.5078125.
\end{aligned}$$

Again, note the changes in the iteration number on the right-hand side of these equations, especially the differences against the Jacobi method.

- What happens if the initial estimate is altered to $\vec{x}^{(0)} = (2, 1)^T$.

Exercise 5.1. Take one iteration of (a) Jacobi iteration; (b) Gauss-Seidel iteration to approximate the solution of the following system using the initial guess $\vec{x}^{(0)} = (1, 2, 3)^T$:

$$\begin{pmatrix} 2 & 1 & 0 \\ 1 & 3 & 1 \\ 0 & 1 & 2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 6 \\ 10 \\ 6 \end{pmatrix}.$$

Note that the exact solution to this system is $x_1 = 2, x_2 = 2, x_3 = 2$.

Remark.

- Here, both methods converge, but relatively slowly. They might not converge at all!
- We will discuss convergence and when to stop later.
- The Gauss-Seidel iteration generally out-performs the Jacobi iteration.
- Performance can depend on the order in which the equations are written.
- Both iterative algorithms can be made faster and more efficient for sparse systems of equations (far more than direct methods).

5.4 Python version of iterative methods

```

1 def jacobi_iteration(A, b, x0, max_iter, verbose=False):
2     """
3         Solve a linear system  $Ax = b$  using the Jacobi iterative method.
4
5         The Jacobi method is an iterative algorithm for solving the linear system:
6
7         .. math::
8             Ax = b
9
10        starting from an initial guess ``x0``. At each iteration, the solution is
11        updated according to:
12
13        .. math::
14            x_i^{(k+1)} = x_i^{(k)} + \frac{1}{A_{ii}} \left( b_i - \sum_{j=0}^{n-1} A_{ij} x_j^{(k)} \right)
15
16    Parameters
17    -----
18
19    A : numpy.ndarray
20        A 2D NumPy array of shape ``n, n`` representing the coefficient
21        matrix.
22
23    b : numpy.ndarray
24        A 1D or 2D NumPy array of shape ``n,`` or ``n, 1`` representing the
25        right-hand side vector.
26
27    x0 : numpy.ndarray
28        Initial guess for the solution, same shape as ``b``.
29
30    max_iter : int
31        Maximum number of iterations to perform.
32
33    verbose : bool, optional
34        If ``True``, prints the value of the solution vector at each iteration.
35        Default is ``False``.
36
37    Returns
38    -----
39
40    x : numpy.ndarray
41        Approximated solution vector after ``max_iter`` iterations.
42
43    n = system_size(A, b)
44
45    x = x0.copy()
46    xnew = np.empty_like(x)

```

```

43     if verbose:
44         print("starting value: ", end="")
45         print_array(x.T, "x.T")
46
47     for iter in range(max_iter):
48         for i in range(n):
49             Ax_i = 0.0
50             for j in range(n):
51                 Ax_i += A[i, j] * x[j]
52             xnew[i] = x[i] + 1.0 / (A[i, i]) * (b[i] - Ax_i)
53             x = xnew.copy()
54
55         if verbose:
56             print(f"after {iter}: ", end="")
57             print_array(x.T, "x.T")
58
59     return x
60
61
62 def gauss_seidel_iteration(A, b, x0, max_iter, verbose=False):
63     """
64     Solve a linear system  $Ax = b$  using the Gauss-Seidel iterative method.
65
66     The Gauss-Seidel method is an iterative algorithm for solving the linear
67     system:
68
69     .. math::
70         Ax = b
71
72     starting from an initial guess ``x0``. At each iteration, the solution is
73     updated sequentially using the most recently computed values:
74
75     .. math::
76         x_{i}^{(k+1)} = x_{i}^{(k)} + \frac{1}{A_{ii}} \left( b_i - \sum_{j=0}^{i-1} A_{ij} x_j^{(k+1)} - \sum_{j=i}^{n-1} A_{ij} x_j^{(k)} \right)
77
78
79     Parameters
80     -----
81     A : numpy.ndarray
82         A 2D NumPy array of shape ``(n, n)`` representing the coefficient
83         matrix.

```

```

85     b : numpy.ndarray
86         A 1D or 2D NumPy array of shape ``n,`` or ``n, 1`` representing the
87         right-hand side vector.
88     x0 : numpy.ndarray
89         Initial guess for the solution, same shape as ``b``.
90     max_iter : int
91         Maximum number of iterations to perform.
92     verbose : bool, optional
93         If ``True``, prints the value of the solution vector at each iteration.
94         Default is ``False``.
95
96     Returns
97     -----
98     x : numpy.ndarray
99         Approximated solution vector after ``max_iter`` iterations.
100
101 """
102 n = system_size(A, b)
103
104 x = x0.copy()
105 xnew = np.empty_like(x)
106
107 if verbose:
108     print("starting value: ", end="")
109     print_array(x.T, "x.T")
110
111 for iter in range(max_iter):
112     for i in range(n):
113         Ax_i = 0.0
114         for j in range(i):
115             Ax_i += A[i, j] * xnew[j]
116         for j in range(i, n):
117             Ax_i += A[i, j] * x[j]
118         xnew[i] = x[i] + 1.0 / (A[i, i]) * (b[i] - Ax_i)
119     x = xnew.copy()
120
121     if verbose:
122         print(f"after {iter}: ", end="")
123         print_array(x.T, "x.T")
124
125 return x

```

```

1 A = np.array([[2.0, 1.0], [-1.0, 4.0]])
2 b = np.array([[3.5], [0.5]])
3 x0 = np.array([[1.0], [1.0]])
4
5 print("jacobi iteration")
6 x = jacobi_iteration(A, b, x0, 5, verbose=True)
7 print()
8
9 print("gauss seidel iteration")
10 x = gauss_seidel_iteration(A, b, x0, 5, verbose=True)
11 print()

```

```

jacobi iteration
starting value: x.T = [ 1.0, 1.0 ]
after iter=0: x.T = [ 1.250, 0.375 ]
after iter=1: x.T = [ 1.5625, 0.4375 ]
after iter=2: x.T = [ 1.53125, 0.51562 ]
after iter=3: x.T = [ 1.49219, 0.50781 ]
after iter=4: x.T = [ 1.49609, 0.49805 ]

gauss seidel iteration
starting value: x.T = [ 1.0, 1.0 ]
after iter=0: x.T = [ 1.2500, 0.4375 ]
after iter=1: x.T = [ 1.53125, 0.50781 ]
after iter=2: x.T = [ 1.49609, 0.49902 ]
after iter=3: x.T = [ 1.50049, 0.50012 ]
after iter=4: x.T = [ 1.49994, 0.49998 ]

```

5.5 Sparse Matrices

We met sparse matrices as an example of a special matrix format when we first thought about systems of linear equations (Example 3.8). Sparse matrices are very common in applications and have a structure which is very useful when used with iterative methods. There are two main ways in which sparse matrices can be exploited in order to obtain benefits within iterative methods.

- The storage can be reduced from $O(n^2)$.
- The cost per iteration can be reduced from $O(n^2)$.

Recall that a sparse matrix is defined to be such that it has at most αn non-zero entries (where α is independent of n). Typically this happens when we know there are at most α non-zero entries in any row.

The simplest way in which a sparse matrix is stored is using three arrays:

- an array of floating point numbers (`A_real` say) that stores the non-zero entries;
- an array of integers (`I_row` say) that stores the row number of the corresponding entry in the real array;
- an array of integers (`I_col` say) that stores the column numbers of the corresponding entry in the real array.

This requires just $3\alpha n$ units of storage - i.e. $O(n)$. This is called the COO (coordinate) format.

Given the above storage pattern, the following algorithm will execute a sparse matrix-vector multiplication ($\vec{z} = A\vec{y}$) in $O(n)$ operations:

```

1 z = np.zeros((n, 1))
2 for k in range(nonzero):
3     z[I_row[k]] = z[I_row[k]] + A_real[k] * y[I_col[k]]

```

- Here `nonzero` is the number of non-zero entries in the matrix.
- Note that the cost of this operation is $O(n)$ as required.

5.5.1 Python experiments

First let's adapt our implementations to use this sparse matrix format:

```

1 def jacobi_iteration_sparse(
2     A_real, I_row, I_col, b, x0, max_iter, verbose=False
3 ):
4     """
5         Solve a sparse linear system Ax = b using the Jacobi iterative method.
6
7         The system is represented in **sparse COO (coordinate) format** with:
8         - `A_real`: non-zero values
9         - `I_row`: row indices of non-zero entries
10        - `I_col`: column indices of non-zero entries
11
12        The Jacobi method updates the solution iteratively:
13
14        .. math::
15            x_i^{(k+1)} = x_i^{(k)} + \frac{1}{A_{ii}} \left( b_i -

```

```

16     \sum_{j=0}^{n-1} A_{ij} x_j^{(k)} \right)
17
18 Parameters
19 -----
20 A_real : array-like
21     Array of non-zero entries of the sparse matrix A.
22 I_row : array-like
23     Row indices corresponding to each entry in `A_real`.
24 I_col : array-like
25     Column indices corresponding to each entry in `A_real`.
26 b : array-like
27     Right-hand side vector of length `n`.
28 x0 : numpy.ndarray
29     Initial guess for the solution vector, same length as `b`.
30 max_iter : int
31     Maximum number of iterations to perform.
32 verbose : bool, optional
33     If ``True``, prints the solution vector after each iteration. Default is
34     ``False``.
35
36 Returns
37 -----
38 x : numpy.ndarray
39     Approximated solution vector after `max_iter` iterations.
40 """
41 n, nonzero = system_size_sparse(A_real, I_row, I_col, b)
42
43 x = x0.copy()
44 xnew = np.empty_like(x)
45
46 if verbose:
47     print("starting value: ", end="")
48     print_array(x.T, "x.T")
49
50 # determine diagonal
51 # D[i] should be A_{ii}
52 D = np.zeros_like(x)
53 for k in range(nonzero):
54     if I_row[k] == I_col[k]:
55         D[I_row[k]] = A_real[k]
56
57 for iter in range(max_iter):

```

```

58     # precompute Ax
59     Ax = np.zeros_like(x)
60     for k in range(nonzero):
61         Ax[I_row[k]] = Ax[I_row[k]] + A_real[k] * x[I_col[k]]
62
63     for i in range(n):
64         xnew[i] = x[i] + 1.0 / D[i] * (b[i] - Ax[i])
65     x = xnew.copy()
66
67     if verbose:
68         print(f"after {iter=}: ", end="")
69         print_array(x.T, "x.T")
70
71     return x
72
73
74 def gauss_seidel_iteration_sparse(
75     A_real, I_row, I_col, b, x0, max_iter, verbose=False
76 ):
77     """
78     Solve a sparse linear system  $Ax = b$  using the Gauss-Seidel iterative method.
79
80     The system is represented in **sparse COO (coordinate) format** with:
81     - `A_real`: non-zero values
82     - `I_row`: row indices of non-zero entries
83     - `I_col`: column indices of non-zero entries
84
85     The Gauss-Seidel method updates the solution sequentially using the most
86     recently computed values:
87
88     .. math::
89         x_{i^{(k+1)}} = x_{i^{(k)}} + \frac{1}{A_{ii}} \left( b_i - \sum_{j=0}^{i-1} A_{ij} x_{j^{(k+1)}} - \sum_{j=i}^{n-1} A_{ij} x_{j^{(k)}} \right)
90
91     Parameters
92     -----
93     A_real : array-like
94         Array of non-zero entries of the sparse matrix A.
95     I_row : array-like
96         Row indices corresponding to each entry in `A_real`.
97     I_col : array-like
98
99

```

```

100     Column indices corresponding to each entry in `A_real`.
101     b : array-like
102         Right-hand side vector of length `n`.
103     x0 : numpy.ndarray
104         Initial guess for the solution vector, same length as `b`.
105     max_iter : int
106         Maximum number of iterations to perform.
107     verbose : bool, optional
108         If ``True``, prints the solution vector after each iteration. Default is
109         ``False``.
110
111     Returns
112     -----
113     x : numpy.ndarray
114         Approximated solution vector after `max_iter` iterations.
115     """
116     n, nonzero = system_size_sparse(A_real, I_row, I_col, b)
117
118     x = x0.copy()
119     xnew = np.empty_like(x)
120
121     if verbose:
122         print("starting value: ", end="")
123         print_array(x.T, "x.T")
124
125     for iter in range(max_iter):
126         # precompute Ax using xnew if i < j
127         Ax = np.zeros_like(x)
128         for k in range(nonzero):
129             if I_row[k] < I_col[k]:
130                 Ax[I_row[k]] = Ax[I_row[k]] + A_real[k] * xnew[I_col[k]]
131             else:
132                 Ax[I_row[k]] = Ax[I_row[k]] + A_real[k] * x[I_col[k]]
133
134         for i in range(n):
135             xnew[i] = x[i] + 1.0 / (A[i, i]) * (b[i] - Ax[i])
136         x = xnew.copy()
137
138         if verbose:
139             print(f"after {iter}: ", end="")
140             print_array(x.T, "x.T")
141

```

```
142     return x
```

Then we can test the two different implementations of the methods:

```
1 # random matrix
2 n = 4
3 nonzero = 10
4 A_real, I_row, I_col, b = random_sparse_system(n, nonzero)
5 print("sparse matrix:")
6 print("A_real =", A_real)
7 print("I_row = ", I_row)
8 print("I_col = ", I_col)
9 print()
10
11 # convert to dense for comparison
12 A_dense = to_dense(A_real, I_row, I_col)
13 print("dense matrix:")
14 print_array(A_dense)
15 print()
16
17 # starting guess
18 x0 = np.zeros((n, 1))
19
20 print("jacobi with sparse matrix")
21 x_sparse = jacobi_iteration_sparse(
22     A_real, I_row, I_col, b, x0, max_iter=5, verbose=True
23 )
24 print()
25
26 print("jacobi with dense matrix")
27 x_dense = jacobi_iteration(A_dense, b, x0, max_iter=5, verbose=True)
28 print()
```

```
sparse matrix:
A_real = [16. 25. 12. 16.  8. 25. 12. 16. 20.  8.]
I_row =  [0 0 1 1 2 2 2 3 3 3]
I_col =  [3 0 2 1 3 2 1 0 3 2]

dense matrix:
A_dense = [ 25.0,  0.0,  0.0, 16.0 ]
           [ 0.0, 16.0, 12.0,  0.0 ]
           [ 0.0, 12.0, 25.0,  8.0 ]
```

```

[ 16.0,  0.0,  8.0, 20.0 ]

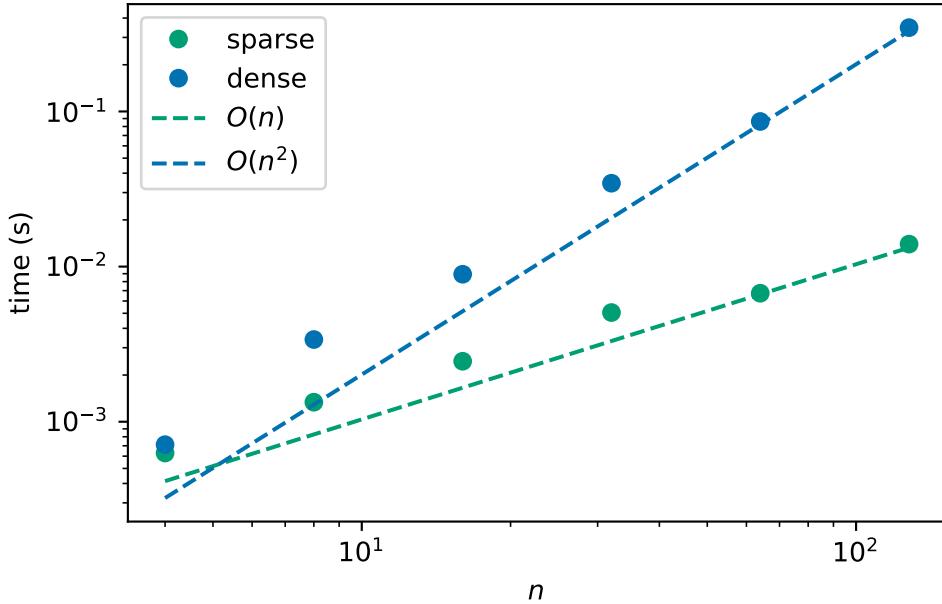
jacobi with sparse matrix
starting value: x.T = [  0.0,  0.0,  0.0,  0.0 ]
after iter=0: x.T = [  1.64,  1.75,  1.80,  2.20 ]
after iter=1: x.T = [  0.232,  0.400,  0.256,  0.168 ]
after iter=2: x.T = [  1.53248,  1.55800,  1.55424,  1.91200 ]
after iter=3: x.T = [  0.41632,  0.58432,  0.44032,  0.35232 ]
after iter=4: x.T = [  1.41452,  1.41976,  1.40678,  1.69082 ]

jacobi with dense matrix
starting value: x.T = [  0.0,  0.0,  0.0,  0.0 ]
after iter=0: x.T = [  1.64,  1.75,  1.80,  2.20 ]
after iter=1: x.T = [  0.232,  0.400,  0.256,  0.168 ]
after iter=2: x.T = [  1.53248,  1.55800,  1.55424,  1.91200 ]
after iter=3: x.T = [  0.41632,  0.58432,  0.44032,  0.35232 ]
after iter=4: x.T = [  1.41452,  1.41976,  1.40678,  1.69082 ]

```

We see that we get the same results!

Now let us see how long it takes to get a solution. The following plot shows the run times of using the two different implementations of the Jacobi method, each for 10 iterations. We see that, as expected, the run time of the dense formulation is $O(n^2)$ and the run time of the sparse formulation is $O(n)$.



We say “as expected” because we have already counted the number of operations per iteration and these implementations compute for a fixed number of iterations. In the next section, we look at alternative stopping criteria.

5.6 Convergence of an iterative method

We have discussed the construction of **iterations** which aim to find the solution of the equations $A\vec{x} = \vec{b}$ through a sequence of better and better approximations $\vec{x}^{(k)}$.

In general the iteration takes the form

$$\vec{x}^{(k+1)} = \vec{F}(\vec{x}^{(k)})$$

here $\vec{x}^{(k)}$ is a vector of values and \vec{F} is some vector-valued function which we have defined.

How can we decide if this iteration has converged? We need $\vec{x} - \vec{x}^{(k)}$ to be small, but we do not have access to the exact solution \vec{x} so we have to do something else!

How do we decide that a vector/array is small? The most common measure is to use the *Euclidean norm* of an array (which you met last year!). The Euclidean norm, or norm for short, is defined to be the square root of the sum of squares of the entries of the array:

$$\|\vec{r}\| = \sqrt{\sum_{i=1}^n r_i^2}.$$

where \vec{r} is a vector with n entries.

Example 5.4. Consider the following sequence $\vec{x}^{(k)}$:

$$\begin{pmatrix} 1 \\ -1 \end{pmatrix}, \begin{pmatrix} 1.5 \\ 0.5 \end{pmatrix}, \begin{pmatrix} 1.75 \\ 0.25 \end{pmatrix}, \begin{pmatrix} 1.875 \\ 0.125 \end{pmatrix}, \begin{pmatrix} 1.9375 \\ -0.0625 \end{pmatrix}, \begin{pmatrix} 1.96875 \\ -0.03125 \end{pmatrix}, \dots$$

- What is $\|\vec{x}^{(1)} - \vec{x}^{(0)}\|$?
- What is $\|\vec{x}^{(5)} - \vec{x}^{(4)}\|$?

Let $\vec{x} = \begin{pmatrix} 2 \\ 0 \end{pmatrix}$.

- What is $\|\vec{x} - \vec{x}^{(3)}\|$?
- What is $\|\vec{x} - \vec{x}^{(4)}\|$?
- What is $\|\vec{x} - \vec{x}^{(5)}\|$?

Rather than decide in advance how many iterations (of the Jacobi or Gauss-Seidel methods) to use, we can use the following stopping criteria:

- A maximum number of iterations.
- The *change* in values is small enough:

$$\|\vec{x}^{(k+1)} - \vec{x}^{(k)}\| < tol,$$

- The *norm of the residual* is small enough:

$$\|\vec{r}\| = \|\vec{b} - A\vec{x}^{(k)}\| < tol$$

In the second and third cases, we call *tol* the **convergence tolerance** and the choice of *tol* controls the accuracy of the solution.

Exercise 5.2 (Discussion). What is a good convergence tolerance?

In general there are two possible reasons that an iteration may fail to converge.

- It may **diverge** - this means that $\|\vec{x}^{(k)}\| \rightarrow \infty$ as k (the number of iterations) increases, e.g.:

$$\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \begin{pmatrix} 4 \\ 2 \end{pmatrix}, \begin{pmatrix} 16 \\ 4 \end{pmatrix}, \begin{pmatrix} 64 \\ 8 \end{pmatrix}, \begin{pmatrix} 256 \\ 16 \end{pmatrix}, \begin{pmatrix} 1024 \\ 32 \end{pmatrix}, \dots$$

- It may *neither* converge nor diverge, e.g.:

$$\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \begin{pmatrix} 2 \\ 0 \end{pmatrix}, \begin{pmatrix} 3 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 2 \\ 1 \end{pmatrix}, \begin{pmatrix} 3 \\ 0 \end{pmatrix}, \dots$$

In addition to testing for convergence it is also necessary to include tests for failure to converge.

- Divergence may be detected by monitoring $\|\vec{x}^{(k)}\|$.
- Impose a maximum number of iterations to ensure that the loop is not repeated forever!

5.7 Summary

Many complex computational problems simply cannot be solved with today's computers using direct methods. Iterative methods are used instead since they can massively reduce the computational cost and storage required to get a "good enough" solution.

These basic iterative methods are simple to describe and program but generally slow to converge to an accurate answer - typically $O(n)$ iterations are required! Their usefulness for general matrix systems is very limited therefore - but we have shown their value in the solution of sparse systems however.

More advanced iterative methods do exist but are beyond the scope of this module - see Final year projects, MSc projects, PhD, and beyond!

5.8 Further reading

- Jason Brownlee: [A gentle introduction to sparse matrices for machine learning](#), Machine learning mastery

Some software implementations:

- `scipy.sparse` custom routines specialised to sparse matrices
- `SuiteSparse`, a suite of sparse matrix algorithms geared toward the direct solution of sparse linear systems
- `scipy.sparse` iterative solvers: [Solving linear problems](#)
- PETSc: [Linear system solvers](#) - a high-performance linear algebra toolkit

6 Complex numbers

This section of the notes supports the final learning outcome around eigenvalues and eigenvectors.

6.1 Basic definitions

A complex number is an element of a number system which extends our familiar real number system. Our motivation will be to find eigenvalues and eigenvectors which is the next topic in this module. To find eigenvalues, we need to solve of polynomial equations and it will turn out to be useful to *always* be able to get a solution to any polynomial equation.

Example 6.1. Consider the polynomial equation

$$x^2 + 1 = 0. \quad (6.1)$$

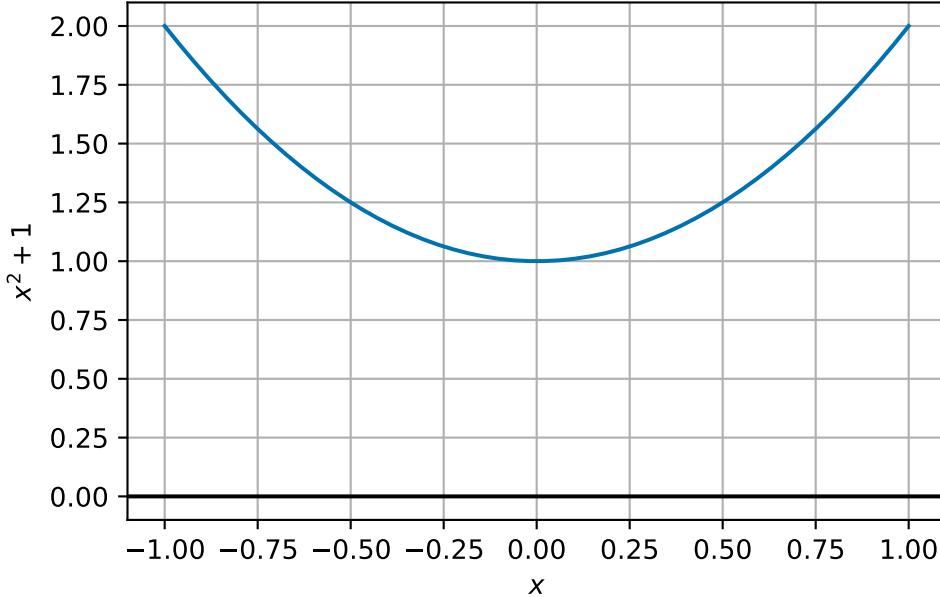


Figure 6.1: Plot of $y = x^2 + 1$.

We can see that this equation has no solution over the real numbers: There are no real values x such that $x^2 + 1 = 0$.

The key idea of complex numbers is to create a new symbol, which we will call i , or the **imaginary unit** which satisfies:

$$i^2 = -1 \quad \sqrt{-1} = i.$$

By taking multiples of this imaginary unit, we can create many more new numbers, like $3i$, $\sqrt{5}i$ or $-12i$. These are examples of **imaginary numbers**.

We form **complex numbers** by adding real and imaginary numbers whilst keeping each part separate – for example, $2 + 3i$, $\frac{1}{2} + \sqrt{5}i$ or $12 - 12i$.

Definition 6.1. Any number that can be written as $z = a + bi$ with a, b real numbers and i the imaginary unit is called *complex number*. In this format, we call a the **real part** of z and b the **imaginary part** of z .

We notice that all real numbers x must also be complex numbers since $x = x + 0i$.

Remark 6.1. Among the first recorded uses of complex numbers in European mathematics was by an Italian mathematician, Gerolamo Cardano, in around 1545. He later described complex numbers as being “as subtle as they are useless” and “mental torment”.

The term imaginary was coined by René Descartes in 1637:

... sometimes only imaginary, that is one can imagine as many as I said in each equation, but sometimes there exist no quantity that matches that which we imagine.

Exercise 6.1. What are the real and imaginary parts of these numbers?

1. $3 + 6i$
2. $-3.5 + 2i$
3. 5
4. $7i$

6.2 Calculations with complex numbers

We can perform the basic operations, such as addition, subtraction, multiplication and division, on complex numbers.

Addition and subtraction are relatively straightforward: we treat the real and imaginary parts separately.

Example 6.2. We can compute that

$$(2 + 3i) + (12 - 12i) = (2 + 12) + (3 - 12)i = 14 - 9i$$

$$(2 + 3i) - (12 - 12i) = (2 - 12) + (3 - (-12))i = -10 + 15i.$$

Exercise 6.2. Compute $(3 + 6i) + (-3.5 + 2i)$ and $(3 + 6i) - (-3.5 + 2i)$.

For multiplying and dividing, we first say that applying these operations between complex and real numbers again follows the usual rules. Let x be a real number and $z = (a + bi)$ be a complex number, then

$$x \times (a + bi) = (a + bi) \times x = (x \times a) + (x \times b)i$$

$$\frac{a + bi}{x} = \frac{a}{x} + \frac{b}{x}i.$$

For multiplication between complex numbers, things are harder. We expand brackets and apply the rule that $i^2 = -1$:

Example 6.3.

$$\begin{aligned} & (2 + 3i) \times (12 - 12i) \\ &= 2 \times 12 + 3i \times 12 + 2 \times -12i + 3i \times -12i && \text{(expand brackets)} \\ &= 2 \times 12 + (12 \times 3)i + (2 \times -12)i + (3 \times -12) \times i^2 && \text{(rearrange)} \\ &= 24 + 36i - 24i - 36 \times i^2 && \text{(compute products)} \\ &= 24 + 36i - 24i + 36 && \text{(use } i^2 = -1\text{)} \\ &= 60 + 12i && \text{(collect terms).} \end{aligned}$$

This leads us to a general formula:

$$(a + bi) \times (c + di) = (ac - bd) + (ad + bc)i.$$

Exercise 6.3. Compute $(3 + 6i) \times (-3.5 + 2i)$.

Division is harder - you may want to skip this on first reading since it is not so important for what follows in these notes. When we divide complex numbers, we try to rewrite the fraction to have a real denominator by “rationalising the denominator”.

Example 6.4. Suppose we want to find $(2 + 3i)/(12 - 12i)$. Our idea is to find a number so that we can write

$$\frac{2 + 3i}{12 - 12i} = \frac{2 + 3i}{12 - 12i} \times \frac{z}{z} = \frac{(2 + 3i)z}{(12 - 12i)z} = \frac{\text{something}}{\text{something real}}.$$

The answer is to use $z = 12 + 12i$ - that is the denominator with the sign of the imaginary part flipped (we will give this a name later on).

We can compute that

$$\begin{aligned}
 & (12 - 12i) \times (12 + 12i) \\
 &= (12 \times 12) + (12 \times 12i) + (-12i \times 12) + (-12i \times 12i) && \text{(expand bracket)} \\
 &= 12 \times 12 + (12 \times 12)i + (-12 \times 12)i + (-12 \times 12)i^2 && \text{(rearrange)} \\
 &= 144 + 144i - 144i - 144i^2 && \text{(compute products)} \\
 &= 144 + 144i - 144i + 144 && \text{(use } i^2 = -1\text{)} \\
 &= 288 + 0i && \text{(collect terms).}
 \end{aligned}$$

So we have that $(12 - 12i) \times (12 + 12i) = 288$ is a real number.

We continue by computing that

$$\begin{aligned}
 & (2 + 3i) \times (12 + 12i) \\
 &= (2 \times 12) + (2 \times 12i) + (3i \times 12) + (3i \times 12i) \\
 &= 2 \times 12 + (2 \times 12)i + (3 \times 12)i + (3 \times 12)i^2 \\
 &= 24 + 24i + 36i + 36i^2 \\
 &= 24 + 24i + 36i - 36 \\
 &= -12 + 60i.
 \end{aligned}$$

Thus we infer that

$$\begin{aligned}
 \frac{2 + 3i}{12 - 12i} &= \frac{2 + 3i}{12 - 12i} \times \frac{12 + 12i}{12 + 12i} \\
 &= \frac{(2 + 3i)(12 + 12i)}{(12 - 12i)(12 + 12i)} \\
 &= \frac{-12 + 60i}{288} \\
 &= \frac{-12}{288} + \frac{60}{288}i \\
 &= -\frac{1}{24} + \frac{5}{24}i.
 \end{aligned}$$

To check we have not done anything silly, we should also check that $(12 + 12i)/(12 + 12i) = 1$. This is left as an exercise.

Exercise 6.4. Find $(3 + 6i)/(-3.5 + 2i)$ and $(12 + 12i)/(12 + 12i)$.

Remark 6.2. One thing to be careful of when considering products is that the identity $i^2 = -1$ appears to break one rule of arithmetic of square roots:

$$i^2 = (\sqrt{-1})^2 = \sqrt{-1}\sqrt{-1} \neq \sqrt{(-1) \times (-1)} = \sqrt{1} = 1.$$

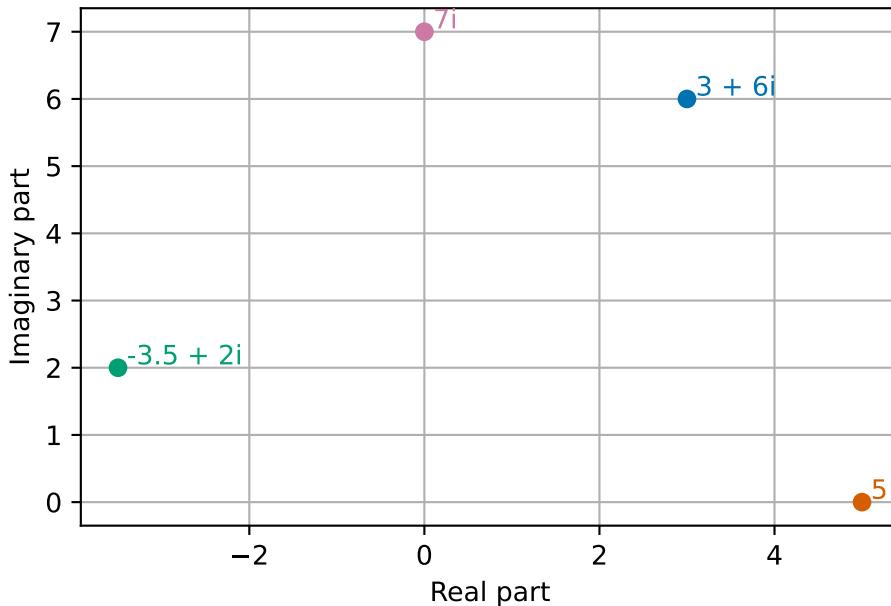
In fact, we have that $\sqrt{x}\sqrt{y} = \sqrt{xy}$ only if $x, y > 0$.

6.3 A geometric picture

The idea of adding complex numbers by considering real and imaginary parts separately is reminiscent of adding two-dimensional vectors. For this reason, it is often helpful to think of complex numbers as points in *the complex plane*.

The complex plane is the two-dimensional space formed by considering the real and imaginary parts of a complex number as two different coordinate axes.

Example 6.5.



Adding complex numbers looks just like adding two dimensional vectors! We can also use this geometric picture to help with some further operations.

The *complex conjugate* of a complex number $z = a + bi$ is given by $\bar{z} = a - bi$. The complex conjugate is that number we used before when working out how to divide complex numbers.

Example 6.6. The complex conjugate of $2 + 3i$ is $2 - 3i$. The complex conjugate of $12 - 12i$ is $12 + 12i$.

Exercise 6.5. Find the complex conjugates of $3 + 6i$ and $-3.5 + 2i$.

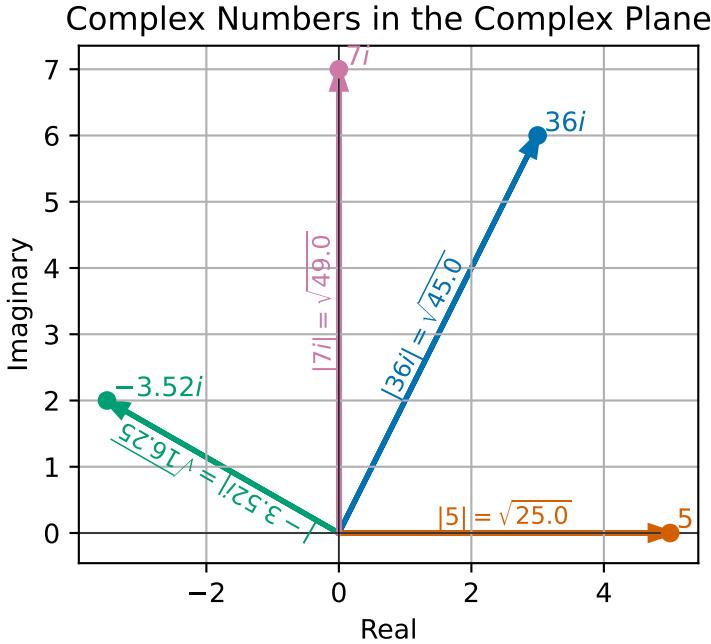
We have already seen that the complex conjugate of a complex number is helpful when performing division of complex numbers. The reason is that computing the product of a number and its conjugate always gives a real, positive number:

$$\begin{aligned}
 & (a + bi) \times (a - bi) \\
 &= (a \times a) + (a \times -bi) + (bi \times a) + (bi \times -bi) \\
 &= (a \times a) + (a \times -b)i + (b \times a)i + (b \times -b)i^2 \\
 &= (a \times a) + (a \times -b + b \times a)i - (b \times -b) \\
 &= a^2 + b^2 + 0i.
 \end{aligned}$$

In fact, we use this same calculation to define the **modulus** (sometimes called the **absolute value**) of a complex number $z = a + bi$

$$|z| = |a + bi| = \sqrt{a^2 + b^2} = \sqrt{z\bar{z}}. \quad (6.2)$$

Example 6.7.



Exercise 6.6. Find the value of

$$|3 + 6i| \quad \text{and} \quad |-3.5 + 2i|. \quad (6.3)$$

Consider two complex numbers $z = a + bi$ and $y = c + di$. Then, we have already seen that

$$zy = (a + bi) \times (c + di) = (ac - bd) + (ad + bc)i.$$

We can compute the square of the modulus of the product zy as

$$\begin{aligned} |zy|^2 &= (ac - bd)^2 + (ad + bc)^2 \\ &= a^2c^2 - 2abcd + b^2d^2 + a^2d^2 + 2abcd + b^2c^2 \\ &= a^2c^2 + b^2d^2 + a^2d^2 + b^2c^2 \\ &= (a^2 + b^2)(c^2 + d^2), \end{aligned}$$

and we have computed that $|zy| = |z||y|$.

In particular, if y has modulus 1, then $|zy| = |z|$. This means that zy and z are the same distance from the origin but ‘point’ in different directions. We can write the real and imaginary parts as $y = c + di = \cos(\theta) + i \sin(\theta)$, where θ is the angle between the positive real axis and the line between 0 and y . Then

$$\begin{aligned} zy &= (ac - bd) + (ad + bc)i \\ &= (a \cos(\theta) - b \sin(\theta)) + (a \sin(\theta) + b \cos(\theta))i. \end{aligned}$$

Recalling the example of a rotation matrix from Example 1.3, we see that multiplying by y is the same as rotating the complex point (z) by an angle of θ radians in the anti-clockwise direction.

This leads us to thinking *polar coordinates* for the complex plane. Polar coordinates are a different form of coordinates that replace the usual x and y -directions (up and across) by two values which represent the distance to the origin (that we call radius) and angle to the positive x -axis (that we call the angle). When talking about a complex number z represented in the complex plane, we know that the modulus $|z|$ represents the radius. The idea of θ above represents the angle of a complex number that we know call the **argument**.

Definition 6.2. Let z be a complex number. The **polar form** of z is $R(\cos \theta + i \sin \theta)$. We call R the modulus of z and θ is the argument of z .

The representation of the angle unique up to adding integer multiples of 2π , since rotating a point by 2π about the origin leaves it unchanged.

Example 6.8. Let $z = 12 - 12i$. Then

$$|z| = |12 - 12i| = \sqrt{12^2 + 12^2} = \sqrt{2 \times 144} = 12\sqrt{2}.$$

We have $\arg z = -\pi/4$ since

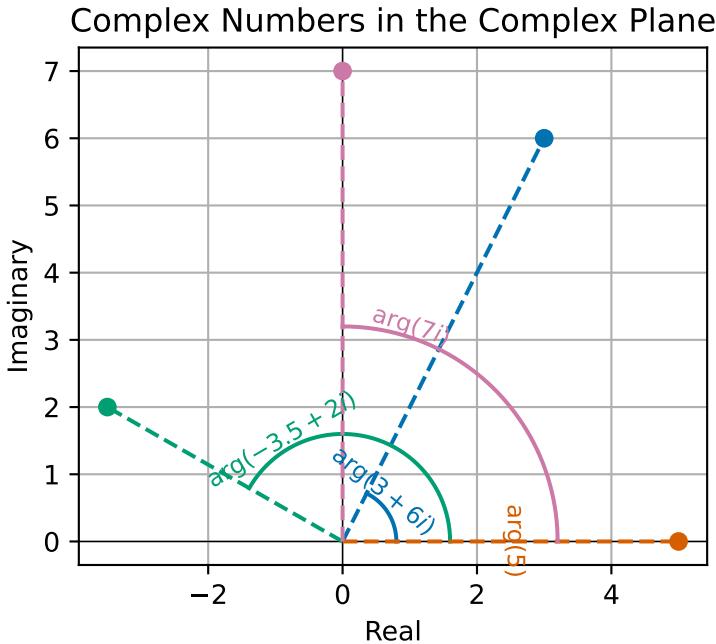
$$\cos(-\pi/4) = \frac{1}{\sqrt{2}}, \quad \text{and} \quad \sin(-\pi/4) = \frac{-1}{\sqrt{2}},$$

so

$$12\sqrt{2}(\cos(-\pi/4) + i \sin(-\pi/4)) = 12\sqrt{2} \left(\frac{1}{\sqrt{2}} + i \frac{-1}{\sqrt{2}} \right) = 12 - 12i.$$

Exercise 6.7. Compute the modulus and argument of 2 , $3i$ and $4 + 4i$.

Example 6.9.



The polar representation of complex numbers then gives us a nice way to understand multiplication of complex numbers. If $y \neq 0$, then we can check that $\left| \frac{y}{|y|} \right| = 1$ and $\arg y = \arg \frac{y}{|y|}$. Then writing $zy = z \frac{y}{|y|} |y|$, we can use our calculations above to infer that multiplying by y corresponds to an anticlockwise rotation by $\arg y$ then scaling by $|y|$.

Exercise 6.8. Check that for any non-zero complex number y , that $\left| \frac{y}{|y|} \right| = 1$ and $\arg y = \arg \frac{y}{|y|}$.

6.4 Euler's formula

The polar form of complex numbers can be further developed thanks to two helpful identities. We only state the identities here. There are some examples on the worksheet to help your understanding here.

Euler's formula relates the polar form of a complex number to complex exponentials: Let x be a real number, then

$$\exp(ix) = \cos x + i \sin x.$$

The result can be shown by showing that the function $f(x) = \exp(-ix)(\cos x + i \sin x)$ is a constant function and that the constant value is 1. For the purposes of this part of the module, you might want to think of $\exp(ix)$ simply as a shorthand for $\cos x + i \sin x$ when used in calculations.

For example, as a consequence of Euler's formula, we can compute powers of complex numbers very simply. Let z be given in polar form by $z = R \exp(i\theta)$ (that is R is the magnitude of z and θ is the argument of z). Then z^p is, by the rule of exponentiation, $z^p = R^p \exp(ip\theta)$.

Euler's formula is the key important step for showing Euler's identity:

$$\exp(i\pi) = -1.$$

This is shown by applying Euler's formula at $x = \pi$. This is a formula which many mathematicians a surprising and beautiful result!

6.5 Solving polynomial equations

As we have mentioned above, we will be using complex numbers when solving polynomial equations to work out eigenvalues and eigenvectors of matrices later in the section. The reason complex numbers are useful here is this very important Theorem:

Theorem 6.1 (The Fundamental Theorem of Algebra). *For any complex numbers a_0, \dots, a_n not all zero, there is at least one complex number z which satisfies:*

$$a_n z^n + \dots + a_1 z + a_0 = 0$$

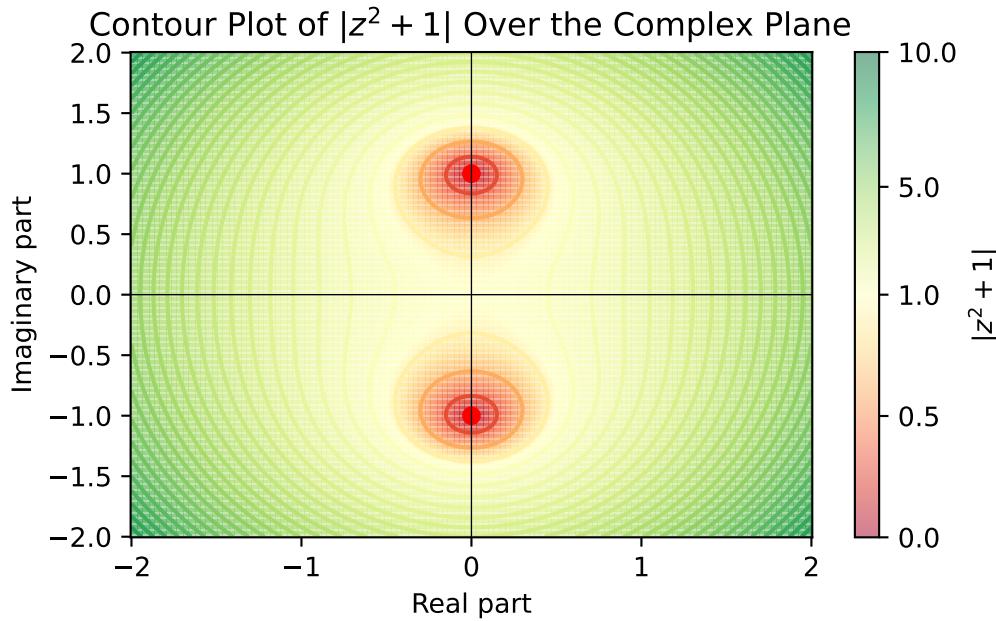
It is really important to note here that this is not true if we want z to be a real number. Let's revisit Example 6.1.

Example 6.10. Consider the polynomial equation

$$x^2 + 1 = 0. \quad (6.4)$$

We saw before that this equation has no solution over the real numbers, but the Fundamental Theorem of Algebra tells us there must be at least one solution which is a complex number. In fact it has two solutions $-i$ and $-i$:

$$\begin{aligned} i^2 + 1 &= 0 \\ (-i)^2 + 1 &= (-1)^2 i^2 + 1 = i^2 + 1 = 0. \end{aligned}$$



Notice that along the real line (Imaginary part = 0), the value of the function is always above 1.

In general, to find complex roots of other quadratic equations, we can apply the quadratic formula:

Example 6.11. To find the values of z which satisfy $z^2 - 2z + 2 = 0$, we see:

$$z = \frac{+2 \pm \sqrt{(-2)^2 - 4 \times 1 \times 2}}{2} = \frac{2 \pm \sqrt{-4}}{2} = \frac{2 \pm 2\sqrt{-1}}{2} = 1 \pm i.$$

Exercise 6.9. Find the value of z which satisfy $z^2 - 4z + 20 = 0$.

We will see in later sections that although this is one possible solution to compute the eigenvalues for 2×2 matrices this approach becomes infeasible for larger size matrices and we need another approach!

6.6 Complex vectors and matrices

Last year you were introduced to vectors of real numbers. In the remaining part of Linear Algebra, we will need to work with complex matrices and vectors. The definitions are mostly what you would expect but with some slight subtleties.

Definition 6.3. A complex matrix is a matrix whose entries are complex numbers. A complex vector is a vector whose entries are complex numbers.

One thing we like to do with vectors is to take scalar products and to find their length. When working with complex vectors, we replace the scalar product with a *Hermitian product*. We write $\langle \vec{a}, \vec{b} \rangle$ for the Hermitian product of two complex n -vectors \vec{a} and \vec{b} and the value is given by

$$\langle \vec{a}, \vec{b} \rangle = \sum_{i=1}^n a_i \bar{b}_i. \quad (6.5)$$

We see that the Hermitian product is the same as taking the scalar product of \vec{a} and the complex conjugate of \vec{b} . If the entries in \vec{b} have no imaginary part (i.e. they are all real numbers), then the Hermitian product of \vec{a} and \vec{b} is equal to the scalar product of \vec{a} and \vec{b} .

Example 6.12. Let $\vec{a} = (1 + 2i, 2 + i, 3 - 4i)^T$ and $\vec{b} = (6 + 2i, 3 + 4i, 1 + i)^T$ then:

$$\begin{aligned} \langle \vec{a}, \vec{b} \rangle &= (1 + 2i) \times (6 - 2i) + (2 + i) \times (3 - 4i) + (3 - 4i) \times (1 - i) \\ &= (10 + 10i) + (10 - 5i) + (-1 - 7i) = 19 - 2i. \end{aligned}$$

Exercise 6.10. Find the Hermitian product of $\vec{c} = (3 + i, -2 + 2i, 4 - i)^T$ and $\vec{d} = (-1 + 3i, 2 + 6i, 2i)^T$.

Recalling the definition of modulus of a complex number (6.2), we can also compute that for a complex n -vector \vec{z} that

$$\langle \vec{z}, \vec{z} \rangle = \sum_{i=1}^n z_i \bar{z}_i = \sum_{i=1}^n |z_i|^2.$$

So for a complex vector, we define the Euclidean norm as

$$\|\vec{z}\| = \sqrt{\sum_{i=1}^n |z_i|^2} = \sqrt{\langle \vec{z}, \vec{z} \rangle}.$$

Recall that for a real *symmetric* $n \times n$ matrix A and any n -vectors \vec{x} and \vec{y} that

$$\begin{aligned}
A\vec{x} \cdot \vec{y} &= \sum_{i=1}^n (A\vec{x})_i y_i && \text{(definition of scalar product)} \\
&= \sum_{i=1}^n \left(\sum_{j=1}^n A_{ij} x_j \right) y_i && \text{(definition of matrix-vector product)} \\
&= \sum_{i=1}^n \sum_{j=1}^n A_{ji} x_j y_i && \text{(symmetry of } A\text{)} \\
&= \sum_{j=1}^n x_j \sum_{i=1}^n (A_{ji} y_i) && \text{(rearranging)} \\
&= \sum_{j=1}^n x_j (Ay)_j && \text{(definition of matrix-vector product)} \\
&= \vec{x} \cdot A\vec{y} && \text{(definition of scalar product).}
\end{aligned}$$

Replacing all terms with complex value and the scalar product with the Hermitian product, we get a similar calculation:

$$\begin{aligned}
\langle A\vec{x}, \vec{y} \rangle &= \sum_{i=1}^n (A\vec{x})_i \bar{y}_i && \text{(definition of Hermitian product)} \\
&= \sum_{i=1}^n \left(\sum_{j=1}^n A_{ij} x_j \right) \bar{y}_i && \text{(definition of matrix-vector product)} \\
&= \sum_{i=1}^n \sum_{j=1}^n A_{ji} x_j \bar{y}_i && \text{(symmetry of } A\text{)} \\
&= \sum_{j=1}^n x_j \sum_{i=1}^n (A_{ji} \bar{y}_i) && \text{(rearranging)} \\
&= \sum_{j=1}^n x_j (\bar{A}\bar{y})_j && \text{(definition of matrix-vector product)} \\
&= \langle \vec{x}, \bar{A}\bar{y} \rangle && \text{(definition of Hermitian).}
\end{aligned}$$

This is quite unsatisfactory (note the extra bar on A in the final equation), and we would like something that generalises the idea of a symmetric matrix to the Hermitian product case too.

The key idea is to generalise the definition of matrix transpose to the complex setting:

Definition 6.4. For a complex n -matrix A , we write A^H for the **conjugate transpose** (also called the **Hermitian transpose**) given by

$$(A^H)_{ij} = \bar{A}_{ji} = \bar{A}^T.$$

If $A^H = A$, then we say that A is **Hermitian**.

Repeating the above calculations, we can see that if A is Hermitian then

$$\langle A\vec{x}, \vec{y} \rangle = \langle \vec{x}, A\vec{y} \rangle.$$

6.7 Summary

In this section, we introduced complex numbers and their algebraic and geometric representations. Key concepts include:

- Definition of complex numbers as combinations of real and imaginary parts.
- Arithmetic operations: addition, subtraction, multiplication, and division.
- Geometric interpretation in the complex plane.
- Complex conjugates and their role in division and modulus.
- Polar representation and argument of complex numbers.
- Application of complex numbers in solving polynomial equations.
- Extension to complex vectors and matrices, including Hermitian products and Hermitian matrices.

These concepts form the foundation for understanding eigenvalues and eigenvectors in the context of complex matrices.

7 Eigenvectors and eigenvalues

Module learning outcome:

Apply algorithms to compute eigenvectors and eigenvalues of large matrices.

This section of the notes will introduce our second big linear algebra problem. Throughout, we will be considering a square ($n \times n$) matrix.

7.1 Key definitions

For this problem, we will think of a matrix A acting on functions \vec{x} :

$$\vec{x} \mapsto A\vec{x}.$$

We are interested in when is the output vector $A\vec{x}$ is *parallel* to \vec{x} .

Definition 7.1. We say that any vector \vec{x} where $A\vec{x}$ is parallel is \vec{x} is called an *eigenvector* of A . Here by parallel, we mean that there exists a number λ (which can be positive, negative or zero, real or complex) such that

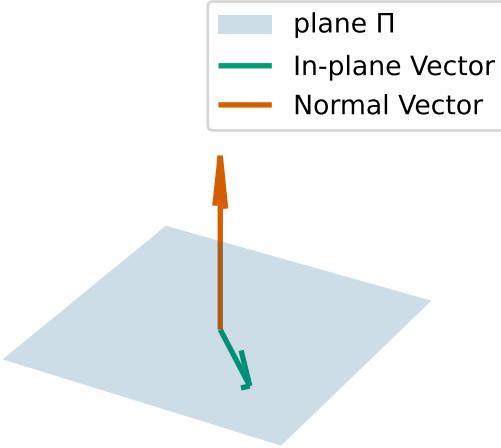
$$A\vec{x} = \lambda\vec{x}. \quad (7.1)$$

We call the associated number λ an *eigenvalue* of A .

We will later see that an $n \times n$ square matrix always has n eigenvalues (which may not always be distinct).

If $A\vec{x} = \vec{0}$, then \vec{x} is an eigenvector associated with the eigenvalue 0. In fact, we know that 0 is an eigenvalue of A if, and only if, A is singular.

Example 7.1. Let P be the 3x3 matrix that represents projection onto a plane $\Pi = \{\vec{x} \in \mathbb{R}^3 : \vec{a} \cdot \vec{x} = 0\}$ (i.e. P maps any point in \mathbb{R}^3 to its nearest point in Π). What are the eigenvalues and eigenvectors of P ?



- if \vec{x} is in the plane Π , then $P\vec{x} = \vec{x}$. This means that \vec{x} is an eigenvector and the associated eigenvalue is 1.
- if \vec{y} is perpendicular to the plane Π , then $P\vec{y} = \vec{0}$. this means that \vec{y} is an eigenvector and the associated eigenvalue is 0.

Let \vec{y} be perpendicular to Π (so that $P\vec{y} = \vec{0}$ and \vec{y} is an eigenvector of P), then for any number s , we can compute

$$P(s\vec{y}) = sP\vec{y} = s\vec{0} = \vec{0}.$$

This means that $s\vec{y}$ is also an eigenvector of P associated to the eigenvalue 0. As a consequence when we compute eigenvectors, we need to take care to *normalise* the vector to ensure we get a unique answer.

We end up with a two-dimensional space of eigenvectors (i.e., the plane Π) associated with eigenvalue 1 and a one-dimensional space of eigenvectors (i.e., the line perpendicular to Π) associated with the eigenvalue 0.

Example 7.2. Let A be the permutation matrix which takes an input two-vector and outputs a two-vector with the components swapped. The matrix is given by

$$A = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

What are the eigenvectors and eigenvalues of A ?

- Let $\vec{x} = (1, 1)^T$, then swapping the components of \vec{x} gives back the same vector \vec{x} . In equations, we can write $A\vec{x} = \vec{x}$. This means that \vec{x} is an eigenvector and the eigenvalue is 1.
- Let $\vec{x} = (-1, 1)^T$, then swapping the components of \vec{x} gives back $(1, -1)^T$ which we can see is $-\vec{x}$. In equations, we can write $A\vec{x} = -\vec{x}$. This means that \vec{x} is an eigenvector of A and the associated eigenvalue is -1 .

{.remark} If we take the product of all eigenvalues of a $n \times n$ matrix A , we get the determinant of the matrix A :

$$\det A = \lambda_1 \cdot \lambda_2 \cdots \lambda_n.$$

If we add up all the eigenvalues of a $n \times n$ matrix, we get the *trace* of the matrix A . We can also find the trace by adding up the diagonal components of the matrix:

$$\lambda_1 + \cdots + \lambda_n = a_{11} + a_{22} + \cdots + a_{nn} = \text{trace}(A).$$

Let A and B be two $n \times n$ matrices. Then, we cannot use the eigenvalues of A and B to work out the eigenvalues of $A + B$ or the eigenvalues of AB , in general. :::

7.2 How to find eigenvalues and eigenvectors

To compute eigenvalues and eigenvectors, we start from (7.1) and move everything to the left-hand side and use the identity matrix (I_n):

$$(A - \lambda I_n)\vec{x} = \vec{0}.$$

This tells us that if we want to find an eigenvalue of A , then we need to find a number λ such that $(A - \lambda I_n)$ can multiply a non-zero vector and give us back the zero-vector. This happens when $(A - \lambda I)$ is *singular* (Theorem 3.3).

As we saw earlier one way to test if a matrix is singular, is if the determinant is 0. This gives us a test we can use to determine eigenvalues:

$$\det(A - \lambda I_n) = 0. \tag{7.2}$$

In fact, this equation no longer depends on the eigenvector \vec{x} , and if we can find solutions λ to this equation then λ is an eigenvalue of A .

We call (7.2) the *characteristic equation* or *eigenvalue equation*. We will see that (7.2) gives us a degree n polynomial equation in λ .

Once we have found an eigenvalue by solving the characteristic equation for a value λ^* , we need to find a vector \vec{x} such that

$$(A - \lambda^*)\vec{x} = \vec{0}.$$

In general, this is possible using a variation of Gaussian elimination with pivoting, but we do not explore this method in this module.

Example 7.3. Let A be the matrix given by

$$A = \begin{pmatrix} 3 & 1 \\ 1 & 3 \end{pmatrix}.$$

Then, we can compute that

$$\begin{aligned} \det(A - \lambda I_n) &= \det \begin{pmatrix} 3 - \lambda & 1 \\ 1 & 3 - \lambda \end{pmatrix} \\ &= (3 - \lambda)(3 - \lambda) - 1 \times 1 \\ &= \lambda^2 + 6\lambda + 8. \end{aligned}$$

So we want to find values λ such that

$$\det(A - \lambda I_n) = \lambda^2 + 6\lambda + 8 = 0.$$

We can read off, by factorisation, that the values of λ are 4 and 2.

We can now start computing the associated eigenvectors.

To find the eigenvector associated with the eigenvalue 4. We see that

$$A - 4I_n = \begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix}.$$

We can identify that $(A - 4I_n)(1, 1)^T = \vec{0}$. So $(1, 1)$ is an eigenvector associated with 4.

To find the eigenvector associated with the eigenvalue 2. We see that

$$A - 2I_n = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}.$$

We can identify that $(A - 2I_n)(-1, 1)^T = \vec{0}$. So $(-1, 1)$ is an eigenvector associated with 2.

We note that this example is actually surprisingly similar to Example 7.2. We see that the eigenvectors are actually the same! We can see that the matrices are related too:

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} - 3I = \begin{pmatrix} 3 & 1 \\ 1 & 3 \end{pmatrix}.$$

So we can compute that if $A\vec{x} = \lambda\vec{x}$ then

$$(A + 3I)\vec{x} = \lambda\vec{x} + 3\vec{x} = (\lambda + 3)\vec{x}.$$

So we see that \vec{x} is also an eigenvector of A and the associated eigenvector is $\lambda + 3$.

Although this procedure gives us back eigenvalues there are cases where we have to be careful. We have seen one example above with a two-dimensional eigenspace associated with one eigenvector (Example 7.1). Here are two other cases we must be careful:

Example 7.4. Let Q denote the 2×2 matrix that rotates any vector by $\pi/2$ ($= 90^\circ$):

$$Q = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}.$$

Our intuition says that there can be no vectors that when rotated by $\pi/2$ give something parallel to the input vector, but we can still compute:

$$\det Q = \det \begin{pmatrix} -\lambda & -1 \\ 1 & -\lambda \end{pmatrix} = \lambda^2 + 1.$$

So we can find eigenvalues by finding the values λ such that

$$\lambda^2 + 1 = 0.$$

We saw in the section on Complex Numbers (Chapter 6) that the solutions to this equation are $\pm i$. This means that a general algorithm for finding eigenvalues and eigenvectors need to handle complex numbers too.

Example 7.5. Let A be the 2×2 matrix given by

$$A = \begin{pmatrix} 3 & 1 \\ 0 & 3 \end{pmatrix}.$$

If we follow our procedure above we get a single repeated eigenvalue 3.

Looking at the shifted matrix, $A - 3I_n$:

$$A - 3I_n = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}.$$

we can identify one eigenvector $(1, 0)^T$, but there is no other eigenvector (in a different direction)! Indeed, we can compute that:

$$(A - 3I_n) \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} y \\ 0 \end{pmatrix}.$$

This tells us that if $(A - 3I_n)(x, y)^T = \vec{0}$ if, and only if, $y = 0$. Thus all eigenvectors have the form $(x, 0)^T$ and point in the same direction as $(1, 0)^T$.

Exercise 7.1. Find the eigenvalues and eigenvectors for the matrix:

$$A = \begin{pmatrix} 9 & -2 \\ -2 & 6 \end{pmatrix}.$$

Example 7.6 (Eigenvalues and eigenvectors of a triangular matrix). Consider an upper triangular matrix (Example 3.7). When forming the characteristic equation, we see that most terms are simply zero:

$$\begin{aligned} & \det \begin{pmatrix} 3-\lambda & 2 \\ 0 & 1-\lambda \end{pmatrix} \\ &= (3-\lambda)(1-\lambda) - 2 \times 0 = (3-\lambda)(1-\lambda) \\ & \det \begin{pmatrix} 3-\lambda & 2 & 4 \\ 0 & 1-\lambda & -1 \\ 0 & 0 & 2-\lambda \end{pmatrix} \\ &= (3-\lambda)((1-\lambda)(2-\lambda) - (-1) \times 0) - 2(0(2-\lambda) - (-1 \times 0)) + 4(0 \times 0 - 1 \times 0) \\ &= (3-\lambda)(1-\lambda)(2-\lambda). \end{aligned}$$

Indeed this is true in general,

$$\begin{aligned} \det(A - \lambda I_n) &= \det \begin{pmatrix} a_{11} - \lambda & a_{12} & a_{13} & \cdots & a_{1n} \\ 0 & a_{22} - \lambda & a_{23} & \cdots & a_{2n} \\ 0 & 0 & a_{33} - \lambda & \cdots & a_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & a_{nn} - \lambda \end{pmatrix} \\ &= \prod_{i=1}^n (a_{ii} - \lambda). \end{aligned}$$

So we can read off that the eigenvalues of an upper triangular matrix are simply the diagonal coefficients.

We can see the eigenvectors are the coordinate directions:

$$\begin{aligned} \begin{pmatrix} 3 & 2 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} &= \begin{pmatrix} 3 \\ 0 \end{pmatrix} \\ \begin{pmatrix} 3 & 2 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} &= \begin{pmatrix} 0 \\ 1 \end{pmatrix} \end{aligned}$$

7.3 Important theory

We have established a way to identify eigenvalues and eigenvectors for an arbitrary square matrix. This method can be used to prove the existence of eigenvalues.

Theorem 7.1. *Any square $n \times n$ matrix has n complex eigenvalues (possibly not distinct).*

Proof. For any matrix the characteristic equation (7.2) is a degree n polynomial. The Fundamental Theorem of Algebra (Theorem 6.1) tells us that any degree n polynomial has n roots over the complex numbers. The n roots of the characteristic equation are the n eigenvalues. \square

The Abel-Ruffini theorem states that there is no solution in the radicals for a general polynomial of degree 5 or higher with arbitrary coefficients. This implies that there is no ‘nice’ closed form for roots of polynomials of degree 5 or higher. So, if we want an algorithm to find eigenvalues and eigenvectors of larger matrices then we need to do something else!

Let’s suppose that we have an $n \times n$ matrix A and we have found n eigenvectors and n eigenvalues (all distinct). Let’s call the eigenvectors by $\vec{x}_1, \dots, \vec{x}_n$ and the eigenvalues $\lambda_1, \dots, \lambda_n$ then we have the equation:

$$A\vec{x}_j = \lambda_j \vec{x}_j.$$

So if we form the matrices S to have columns equal to each eigenvector in turn and Λ (pronounced lambda) to be the diagonal matrix with the eigenvalues listed along the diagonal we see that we have:

$$AS = S\Lambda.$$

If S is invertible, we can multiply on the right by S^{-1} to see that we have

$$A = S\Lambda S^{-1}. \quad (7.3)$$

This formula shows another factorisation of the matrix A into simpler matrices, very much like we had when we computed the LU-factorisation matrix (Section 4.7).

The equation (7.3) is an example of a more general idea of *similar matrices*. We say that two matrices A and B are similar if there exists an invertible $n \times n$ matrix P such that

$$B = P^{-1}AP.$$

Since P is invertible, we can pre-multiply this equation by P and post-multiply by P^{-1} and see that being similar is a symmetric property.

Lemma 7.1. *The matrix A is similar to the diagonal matrix Λ formed by the eigenvalues of A .*

Proof. From (7.3), we have that

$$\Lambda = S^{-1}AS.$$

□

This leads to a nice theorem which we will use to help compute eigenvectors and eigenvalues of larger matrices:

Theorem 7.2. *If A and B are similar matrices then A and B have the same eigenvalues.*

Proof. We start by writing $B = P^{-1}AP$. Then we can compute that

$$BP^{-1} = P^{-1}A. \quad (7.4)$$

Let λ be an eigenvalue of A with eigenvector \vec{x} and write $\vec{y} = P^{-1}\vec{x}$. Then we have that

$$\begin{aligned} B\vec{y} &= BP^{-1}\vec{x} && (\text{definition of } \vec{y}) \\ &= P^{-1}A\vec{x} && (\text{from (7.4)}) \\ &= P^{-1}(\lambda\vec{x}) && (\text{since } \vec{x} \text{ is an eigenvector}) \\ &= \lambda P^{-1}\vec{x} && (\text{rearranging}) \\ &= \lambda\vec{y} && (\text{definition of } \vec{y}). \end{aligned}$$

This shows that any eigenvalue of A is an eigenvalue of B . It also gives a formula for how eigenvectors change between A and B .

To show any eigenvalue of B is an eigenvalue of A , we repeat the calculation with A and B swapped. \square

The key idea of the methods we will use to compute eigenvalues to apply a sequence of matrices to convert a matrix A into a form similar to A for which reading off the eigenvalues is easier. However, the quality of the algorithms we apply depend heavily on properties of the matrix A .

7.4 Why symmetric matrices are nice

Whilst all our methods are developed for complex matrices, when we restrict to real-valued symmetric matrices, we have this nice result.

Theorem 7.3. *Let A be a symmetric matrix ($A^T = A$) with real entries. Then A has n real eigenvalues (zero imaginary part) and any distinct eigenvectors are orthogonal.*

Proof. Let λ be an eigenvalue of A with eigenvector \vec{x} . Recall that $\vec{x} \neq 0$. Then, since A has real values, we can compute that:

$$(\bar{A}\vec{x})_i = \left(\sum_{j=1}^n \bar{A}_{ji}x_i \right) = \sum_{j=1}^n A_{ji}\bar{x}_i = (A\bar{\vec{x}})_i.$$

We also note that any real, symmetric matrix is automatically Hermitian.

Then we see that

$$\begin{aligned}
\lambda \langle \vec{x}, \vec{x} \rangle &= \langle (\lambda \vec{x}), \vec{x} \rangle && \text{(from definition of Hermitian product)} \\
&= \langle (A \vec{x}), \vec{x} \rangle && \text{(definition of eigenvalue and eigenvector)} \\
&= \langle \vec{x}, A \vec{x} \rangle && \text{(symmetry of } A) \\
&= \langle \vec{x}, \lambda \vec{x} \rangle && \text{(definition of eigenvalue and eigenvector)} \\
&= \bar{\lambda} \langle \vec{x}, \vec{x} \rangle && \text{(from definition of Hermitian product).}
\end{aligned}$$

Since, $\langle \vec{x}, \vec{x} \rangle > 0$ (recall $\vec{x} \neq 0$), we can divide by $\langle \vec{x}, \vec{x} \rangle$ so infer that

$$\lambda = \bar{\lambda}.$$

Next, let \vec{x} and \vec{y} be eigenvectors of A with distinct, eigenvalues λ and μ , respectively. From the first part of the proof, we know that λ and μ are real. We compute that

$$\begin{aligned}
\lambda \langle \vec{x}, \vec{y} \rangle &= \langle \lambda \vec{x}, \vec{y} \rangle \\
&= \langle A \vec{x}, \vec{y} \rangle \\
&= \langle \vec{x}, A^H \vec{y} \rangle \\
&= \langle \vec{x}, A \vec{y} \rangle \\
&= \langle \vec{x}, \mu \vec{y} \rangle \\
&= \bar{\mu} \langle \vec{x}, \vec{y} \rangle \\
&= \mu \langle \vec{x}, \vec{y} \rangle.
\end{aligned}$$

Subtracting the right-hand side from the left hand side we see that

$$(\lambda - \mu) \langle \vec{x}, \vec{y} \rangle = 0.$$

This implies that if λ and μ are distinct, then $\langle \vec{x}, \vec{y} \rangle = 0$. \square

Corollary 7.1. *Let A be a symmetric $n \times n$ matrix with real entries. Then the eigenvectors of A form a basis of \mathbb{R}^n .*

Proof. We can only give an incomplete proof of this result. We will show that the eigenvectors are linearly independent. The proof is completed by showing that if you have any n linearly independent vectors in \mathbb{R}^n then you must have a basis.

Denote by $\vec{x}^{(1)}, \dots, \vec{x}^{(n)}$ the n eigenvectors of A . We want to show that the eigenvectors are linearly independent. Suppose that we have real numbers $\alpha_1, \alpha_2, \dots, \alpha_n$ such that:

$$\sum_{i=1}^n \alpha_i \vec{x}^{(i)} = \vec{0}. \tag{7.5}$$

To show the eigenvectors are linearly independent, we need to show that all $\alpha_i = 0$. We can do this by taking the inner product of (7.5) with $\vec{x}^{(j)}$ for *any* j :

$$0 = \vec{0} \cdot \vec{x}^{(j)} = \left(\sum_{i=1}^n \alpha_i \vec{x}^{(i)} \right) \cdot \vec{x}^{(j)} = \sum_{i=1}^n \alpha_i (\vec{x}^{(i)} \cdot \vec{x}^{(j)}) = \alpha_j \vec{x}^{(j)} \cdot \vec{x}^{(j)}.$$

Since we have that $|\vec{x}^{(j)}| > 0$, we have $\alpha_j = 0$ and we have shown that the eigenvectors are linearly independent. \square

8 Eigenvectors and eigenvalues: practical solutions

Tip

Module learning outcome: apply algorithms to compute eigenvectors and eigenvalues of large matrices.

In the previous lecture, we defined the eigenvalue problem for a matrix A : Finding numbers λ (eigenvalues) and vectors \vec{x} (eigenvectors) which satisfy the equation:

$$A\vec{x} = \lambda\vec{x}. \quad (8.1)$$

We saw one starting point for finding eigenvalues is to find the roots of the characteristic equation: a polynomial of degree n for an $n \times n$ matrix A . However, we have already seen that this approach will be infeasible for large matrices. Instead, we will find a sequence of similar matrices to A such that we can read off the eigenvalues from the final matrix.

In equations, we can say our “grand strategy” is to find a sequence of matrices P_1, P_2, \dots to form a sequence of matrices:

$$A, P_1^{-1}AP, P_2^{-1}P_1^{-1}AP_1P_2, P_3^{-1}P_2^{-1}P_1^{-1}AP_1P_2P_3, \dots \quad (8.2)$$

We aim to get all the way to a simple matrix where we read off the eigenvalues and eigenvectors.

For example, if at level m , say, we have transformed A into a diagonal matrix the eigenvalues are the diagonal of the matrix

$$P_m^{-1}P_{m-1}^{-1} \cdots P_2^{-1}P_1^{-1}AP_1P_2 \cdots P_{m-1}P_m,$$

and the eigenvectors are the columns of the matrix

$$S_m = P_1P_2 \cdots P_{m-1}P_m.$$

We have seen a similar example for upper triangular matrices (Example 7.6).

Remark 8.1. In the example below, and many others, we see that we typically want the matrices P_j to be **orthogonal** or **orthonormal**.

A (real-valued) matrix Q is orthogonal if $Q^T Q$ is diagonal and a (real-valued) matrix Q is orthonormal if $Q^T Q = I_n$.

In other words, if denote by $\vec{q}^{(1)}, \dots, \vec{q}^{(n)}$ the columns of Q , then Q is orthogonal if

$$\vec{q}^{(i)} \cdot \vec{q}^{(j)} = 0 \quad \text{if } i \neq j,$$

and Q is orthonormal if

$$\vec{q}^{(i)} \cdot \vec{q}^{(j)} = \begin{cases} 0 & \text{if } i \neq j \\ 1 & \text{if } i = j. \end{cases}$$

Orthonormal matrices have the nice property that $Q^{-1} = Q^T$ so we can very easily compute their inverse! They also always have a determinant of 1. Importantly, we can apply them (or their inverses) without worrying about adding extra problems from finite precision.

Examples of orthonormal matrices include matrices which describe rotations.

Exercise 8.1. Show that the rotation matrix $R(\theta)$ from Example 1.3 is orthonormal.

8.1 QR algorithm

The QR algorithm is an iterative method for computing eigenvalues and eigenvectors. At each step a matrix is factored into a product in a similar fashion to LU factorisation (Section 4.7). In this case, we factor a matrix, A into a product of an orthonormal matrix, Q , and an upper triangular matrix, R :

$$A = QR.$$

This is *QR factorisation*.

Given a matrix A , the algorithm repeatedly applies QR factorisation. First, we set $A^{(0)} = A$, then we successively perform for $k = 0, 1, 2, \dots$:

1. Compute the QR factorisation of $A^{(k)}$ into an orthonormal part and upper triangular part

$$A^{(k)} = Q^{(k)} R^{(k)};$$

2. Update the matrix $A^{(k+1)}$ recombining Q and R in the reverse order:

$$A^{(k+1)} = R^{(k)} Q^{(k)}.$$

As we take more and more steps, we hope that $A^{(k)}$ converges to an upper triangular matrix whose diagonal entries are the eigenvalues of the original matrix.

Rearranging the first step within each iteration, we see that

$$R^{(k)} = (Q^{(k)})^{-1} A^{(k)} = (Q^{(k)})^T A^{(k)}.$$

Substituting this value of $R^{(k)}$ into the second step gives

$$A^{(k+1)} = (Q^{(k)})^{-1} A^{(k)} Q^{(k)},$$

and we see that at each step we are finding a sequence of similar matrices, all with the same eigenvalues (Theorem 7.2). We can additionally find the eigenvectors of A by forming the product

$$Q = Q^{(1)} Q^{(2)} \cdots Q^{(m)}.$$

The hard part of the method is computing the QR factorisation. One classical way to get a QR factorisation is to use the Gram-Schmidt process. In general, the Gram-Schmidt process is used to take a sequence of vectors and form a new sequence which is orthonormal. We can apply this to the columns of A to form an orthonormal matrix. If we track this process as a matrix-matrix product, we find that the other factor is upper triangular.

8.1.1 The Gram-Schmidt process

The key idea is shown in Figure 8.1. Given a vector \vec{a} (blue) and a vector \vec{q} (green) with length 1. We can compute the projection of \vec{a} onto the direction \vec{q} (orange) by

$$(\vec{a} \cdot \vec{q})\vec{q}.$$

If we subtract this term from \vec{a} . We end up with a vector \vec{u} with $\vec{u} \cdot \vec{q} = 0$. The difference \vec{u} is given by

$$\vec{u} = \vec{a} - (\vec{a} \cdot \vec{q})\vec{q},$$

and we can compute that

$$\begin{aligned} \vec{u} \cdot \vec{q} &= (\vec{a} - (\vec{a} \cdot \vec{q})\vec{q}) \cdot \vec{q} \\ &= (\vec{a} \cdot \vec{q}) - (\vec{a} \cdot \vec{q})(\vec{q} \cdot \vec{q}) && \text{(properties of scalar product)} \\ &= (\vec{a} \cdot \vec{q}) - (\vec{a} \cdot \vec{q}) && \text{(since } \|\vec{q}\| = 1\text{)} \\ &= 0. \end{aligned}$$

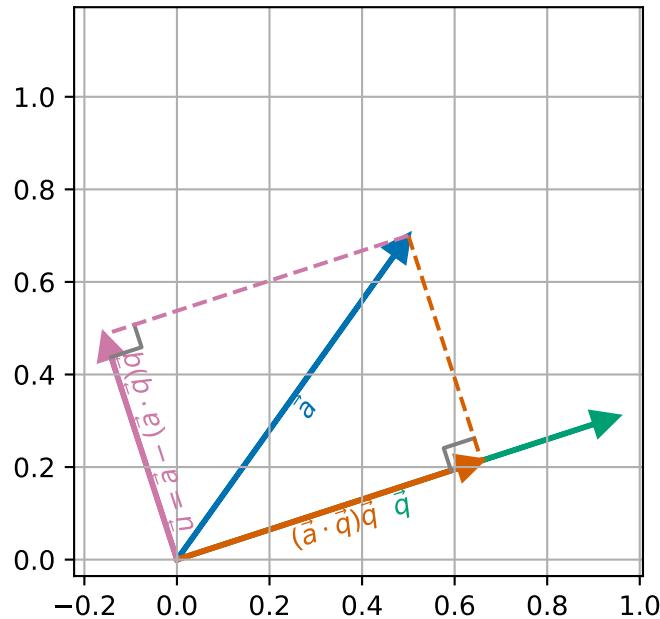
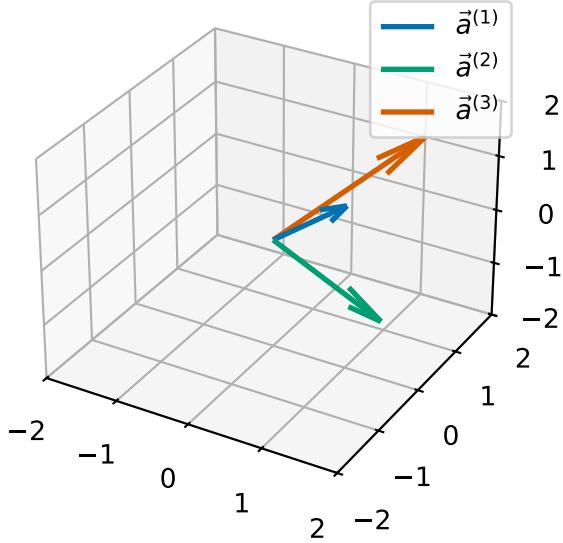


Figure 8.1: Projection of \vec{a} away from \vec{q} onto \vec{u} .

Example 8.1. Consider the sequence of vectors

$$\vec{a}^{(1)} = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \vec{a}^{(2)} = \begin{pmatrix} 2 \\ -1 \\ 0 \end{pmatrix}, \vec{a}^{(3)} = \begin{pmatrix} 1 \\ 2 \\ 1 \end{pmatrix}.$$

We will manipulate these vectors to form three orthonormal vectors.



First, we set $\vec{q}^{(1)} = \vec{a}^{(1)} / \|\vec{a}^{(1)}\|$:

$$\|\vec{a}^{(1)}\| = \sqrt{1^2 + 0^2 + 1^2} = \sqrt{2},$$

so

$$\vec{q}^{(1)} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix}.$$

Second, we want to find $\vec{q}^{(2)}$ which must satisfy that $\vec{q}^{(2)} \cdot \vec{q}^{(1)} = 0$. We can do this by subtracting from $\vec{a}^{(2)}$ the portion of $\vec{a}^{(2)}$ which points in the direction $\vec{q}^{(1)}$. We call this $\vec{u}^{(2)}$:

$$\begin{aligned} \vec{u}^{(2)} &= \vec{a}^{(2)} - (\vec{a}^{(2)} \cdot \vec{q}^{(1)}) \vec{q}^{(1)} \\ &= \begin{pmatrix} 2 \\ -1 \\ 0 \end{pmatrix} - \left(\begin{pmatrix} 2 \\ -1 \\ 0 \end{pmatrix} \cdot \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix} \right) \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix} \\ &= \begin{pmatrix} 2 \\ -1 \\ 0 \end{pmatrix} - \frac{2}{\sqrt{2}} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix} \\ &= \begin{pmatrix} 2 - \frac{2}{\sqrt{2}} \frac{1}{\sqrt{2}} \\ -1 - \frac{2}{\sqrt{2}} 0 \\ 0 - \frac{2}{\sqrt{2}} \frac{1}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} 1 \\ -1 \\ -1 \end{pmatrix}. \end{aligned}$$

We then normalise $\vec{u}^{(2)}$ to get a unit-length vector $q^{(2)}$:

$$\vec{q}^{(2)} = \vec{u}^{(2)} / \|\vec{u}^{(2)}\| = \begin{pmatrix} \frac{1}{\sqrt{3}} \\ \frac{-1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \\ \frac{-1}{\sqrt{3}} \end{pmatrix}.$$

Third, we will find $q^{(3)}$ which we need to check satisfies $\vec{q}^{(3)} \cdot \vec{q}^{(2)} = 0$ and $\vec{q}^{(3)} \cdot \vec{q}^{(1)} = 0$. We can do this by subtracting from $\vec{a}^{(3)}$ the portion of $\vec{a}^{(3)}$ which points in the direction $\vec{q}^{(1)}$ and the portion of $\vec{a}^{(3)}$ which points in the direction $\vec{q}^{(2)}$. We call this term $\vec{u}^{(3)}$

$$\begin{aligned} \vec{u}^{(3)} &= \vec{a}^{(3)} - (\vec{a}^{(3)} \cdot \vec{q}^{(1)}) \vec{q}^{(1)} - (\vec{a}^{(3)} \cdot \vec{q}^{(2)}) \vec{q}^{(2)} \\ &= \begin{pmatrix} 1 \\ 2 \\ 1 \end{pmatrix} - \left(\begin{pmatrix} 1 \\ 2 \\ 1 \end{pmatrix} \cdot \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix} \right) \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix} - \left(\begin{pmatrix} 1 \\ 2 \\ 1 \end{pmatrix} \cdot \begin{pmatrix} \frac{1}{\sqrt{3}} \\ \frac{-1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \end{pmatrix} \right) \begin{pmatrix} \frac{1}{\sqrt{3}} \\ \frac{-1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \end{pmatrix} \\ &= \begin{pmatrix} 1 \\ 2 \\ 1 \end{pmatrix} - \left(\frac{2}{\sqrt{2}} \right) \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix} - \left(\frac{-2}{\sqrt{3}} \right) \begin{pmatrix} \frac{1}{\sqrt{3}} \\ \frac{-1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \end{pmatrix} \\ &= \begin{pmatrix} 1 \\ 2 \\ 1 \end{pmatrix} - \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} - \begin{pmatrix} -2/3 \\ 2/3 \\ 2/3 \end{pmatrix} = \begin{pmatrix} 2/3 \\ 4/3 \\ -2/3 \end{pmatrix}. \end{aligned}$$

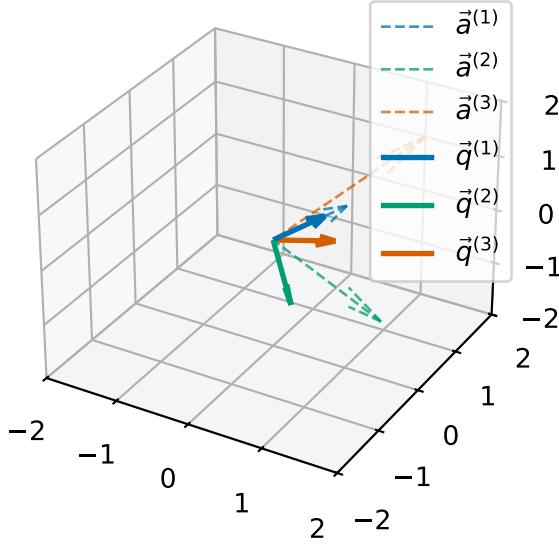
Again, we normalise $\vec{u}^{(3)}$ to get $\vec{q}^{(3)}$:

$$\begin{aligned} \|\vec{u}^{(3)}\| &= \sqrt{(2/3)^2 + (4/3)^2 + (-2/3)^2} = \sqrt{4/9 + 16/9 + 4/9} = \sqrt{24/9} \\ &= \frac{2}{3}\sqrt{6}, \end{aligned}$$

so

$$\vec{q}^{(3)} = \begin{pmatrix} \frac{1}{\sqrt{6}} \\ \frac{2}{\sqrt{6}} \\ \frac{-1}{\sqrt{6}} \end{pmatrix}.$$

Exercise 8.2. Verify the orthonormality conditions for $\vec{q}^{(1)}, \vec{q}^{(2)}$ and $\vec{q}^{(3)}$.



Now we have applied the Gram-Schmidt process to convert from the vectors $\vec{a}^{(j)}$ to the vectors $\vec{q}^{(j)}$. We can consider the matrix Q whose columns are the vectors $\vec{q}^{(j)}$ and the matrix A whose columns are the vectors $\vec{a}^{(j)}$:

$$Q = \begin{pmatrix} \vec{q}^{(1)} & \vec{q}^{(2)} & \vec{q}^{(3)} \end{pmatrix} \quad \text{and} \quad A = \begin{pmatrix} \vec{a}^{(1)} & \vec{a}^{(2)} & \vec{a}^{(3)} \end{pmatrix}$$

Then we can compute that

$$(Q^T A)_{ij} = \vec{q}^{(j)} \cdot \vec{a}^{(i)}.$$

So

$$\begin{aligned} (Q^T A) &= \begin{pmatrix} (1, 0, 1)^T \cdot (\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}})^T & (2, -1, 0)^T \cdot (\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}})^T & (1, 2, 1)^T \cdot (\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}})^T \\ (1, 0, 1)^T \cdot (\frac{1}{\sqrt{3}}, \frac{-1}{\sqrt{3}}, \frac{-1}{\sqrt{3}})^T & (2, -1, 0)^T \cdot (\frac{1}{\sqrt{3}}, \frac{-1}{\sqrt{3}}, \frac{-1}{\sqrt{3}})^T & (1, 2, 1)^T \cdot (\frac{1}{\sqrt{3}}, \frac{-1}{\sqrt{3}}, \frac{-1}{\sqrt{3}})^T \\ (1, 0, 1)^T \cdot (\frac{1}{\sqrt{6}}, \frac{2}{\sqrt{6}}, \frac{-1}{\sqrt{6}})^T & (2, -1, 0)^T \cdot (\frac{1}{\sqrt{6}}, \frac{2}{\sqrt{6}}, \frac{-1}{\sqrt{6}})^T & (1, 2, 1)^T \cdot (\frac{1}{\sqrt{6}}, \frac{2}{\sqrt{6}}, \frac{-1}{\sqrt{6}})^T \end{pmatrix} \\ &= \begin{pmatrix} \frac{2}{\sqrt{2}} & \frac{2}{\sqrt{2}} & \frac{2}{\sqrt{2}} \\ 0 & \frac{3}{\sqrt{3}} & \frac{-2}{\sqrt{3}} \\ 0 & 0 & \frac{4}{\sqrt{6}} \end{pmatrix}. \end{aligned}$$

Hence we have found an upper triangular matrix $R = Q^T A$. Since Q is orthonormal, we know $Q^{-1} = Q^T$ and we have a factorisation:

$$A = QR.$$

Exercise 8.3. Continue the QR-factorisation process by computing $B = RQ$ and apply the Gram-Schmidt process to the columns of B .

Remark. The Gram-Schmidt algorithm relies on the fact that after each projection there should be something left - i.e. $\vec{u}^{(j)}$ should be non-zero. If $\vec{a}^{(j)}$ is in the span of $\{\vec{q}^{(1)}, \dots, \vec{q}^{(j-1)}\}$, then the projection onto $\vec{u}^{(j)}$ will give $\vec{0}$. There are a few ways to test this, but the key idea is that if A is non-singular then we will always have $\vec{u}^{(j)} \neq \vec{0}$ – at least in exact-precision calculations...

8.1.2 Python QR factorisation using Gram-Schmidt

```

1 def gram_schmidt_qr(A):
2     """
3         Compute the QR factorisation of a square matrix using the classical
4         Gram-Schmidt process.
5
6     Parameters
7     -----
8     A : numpy.ndarray
9         A square 2D NumPy array of shape ``(n, n)`` representing the input
10        matrix.
11
12    Returns
13    -----
14    Q : numpy.ndarray
15        Orthonormal matrix of shape ``(n, n)`` where the columns form an
16        orthonormal basis for the column space of A.
17    R : numpy.ndarray
18        Upper triangular matrix of shape ``(n, n)``.
19    """
20    n, m = A.shape
21    if n != m:
22        raise ValueError(f"the matrix A is not square, {A.shape=}")
23
24    Q = np.empty_like(A)
25    R = np.zeros_like(A)
26
27    for j in range(n):
28        # Start with the j-th column of A
29        u = A[:, j].copy()
30
31        # Orthogonalize against previous q vectors
32        for i in range(j):
33            R[i, j] = np.dot(Q[:, i], A[:, j]) # projection coefficient
34            u -= R[i, j] * Q[:, i] # subtract the projection

```

```

35
36     # Normalize u to get q_j
37     R[j, j] = np.linalg.norm(u)
38     Q[:, j] = u / R[j, j]
39
40     return Q, R

```

Let's test it without our example above:

```

A = [ 1.0,  2.0,  1.0 ]
      [ 0.0, -1.0,  2.0 ]
      [ 1.0,  0.0,  1.0 ]
QR factorisation:
Q = [ 0.70711,  0.57735,  0.40825 ]
      [ 0.00000, -0.57735,  0.81650 ]
      [ 0.70711, -0.57735, -0.40825 ]
R = [ 1.41421,  1.41421,  1.41421 ]
      [ 0.00000,  1.73205, -1.15470 ]
      [ 0.00000,  0.00000,  1.63299 ]
Have we computed a factorisation? (A == Q @ R?) True
Is Q orthonormal? (Q.T @ Q == np.eye(3)) True

```

8.2 Finding eigenvalues and eigenvectors

The algorithm given above says that we use the QR factorisation to iteratively find a sequence of matrices $A^{(j)}$ which *should* converge to an upper-triangular matrix.

```

1 def gram_schmidt_eigen(A, maxiter=100, verbose=False):
2     """
3         Compute the eigenvalues and eigenvectors of a square matrix using the QR
4         algorithm with classical Gram-Schmidt QR factorisation.
5
6         This function implements the basic QR algorithm:
7
8         1. Factorise the matrix `A` into `Q` and `R` using Gram-Schmidt QR
9             factorisation.
10        2. Update the matrix as:
11
12            .. math::
13                A_{\{k+1\}} = R_k Q_k

```

```

14
15     3. Accumulate the orthonormal transformations in `V` to compute the
16        eigenvectors.
17     4. Iterate until `A` becomes approximately upper triangular or until the
18        maximum number of iterations is reached.
19
20 Once the iteration converges, the diagonal of `A` contains the eigenvalues,
21 and the columns of `V` contain the corresponding eigenvectors.
22
23 Parameters
24 -----
25 A : numpy.ndarray
26     A square 2D NumPy array of shape `` $(n, n)$ `` representing the input
27     matrix. This matrix will be **modified in place** during the
28     computation.
29 maxiter : int, optional
30     Maximum number of QR iterations to perform. Default is 100.
31 verbose : bool, optional
32     If ``True``, prints intermediate matrices (`A`, `Q`, `R`, and `V`) at
33     each iteration. Useful for debugging and understanding convergence.
34     Default is ``False``.
35
36 Returns
37 -----
38 eigenvalues : numpy.ndarray
39     A 1D NumPy array of length `` $n$ `` containing the eigenvalues of `A`.
40     These are the diagonal elements of the final upper triangular matrix.
41 V : numpy.ndarray
42     A 2D NumPy array of shape `` $(n, n)$ `` whose columns are the normalized
43     eigenvectors corresponding to the eigenvalues.
44 it : int
45     The number of iterations taken by the algorithm.
46 """
47 # identity matrix to store eigenvectors
48 V = np.eye(A.shape[0])
49
50 if verbose:
51     print_array(A)
52
53 it = -1
54 for it in range(maxiter):
55     if verbose:

```

```

56     print(f"\n\n{it}"))
57
58     # perform factorisation
59     Q, R = gram_schmidt_qr(A)
60     if verbose:
61         print_array(Q)
62         print_array(R)
63
64     # update A and V in place
65     A = R @ Q
66     V = V @ Q
67
68     if verbose:
69         print_array(A)
70         print_array(V)
71
72     # test for convergence: is A upper triangular up to tolerance 1.0e-8?
73     if np.allclose(A, np.triu(A), atol=1.0e-8):
74         break
75
76     eigenvalues = np.diag(A)
77     return eigenvalues, V, it

```

We test this out in code first for the matrix from Example 7.3:

```

1 A = np.array([[3.0, 1.0], [1.0, 3.0]])
2 print_array(A)
3
4 eigenvalues, eigenvectors, it = gram_schmidt_eigen(A)
5 print_array(eigenvalues)
6 print_array(eigenvectors)
7 print("iterations required:", it)

```

```

A = [ 3.0,  1.0 ]
      [ 1.0,  3.0 ]
eigenvalues = [ 4.0 ]
              [ 2.0 ]
eigenvectors = [  0.7071, -0.7071 ]
                  [  0.7071,  0.7071 ]
iterations required: 27

```

These values agree with those from Example 7.3. Note that this code normalises the eigenvectors to have length one, so we have slightly different values for the eigenvectors but still in the same directions.

8.3 Correctness and convergence

Let's see what happens when we try this same approach for a bigger symmetric matrices. Here we have a test that samples ten different random matrices and computes the average number of iterations, average run time and maximum error in the eigenvalue equation.

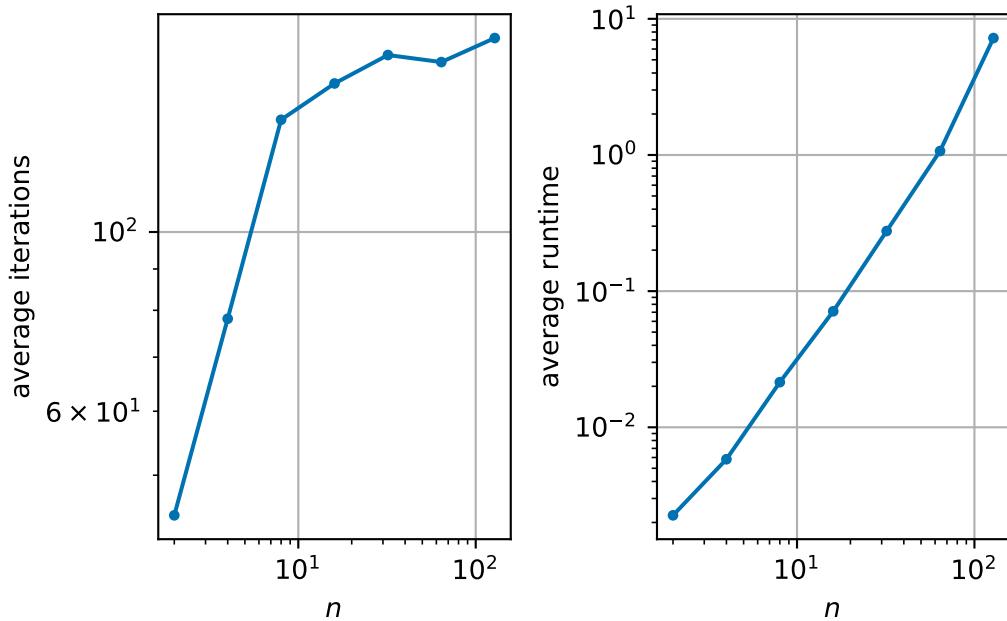
```
1 # replicable random seed
2 np.random.seed(42)
3
4
5 def test_accuracy_of_eigensolve(A, eigenvalues, eigenvectors):
6     """
7         test accuracy of solution of eigenvalue problem
8     """
9     residuals = []
10    for i in range(len(eigenvalues)):
11        residual = np.linalg.norm(
12            A @ eigenvectors[:, i] - eigenvalues[i] * eigenvectors[:, i]
13        )
14        residuals.append(residual)
15    return max(residuals)
16
17
18 # replicable seed
19 repeats = 10
20
21 # restart the seed
22 np.random.seed(42)
23
24
25 def random_symmetric_matrix(n):
26     # generate a random matrix
27     S = special_ortho_group.rvs(n)
28     D = np.diag(np.random.randint(1, 10, (n,)) / 2)
29     A = S.T @ D @ S
30     return A
31
```

```

32
33 print("size  time (s)      iter  error")
34
35 n_values = [2**j for j in range(1, 8)]
36 it_values = []
37 runtime_values = []
38
39 for n in n_values:
40     runtime = 0.0
41     total_its = 0
42     max_error = 0.0
43
44     for _ in range(repeats):
45         # generate new random matrix
46         A = random_symmetric_matrix(n)
47
48         # do and time the solve, ensure converged
49         maxiter = 1000_000
50         start = time.perf_counter()
51         eigenvalues, eigenvectors, it = gram_schmidt_eigen(A, maxiter=maxiter)
52         end = time.perf_counter()
53
54         if it == maxiter - 1:
55             # skip
56             continue
57
58         # store the data
59         runtime += end - start
60         total_its += it
61         max_error = max(
62             max_error,
63             test_accuracy_of_eigensolve(A, eigenvalues, eigenvectors),
64         )
65
66         runtime /= repeats
67         average_it = total_its / repeats
68
69         it_values.append(average_it)
70         runtime_values.append(runtime)
71
72 print(f"{n:4d}  {runtime:.6e}  {average_it:5.1f}  {max_error:.6e}")

```

size	time (s)	iter	error
2	2.256768e-03	44.6	9.319111e-09
4	5.824034e-03	78.1	9.895223e-09
8	2.144682e-02	137.7	1.212740e-08
16	7.111746e-02	152.7	1.346641e-08
32	2.763023e-01	165.6	1.246268e-08
64	1.069227e+00	162.3	1.646202e-08
128	7.222554e+00	173.8	1.478504e-08



We see that the method converges very well with a good low accuracy.