Numerical Methods

Xuemei Chen

New Mexico State University

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Notations

Before this course, you need to be familiar with

- Calculus I
- Calculus II: Integrations. Sequences and Series.
- It is not necessary, but helpful to know some multivariate Calculus
- Some basic Linear Algebra.

Notations

- $\{x|$ descriptions of $x\}$ is the set of all x that meets the description after the ":" sign. For example, $\{x|x^2-1<0\}$ is the set of all number x such that $x^2-1<0$. We can solve this inequality further and see that $\{x|x^2-1<0\}=(-1,1)$

  Remark: Some books use colon instead of verticle bar as $\{x:$ descriptions of $x\}$
- $\in$: belongs to/is contained in. For example, $a\in\{x|x^2-1<0\}$ means that a is a number satisfying $a^2-1<0$.
- A vector in $\mathbb{R}^n$ is a column vector in default.
- In all exercises at the end of each chapter, * means extra credit problems.

Chapter 1

Floating Point Arithmetic

The arithmetic performed by a calculator or computer is different from the arithmetic that we use in our algebra or calculus class. In the ideal world, we permit numbers with an infinite number of digits. For example, $\sqrt{2}$ is the unique positive number that, when multiplied by itself, produces the integer 2. It is an irrational number, which means that there are infinitely many digits associated with $\sqrt{2}$ when represented in decimals. In the computational world, we are only able to assign a fixed and finite number of digits to each number.

Try add up 0.1 and 0.2 in Python, you will get

```
>>> 0.1 + 0.2
0.30000000000000004
```

This can cause serious issues and create bugs. See Section 5.1 of [2]. The above error is caused by rounding in floating point numbers, with which numerical analysis is traditionally concerned.

1.1 Floating Point Representation

Floating point numbers are represented in terms of a base β, a precision p, and an exponent e. For example, in base 10, 0.34 can be represented as 3.4×10^{-1} or 34×10^{-2}. In order to guarantee uniqueness, we take a floating point number to have the specific form.

$$\pm \left(d_0 + d_1\beta^{-1} + \cdots + d_{p-1}\beta^{-(p-1)}\right) \times \beta^e, \tag{1.1}$$

where each d_i is an integer in $[0, \beta)$ and $d_0 \neq 0$. Such a representation is said to be a *normalized floating point number*. In this representation, $d_0 + d_1\beta^{-1} + \cdots + d_{p-1}\beta^{-(p-1)}$ is called *mantissa* (or *significand*). Here are a few examples where $\beta = 10, p = 5$ and e is in the range $-10 \leq e \leq 10$:

$$1.2345 \times 10^8, \qquad 3.4000 \times 10^{-2}, \qquad -5.6780 \times 10^5$$

In the above examples, we are using base $\beta = 10$ to ease into the material. Computers work more naturally in binary (base 2). When $\beta = 2$, each digit d_i is 0 or 1 in equation (1.1). I will leave it to the readers to review binary representation, but some examples are listed below:

- Conversion from binary to decimal:
  a. $11.0101_2 = 1 \cdot 2^1 + 1 \cdot 2^0 + 0 \cdot 2^{-1} + 1 \cdot 2^{-2} + 0 \cdot 2^{-3} + 1 \cdot 2^{-4} = 2 + 1 + 0.25 + 0.0625 = 3.3125$
  b. $1100_2 = 1.1_2 \times 2^3 = (1 \cdot 2^0 + 1 \cdot 2^{-1}) \cdot 2^3 = 12$
  c. $0.01_2 = 1.00_2 \times 2^{-2} = 0.25$

- Conversion from decimal to binary:

  a. $41 = 2^5 + 9 = 1 * 2^5 + 1 * 2^3 + 1 * 2^0 = 101001_2$

  b. To figure out the binary representation for 0.1, we first observe that $2^{-4} = 0.0625$ is the biggest component of 0.1. The leftover $0.1 - 0.0625 = 0.0375 > 2^{-5}$. So $0.1 = 2^{-4} + 2^{-5} + 0.00625 = 2^{-4} + 2^{-5} + 2^{-4} * 0.1 = 2^{-4} + 2^{-5} + 2^{-4}(2^{-4} + 2^{-5} + 2^{-4} * 0.1)$. This can keep going, so

$$0.1 = 2^{-4} + 2^{-5} + 2^{-8} + 2^{-9} + \cdots = 0.0\overline{0011}_2 = 1.\overline{1001}_2 \times 2^{-4}. \tag{1.2}$$

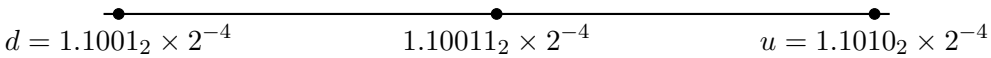
As seen, if a base (subscript) is not specified, then it is understood that it is a decimal number.

The representation in (1.2) has to be rounded at some point, and this is causing the computation inaccuracy at the beginning of this chapter.

There are usually 4 rounding models: rounding down, rounding up, rounding towards 0, and rounding to nearest. rounding to the nearest is, either round down or round up, whichever is closer. In case of a tie, we choose the one whose least significant (rightmost) bit is smaller. Given a real number x, we denote its floating point representation by $\text{fl}(x)$. For convenience of illustration, we use examples where we retain 4 digits after the binary point (this means the representation has precision $p = 5$).

Example 1.1. Round $0.1 = 1.1001100\cdots_2 \times 2^{-4}$ to the nearest so that there are only 4 digits after the binary point. This means that in this machine, $p = 5$.

Rounding up will be $u = 1.1010_2 \times 2^{-4}$. Rounding down will be $d = 1.1001_2 \times 2^{-4}$. To see which one is nearest, we can compute the midpoint of u and d.



0.1 is clearly bigger than the middle point, so we pick $1.1010_2 \times 2^{-4}$ with rounding to the nearest. We can write $\text{fl}(0.1) = 1.1010_2 \times 2^{-4}$ in this particular machine.

Question: In this same machine, meaning we still have $p = 5$ and we still use rounding to the nearest, what is $\text{fl}(1.10011_2 \times 2^{-4})$? (Hint: in binary, we break the tie by choosing the one whose least significant (rightmost) bit is 0.)

In the model where $\beta = 10, p = 5$, 1 is represented as 1.0000×10^0, the number that is closest to 1 (and bigger than 1) is 1.0001×10^0. There is a gap 10^{-4}. This gap is relative. The closest number to 1.0000×10^4 is 1.0001×10^4 (taking the bigger one again). This means we cannot represent any number between 10000 and 10001 with this machine. The gap (=1) is a lot bigger now, but the relative gap is still $1/10000 = 10^{-4}$.

In general, with base β and precision level p, this gap (between 1 and its closest number) is defined to be the *machine precision* or *machine epsilon* ϵ_m.[1] We have $\epsilon_m = \beta^{1-p}$. Machine epsilon is related to the *round-off error*, which is the error that results from replacing a number with its floating point form. The approximation x^* to x has *absolute error* $|x - x^*|$ and *relative error* $\dfrac{|x - x^*|}{|x|}$, provided that $x \neq 0$.

Example 1.2. Let us use base 10 with $p = 3$, in which case the machine precision is $\epsilon_m = 10^{-2}$. If we use the rounding to nearest method, 1.345 becomes 1.34 (both 1.34 and 1.35 are equally

[1] Some sources define the machine precision to be half of this gap.

close, we break the tie by choosing the number whose right most bit is smaller). Relative error $= \left|\frac{1.345 - 1.34}{1.345}\right| < \frac{0.005}{1} = 0.5 * \epsilon_m$ (The relative error is about 0.003.)

The number 1.345×10^4 will be rounded to 1.34×10^4. The absolute error is very big, but the relative error is $\left|\frac{1.345 \times 10^4 - 1.34 \times 10^4}{1.345 \times 10^4}\right| = \left|\frac{1.345 - 1.34}{1.345}\right|$, the same as before.

Example 1.3. Following Example 1.1, the absolute error in representing 0.1 is $|0.1 - \text{fl}(0.1)|$, which is less than half of the difference between u and d. The relative error is

$$\frac{|0.1 - \text{fl}(0.1)|}{0.1} < \frac{2^{-1}(u-d)}{d} = \frac{2^{-5} \cdot 2^{-4}}{1.1001_2 \times 2^{-4}} < 2^{-5}.$$

If we use rounding to the nearest, one has

$$\frac{|\text{fl}(x) - x|}{|x|} \leq 0.5\epsilon_m. \tag{1.3}$$

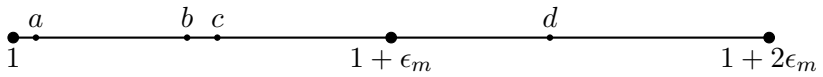
In other words, we may write

$$\text{fl}(x) = x(1+\epsilon), \quad \text{where } |\epsilon| < 0.5\epsilon_m.$$

The idea of machine epsilon is that

- Two numbers may be indistinguishable in a machine if their relative error is less than $0.5\epsilon_m$;
- Two numbers are definitely distinguishable in a machine if their relative error is more than ϵ_m.

Let's consider four numbers a, b, c, d as indicated below:



Using rounding to the nearest, $\text{fl}(a) = \text{fl}(b) = 1$ and a, b are within $0.5\epsilon_m$ relative error. $\text{fl}(b) \neq \text{fl}(c)$ even though they are within $0.5\epsilon_m$ relative error. $\text{fl}(c) = \text{fl}(d)$ even though they are almost ϵ_m apart. The only way to guarantee that two numbers have different representations is make sure they are relatively ϵ_m apart, like b and d.

1.2 Floating Point Operations

On a computer, all computations are reduced to $+, -, \times$, or $/$. Due to rounding, floating point arithmetic are different from the classical ones, and we will denote these *floating point operations (flop)* by $\oplus, \ominus, \otimes, \oslash$.

Example 1.4 (Addition)**.** Suppose we retain 4 digits after the binary point. To add up two numbers with different powers, we first need to adjust one of the numbers to align the mantissa (use bigger power), as:

$1.1000_2 \times 2^1 \oplus 1.1001_2 \times 2^{-1} = 1.1000_2 \times 2^1 \oplus \text{fl}(0.011001_2) \times 2^1 = 1.1000_2 \times 2^1 \oplus 0.0110_2 \times 2^1 = \text{fl}(1.1110_2) \times 2^1 = 1.1110_2 \times 2^1$.

Fundamental axiom of floating point arithmetic: Let $*$ be one of the operations $(+, -, \times, /)$, and let $\circledast$ be its floating point analogue, then for all **floating point numbers** x, y, we have that

$$x \circledast y = (x * y)(1 + \epsilon), \text{ for some } \epsilon \text{ such that } |\epsilon| \leq \epsilon_m.$$

or equivalently

$$\left| \frac{x \circledast y - x * y}{x * y} \right| \leq \epsilon_m.$$

We will not prove this, but we will quickly check this axiom in one example.

Example 1.5. We assume a machine, base 2, can only have 4 digits precision after the binary point, rounding to the nearest. Let $x = 1.1010_2 \times 2^{-4}$ and $y = 1.1010_2 \times 2^{-3}$ be two floating point numbers. (x is the floating point representation of 0.1 by Example 1.1 and y is the floating point representation of 0.2.)

Similar to Example 1.4, we first rewrite x as $0.11010_2 \times 2^{-3}$, which rounds to $0.1110_2 \times 2^{-3}$ (break the tie by picking the one whose right most bit is 0).

$x \oplus y = \text{fl}(0.1110_2 \times 2^{-3} + 1.1010_2 \times 2^{-3}) = \text{fl}(10.1000_2 \times 2^{-3}) = 1.0100_2 \times 2^{-2} = 0.3125$.

The relative error for this addition is

$$\left| \frac{x \oplus y - (x + y)}{x + y} \right| = \left| \frac{1.0100_2 \times 2^{-2} - 1.001110_2 \times 2^{-2}}{1.001110_2 \times 2^{-2}} \right| = \frac{0.000010_2}{1.001110_2} < 2^{-5} < 2^{-4} = \epsilon_m.$$

Finally, we present the example of adding 0.1 and 0.2, but in a "very outdated" machine.

Example 1.6. If we assume a machine, base 2, precision 5. This is how it adds up 0.1 and 0.2.

Step 1: 0.1 is rounded to $\text{fl}(0.1) = 1.1010_2 \times 2^{-4}$ as shown in Example 1.1.

Step 2: $\text{fl}(0.2) = 1.1010_2 \times 2^{-3}$ since 0.2 is twice of 0.1.

Step 3: $\text{fl}(0.1) \oplus \text{fl}(0.2) = 0.3125$ as shown in Example 1.5.

The overall relative error is $|0.3 - 0.3125|/0.3 \approx 0.042$.

To sum up, if we use $m(\cdot)$ to indiate the machine output using floating pont numbers, then $m(x + y) = \text{fl}(x) \oplus \text{fl}(y) = (x(1 + \epsilon_1) + y(1 + \epsilon_2))(1 + \epsilon_3)$

1.3 IEEE 754 Standard

In 1985, the Institute for Electrical and Electronic Engineers (IEEE) published the *Binary Floating Point Arithmetic Standard 754-1985* which is followed by all microcomputer manufacturers. The double precision real numbers require a 64-bit representation. The first bit is a sign indicator, denoted s. This is followed by an 11-bit exponent c, and a 52-bit binary fraction f (also named mantissa or significand). See the following example:

$$0.1 = +1.\underbrace{1001100110011001100110011001100110011001100110011010_2}_{\text{52 digits mantissa}} \times 2^{-4},$$

This is `0.1000000000000000055511151231257827021181583404541015625` in decimal. In the IEEE 754 standard, $p = 53, \epsilon_m = 2^{-52} \approx 2.22 \times 10^{-16}$. To retrieve this machine epsilon, type `eps = numpy.finfo(float).eps` in Python. Moreover, execute `1 + 0.4*eps`, what do you get?

The default IEEE standard is rounding to nearest. The 11-bit exponent can represent $2^{11} = 2048$ numbers. The numbers 0 and 2047 are reserved for other use (like $0, \infty$, NaN), so c can only take on integers ranging from 1 to 2046. In order to include both positive and negative exponents,

we will subtract 1023 from c and the actual exponent can be all integers from -1022 to 1023. To summarize, a double precision number has the form

$$(-1)^s * 2^{c-1023} * (1+f) \tag{1.4}$$

Consider the machine number

$$\underbrace{0}_{s} \quad \underbrace{10000000011}_{\text{11-bit } c} \quad \underbrace{1011100100010000000000000000000000000000000000000000}_{\text{52-bit } f},$$

converted to decimal, $c = 2^{10} + 2^1 + 2^0 = 1027$, $f = 2^{-1} + 2^{-3} + 2^{-4} + 2^{-5} + 2^{-8} + 2^{-12}$, so this number in decimal form is

$$(-1)^0 * 2^{1027-1023} * (1 + 2^{-1} + 2^{-3} + 2^{-4} + 2^{-5} + 2^{-8} + 2^{-12}) = 27.56640625.$$

The smallest positive number that can be represented is $s = 0, c = 1, f = 0$, which is $2^{-1022} \approx 2.225 \times 10^{-308}$.

1.4 Errors in Scientific Computing

Example 1.7. The quadratic formula states that the roots of $ax^2 + bx + c = 0$ are

$$x_1 = \frac{-b + \sqrt{b^2 - 4ac}}{2a}, \quad x_2 = \frac{-b - \sqrt{b^2 - 4ac}}{2a}. \tag{1.5}$$

Let us apply this formula to the equation $x^2 + 80x + 1 = 0$, whose roots are approximately $x_1 = -0.01250195, x_2 = -79.98750$.

If the roots are computed in a machine with $\beta = 10, p = 4$. We would get

$$\text{fl}(x_1) = \frac{-80.00 + \text{fl}(\sqrt{6400 - 4.000})}{2.000} = \frac{-80.00 + 79.97}{2.000} = -0.015$$

whose relative error is about 0.0025/0.0125=20%. This is quite large of an error. This big roundoff error is caused by subtracting two nearly equal number. (In this example, we have b^2 much larger than $4ac$, so b and $\sqrt{b^2 - 4ac}$ are nearly equal.)

On the other hand, the calculation of x_2 involves the addition of two nearly equal numbers, which presents no problem as

$$\text{fl}(x_2) = \frac{-80.00 - \text{fl}(\sqrt{6400 - 4.000})}{2.000} = \frac{-80.00 - 79.97}{2.000} = -79.98$$

with a small relative error $\approx 0.01/79.99 = 1.25 \times 10^{-4}$.

There is a way to get a more accurate approximation for x_1 in this same machine!

$$x_1 = \frac{-b + \sqrt{b^2 - 4ac}}{2a} \cdot \frac{-b - \sqrt{b^2 - 4ac}}{-b - \sqrt{b^2 - 4ac}} = \frac{-2c}{b + \sqrt{b^2 - 4ac}}. \tag{1.6}$$

This is an equivalent formula for x_1, but makes a big difference in a computer since (1.6) **avoids subtracting two nearly equal numbers**. By (1.6), we have

$$\text{fl}(x_1) = \frac{-2.000}{80.00 + \text{fl}(\sqrt{6400 - 4.000})} = \frac{-2.000}{80.00 + 79.97} = -0.01250.$$

This is a much better approximation.

Due to rounding, subtracting two nearly equal numbers will cause a big relative error. Such an error is called cancellation error and we should try to avoid it if possible. As shown in Example 1.7, rationalizing a formula could be used when appropriate.

Chapter 1 Exercises

1. Convert binary to decimal.
   (a) 110_2
   (b) 11.0101_2
2. Convert decimal to binary
   (a) 11.5
   (b) 1.3125
3. Find the **normalized** floating point representation
   (a) 10.345, base 10, $p = 4$, rounding to the nearest.
   (b) 10.395, base 10, $p = 4$, rounding to the nearest.
   (c) 295, base 10, $p = 2$, rounding to the nearest.
   (d) 1.0101_2, base 2, $p = 3$, rounding up.
   (e) 1.0101_2, base 2, $p = 3$, rounding down.
   (f) 1.0101_2, base 2, $p = 3$, rounding to the nearest.
   (g) 1.0101_2, base 2, $p = 4$, rounding to the nearest.
4. Let us use base 10 with $p = 2$. If we use the rounding to the nearest method, what is the relative error of 1.23? What is the relative error of 10.61?
5. Following Exercise 3(g), what is the machine epsilon? what is the relative error in rounding this number? Does the rule (1.3) check out?
6. Directly add in binary (No rounding involved).
   (a) $0.111_2 + 11.101_2$
   (b) $1.1010_2 \times 2^{-4} + 1.1010_2 \times 2^{-3}$.
7. What is the biggest number that can be represented in IEEE 754 standard using double precision? Express this number in the form of $2^a - 2^b$.
8. In a machine of $\beta = 2, p = 3$, compute the machine result of 0.1+0.2 (rounding to the nearest).
9. In a machine of $\beta = 10, p = 4$, compute the machine result of $6400.1 + 4.12$ (rounding to the nearest).
10. This problem is from Chapter 5 problem 15 of [2].

    In the 1991 Gulf War, the Patriot misslie defense system failed due to roundoff error. The troubles stemmed from a computer that performed the tracking calculations with an internal clock whose integer values in tenths of a second were converted to seconds by multiplying by a 24-bit binary approximation to 0.1:

    $$0.1 \approx 0.00011001100110011001100_2$$

    (a) Convert the binary number above to a fraction. Call it x.

(b) Compute the absolute difference between 0.1 and x.

(c) What is the time error in seconds after 100 hours of operation (i.e., the value of $|360,000 - 3,600,000x|$)?

On February 25, 1991, a Patriot battery system, which was to protet the Dhahran Air Base, had been operating for over 100 consecutive hours. The roundoff error caused the system not to track an incoming Scud missle, which slipped through the defense system and detonated on US Army barracks, killing 28 American soldiers.

11. Find the most accurate approximation of the roots of $x^2 - 75.7x + 1$ with $p = 4$. Compute the relative errors for both roots.

12. Given $p(x) = 1 + 2x + 3x^2 + 3x^3 + 4x^4$,

    (a) Find the nested form of $p(x)$.

    (b) How many flops are needed to evaluate this polynomial at one point, in the original form, and in the nested form?

Chapter 1 Python Exercises

13. (a) Define a vector v whose entries are [1, 0.01, 0.02, ... , 5]. Do not print.

    (b) Define a 10×10 matrix whose entries are the integers 1 to 100 ordered column-wise. Print the matrix. [Hint: look up `np.reshape`]

    (c) Plot $y = \cos x$ and $y = x$ on the interval [0,1] in the same graph.

14. Given the equation $x^2 - 100000x + 1 = 0$, use formula (1.5) and formula (1.6) to compute two different approximations of x_1. Print both values in the exponential notation with 15 digits after the decimal point. Which formula produces a better approximation of x_1?

15. Given $p(x) = x^9 - 18x^8 + 144x^7 - 672x^6 + 2016x^5 - 4032x^4 + 5376x^3 - 4608x^2 + 2304x - 512$.

    (a) Let $n(x)$ be the nested form of $p(x)$. Define $p(x), n(x)$, and $s(x) = (x - 2)^9$. All 3 functions need to be able to take in arrays.

    (b) $p(x) = n(x) = s(x)$ algebraically, but makes a difference in computers. Plot all three functions on the interval [1.92, 2.08] (with 0.001 increment). You need to place all 3 plots in a 1×3 grid. Be sure to give a title to each subplot to indicate which is which.

    (c) Explain the difference in three plots in (b).

Chapter 2

Solving nonlinear equations

If we recall the equations that we are able to solve, probably we would realize that there are very few. We can surely solve $x^2 - x - 1 = 0$ using the famous quadratic formula, but have you ever wondered formulas for finding roots of polynomials whose degree is higher than 2? Unfortunately, even as simple as a polynomial equation $x^5 - x - 1 = 0$, a math Ph.D feels hopeless to find an exact answer by analysis. In fact, there are no formula for finding roots of polynomials of degree bigger than 4. Equations like $\cos x = x$ do not have a closed form solution either.

A linear equation has the form $ax = b$. It is trivial to solve if x is a scalar. When x is a vector, we often write $Ax = b$, and is a major topic itself.

In this chapter, we discuss several iterative methods for solving nonlinear equations when x is a scalar. Direct methods are formula or procedures that will produce the exact solution. Iterative methods produce a sequence $\{x_1, x_2, \cdots, x_n, \cdots\}$ that (hopefully) converges to the true solution x.

2.1 The Bisection Method

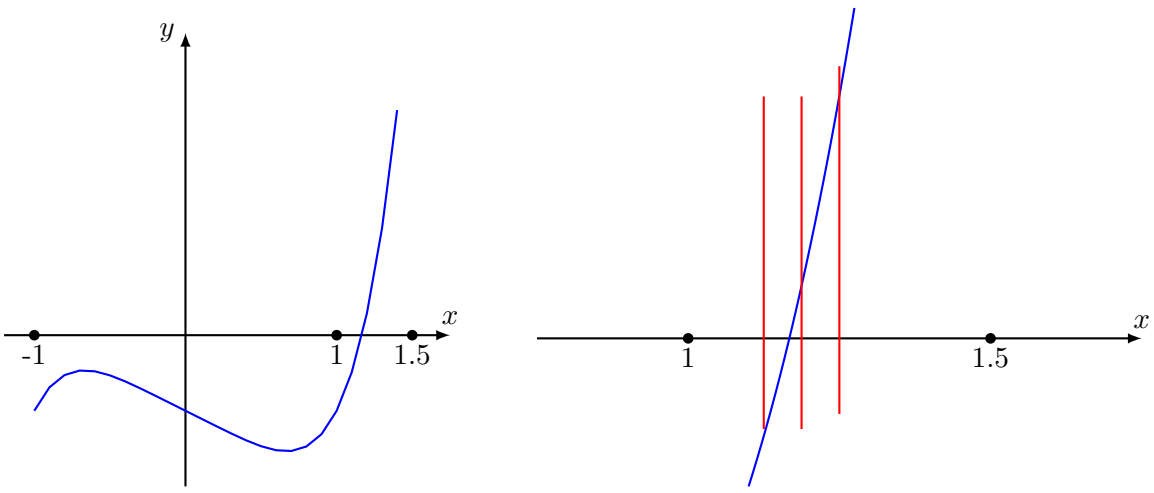


Figure 2.1: Bisection Method. The right is an enlargement of the left.

This is a simple, yet efficient method that is often covered in Calculus I as an application of the Intermediate Value Theorem (IVT). See Theorem 4.1.

Take $f(x) = x^5 - x - 1$ as an example, whose graph is shown on the left of Figure 2.1. Since $f(1) = -1 < 0$ and $f(1.5) \approx 5.09 > 0$, then by the IVT, there is $c \in [1, 1.5]$ such that $f(c) = 0$, or

equivalently, f has a root c in [1,1.5].

To have a more precise estimate of c, we evaluate f at the middle point $\frac{1+1.5}{2} = 1.25$. $f(1.25) \approx 0.8 > 0$. By the IVT again, we conclude that the root $c \in [1, 1.25]$. We can keep bisecting the interval and eventually find the root to a sufficient precision. See the right of Figure 2.1.

Note that the key of the Bisection method is:

1. The function needs to be continuous.
2. One needs to be given initial points a, b such that $f(a)$ and $f(b)$ have different signs.

The Bisection Algorithm

Input:	a_0, b_0 such that $f(a_0), f(b_0)$ have different signs.
Output:	an approximation of a root of f
Repeat:	for $n \geq 0$
	1. $p_n = \frac{a_n + b_n}{2}$
	2. if $f(a_n)f(p_n) < 0$, set $a_{n+1} = a_n, b_{n+1} = p_n$
	otherwsie, set $a_{n+1} = p_n, b_{n+1} = b_n$
	until a stopping criteria has been reached

Example 2.1. Find a solution of $2^{-x} = x$.

This is equivalent to finding a root of $f(x) = (\frac{1}{2})^x - x$. We have $f(0) = 1 - 0 > 0, f(1) = 0.5 - 1 < 0$, so we will let $a_0 = 0, b_0 = 1$. Therefore $p_0 = 1/2$.

$f(1/2) = \frac{1}{\sqrt{2}} - \frac{1}{2} > 0$, so $a_1 = 1/2, b_1 = 1, p_1 = 3/4$.

$f(3/4) = (0.5)^{3/4} - 3/4 < 0$, so $a_2 = 1/2, b_2 = 3/4, p_2 = 5/8$

After only two iterations, we get a coarse approximate of the root: $p_2 = 5/8 = 0.625$. For the reference, the actual root is 0.6411857445.

If we predetermine a tolerance level tol so that the algorithm will terminate if $|p_n - p_{n+1}| < \text{Tol}$, then this can be achieved when

$$|p_n - p_{n+1}| = \frac{b_n - a_n}{4} = \frac{b_0 - a_0}{2^{n+2}} < \text{Tol} \iff n \geq \log_2(\frac{b_0 - a_0}{4\text{Tol}}) \tag{2.1}$$

If p is the actual root, then we have

$$|p_n - p| \leq \frac{b_n - a_n}{2} = 2|p_n - p_{n+1}| < 2\text{Tol}.$$

Therefore the number of iterations needed can be computed via (2.1).

2.2 The Newton's Method

Newton's method (also called the Newton-Raphson method) is a little more sophisticated: it involves derivatives, but it is still Calculus material. This is usually how a calculator or a computer finds a root.

If we are to find the root of $y = f(x)$, we start with a random initial guess x_0. Consider the the tangent line to the curve $y = f(x)$, at $P_0 = (x_0, f(x_0))$. The idea behind Newton's method is linearization. Since the tangent line (linearization of f) is close to f, then its x-intercept, x_2, is close to the x-intercept of the curve $y = f(x)$. We can easily find x_2.

The tangent line at the point $(x_0, f(x_0))$ is

$$y - f(x_0) = f'(x_0)(x - x_0).$$

Plugging in $y = 0$ to solve for the x-intercept:

$$0 - f(x_0) = f'(x_0)(x - x_0) \Longrightarrow x = x_0 - \frac{f(x_0)}{f'(x_0)}.$$

So $x_1 = x_0 - \dfrac{f(x_0)}{f'(x_0)}$. We use x_1 as the next approximation and keep repeating this process, as shown in Figure 2.2, where we gain this iteration formula

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}, \quad k \geq 0. \tag{2.2}$$

Note that we require $f'(x_k) \neq 0$ which is not a trivial condition.

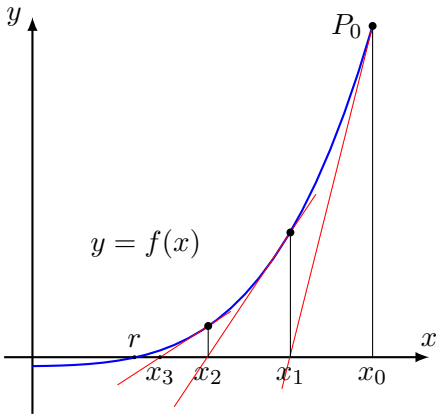


Figure 2.2: Newton's method

Example 2.2. Use the Newton's method to approximate $\sqrt{2}$.

Let $f(x) = x^2 - 2$, which makes $\sqrt{2}$ a root of $f(x)$. We can compute that $f'(x) = 2x$. Let $x_0 = 4$. We can simplify (2.2) to

$$x_{k+1} = x_k - \frac{x_k^2 - 2}{2x_k} = \frac{x_k}{2} + \frac{1}{x_k}.$$

$x_1 = 2 + 1/4 = 9/4 = 2.25$
$x_2 = 9/8 + 4/9 = 113/72 = 1.569\dot{4}$
$x_3 = 1.569\dot{4}/2 + 1/1.569\dot{4} \approx 1.42189$

If we use the Bisection method for this problem starting at $a_0 = 0, b_0 = 4$, we then have $p_0 = 2, p_1 = 1, p_2 = 1.5, p_3 = 1.25$. This is a much worse approximation after the same number of iterations. See Table 2.1 for error comparison. This table also includes the secant method that will be introduced later.

The two drawbacks of the Newton's method are: (1) It requires the knowledge of the derivative function; (2) It may not converge if you have an unlucky initial guess x_0. For example, if one picks $x_0 = 0$ for finding root of $y = x^5 - x - 1$, the sequence will not converge to the root (try to draw tangent lines on your own). However, if the initial guess is close enough, the Newton's method does enjoy fast convergence (faster than the Bisection method as shown in Example 2.2) .

n	Bisection $\lvert p_n - \sqrt{2}\rvert$	Newton $\lvert x_n - \sqrt{2}\rvert$	Secant
0	0.585786438	2.585786438	
1	0.414213562	0.835786438	
2	0.085786438	0.155230882	0.414213562
3	0.164213562	0.007676801	0.080880229
4	0.039213562	0.000020723	0.014357866
5	0.023286438	0.000000000	0.000420459

Table 2.1: Accuracy Comparison of Example 2.2

Definition 2.3. A method that produces a sequence $\{x_n\}$ that converges to a number x *linearly* if there exists $L \in (0,1)$ such that for large values of n

$$|x_{n+1} - x| \leq L|x_n - x|.$$

The sequence converges to x *quadratically* if there exists $Q > 0$ such that for large values of n

$$|x_{n+1} - x| \leq Q|x_n - x|^2.$$

For example, the sequence $\{3^{-n}\}_{n=1}^{\infty}$ converges to 0 linearly. The sequence $\{b_n = 3^{-2^n}\}_{n=1}^{\infty}$ converges quadratically to 0.

Theorem 2.4. *Let $f(x)$ be a function whose second derivative is continuous, and r be a root of $f(x)$. Let I be an interval contains r such that $|f''(x)| \leq M$ for any $x \in I$. If $x_k \in I$, then the Newton's method converges to r quadratically as*

$$|x_{k+1} - r| \leq \frac{M}{2|f'(x_k)|}|x_k - r|^2. \tag{2.3}$$

Proof. Expand f in the first Taylor polynomial ($n = 1$ in (4.1)) at x_k gives

$$0 = f(r) = f(x_k) + f'(x_k)(r - x_k) + \frac{f''(\xi)}{2}(r - x_k)^2,$$

where ξ lies between x_k and r. Consequently, if $f'(x_k) \neq 0$, we have

$$r - x_k + \frac{f(x_k)}{f'(x_k)} = -\frac{f''(\xi)}{2f'(x_k)}(r - x_k)^2.$$

Combined with (2.2), we have

$$r - x_{k+1} = -\frac{f''(\xi)}{2f'(x_k)}(r - x_k)^2 \Longrightarrow |r - x_{k+1}| \leq \frac{M}{2|f'(x_k)|}|r - x_k|^2$$

since ξ is in between x_k and r, hence $\xi \in I$. □

This implies that the Newton's method has the tendency to approximately double the number of digits of accuracy with each successive approximation, as demonstrated in Table 2.1.

The order of convergence for linear methods (like Bisection) is 1 and the order of convergence for quadratic methods (like Newton) is 2.

2.3 The Secant Method

As mentioned, one of the drawbacks of the Newton's method is that we have to know its derivative. For the simple example presented above, this is not difficult. In many problems, however, f can get complicated, or worse, cannot be written down analytically. In such scenarios, differentiating f analytically is difficult or impossible. For such problems, we approximate the derivatives. Iterations of the form

$$x_{k+1} = x_k - \frac{f(x_k)}{g(x_k)}, \quad \text{where } g_k \approx f'(x_k)$$

are called *quasi-Newton* methods.

Among many quasi-Newton methods, the *secant method* is defined by taking $f'(x_k)$ to be

$$f'(x_k) \approx \frac{f(x_k) - f(x_{k-1})}{x_k - x_{k-1}}.$$

So the iteration formula for the secant method is:

$$x_{k+1} = x_k - \frac{f(x_k)(x_k - x_{k-1})}{f(x_k) - f(x_{k-1})}, \quad k \geq 1.$$

To begin the secant method, one needs two starting points x_0, x_1.

It turns out that the order of convergence of the secant method is in between Bisection and Newton. In fact, the order is $\dfrac{1+\sqrt{5}}{2} \approx 1.62$ the Golden ratio as for the secant method the iterates satisfy

$$|x_{n+1} - x| \leq M|x_n - x|^{\frac{1+\sqrt{5}}{2}}.$$

Interested readers can find a proof in [2, Section 4.3.3].

We will use the secant method on the same example.

Example 2.5. Use the secant method to find the positive root of $f(x) = x^2 - 2$ with initial $x_0 = 0, x_1 = 2$.

$$x_{k+1} = x_k - \frac{f(x_k)(x_k - x_{k-1})}{f(x_k) - f(x_{k-1})} = x_k - \frac{(x_k^2 - 2)(x_k - x_{k-1})}{x_k^2 - x_{k-1}^2} = x_k - \frac{x_k^2 - 2}{x_k + x_{k-1}} = \frac{x_k x_{k-1} + 2}{x_k + x_{k-1}}.$$

$$x_2 = \frac{0+2}{2} = 1.$$

$$x_3 = \frac{2+2}{1+2} = 4/3.$$

$$x_4 = \frac{4/3+2}{7/3} = 10/7.$$

$$x_5 = \frac{\frac{10}{7}\frac{4}{3}+2}{\frac{10}{7}+\frac{4}{3}} = \frac{40+42}{30+28} = \frac{41}{29}.$$

The errors are listed in the third column of Table 2.1.

Chapter 2 Exercises

Python Exercises

1. Bisection and Newton comparison.

(a) Use the Bisection method to do Example 2.1, with the stopping criteria $|p_{n+1} - p_n| \leq$1e-5, and initial interval $a_0 = 0, b_0 = 1$. How many iterations was run? (meaning what is the n value when $|p_{n+1} - p_n| \leq$1e-5 is reached?) How is this compared to the theoretical value in (2.1)?

(b) Use the Newton's method to do Example 2.1, with the stopping criteria $|x_{n+1} - x_n| \leq$1e-5, and initial value $x_0 = 1$. How many iterations was run?

2. Newton's method fails for finding a root of $y = x^5 - x - 1$ with $x_0 = 0$. Print the first 6 approximations to illustrate this.

Other Exercises

3. Use the Bisection method to find a solution of $\cos x = x$ with initial interval $[0, \pi]$. Find $p_i, i = 0, 1, 2$. Use (2.1) to compute how many iterations are needed if tol=0.01.

4. Let $f(x) = 3(x+1)(x-1/2)(x-1)$. Use the Bisection method to find p_3 on the interval [-2, 1.5]. [Since f is factored, we know its roots right away. This problem is more of an exercise such that the function's sign can be determined easily.]

5. Write down the first 3 iterations (x_1, x_2, x_3) of the Newton's method for solving $x^2 - 3 = 0$, starting with $x_0 = 1$. Write your answers in terms of fractions.

6. Prove that Newton's method will converge to 0 given any initial value x_0 if we are solving $x^2 = 0$.

7. Write down the first three iterates (2, 3, 4) of the secant method for solving $x^2 - 3 = 0$, starting with $x_0 = 0$ and $x_1 = 1$. Write your answer in terms of fractions.

8. Show that $\{3^{-n}\}_{n=1}^{\infty}$ converges to 0 linearly, and the sequence $\{b_n = 3^{-2^n}\}_{n=1}^{\infty}$ converges to 0 quadratically.

9. We can compute 1/3 by solving $f(x) = 0$ with $f(x) = x^{-1} - 3$.

   (a) Write down the Newton iteration for this problem, and compute by hand the first 2 Newton iterates for approximating 1/3, starting with $x_0 = 0.5$.

   (b) What happens if you start with $x_0 = 1$?

   (c) *In the case of (b), show that the iterates $x_k \to -\infty$ as $k \to \infty$.

10. Problems involving the amount of money required to pay off a mortgage over a fixed period of time involve the formula

$$A = \frac{P}{i}[1 - (1+i)^{-n}],$$

known as an *ordinary annuity equation.* In this equation A is the amount of the mortgage, P is the amount of each payment, and i is the interest rate per period for the n payment periods. Suppose that a 30-year home mortgage in the amount of $135,000 is needed and that the borrower can afford house payments of at most $1000 per month. What is the maximal interest rate the borrower can afford to pay? (You can use `scipy.optimize.newton` to solve the equation in the end.)

Chapter 3

Solving system of linear equations: Direct methods

Solving a linear system $Ax = b$ is everywhere in many applications. There are generally two approaches: Direct methods and iterative (indirect) methods. Direct methods give a direct answer at the end of the algorithm, whereas iterative methods follow an iterative formula where the iterates are approaching the real solution.

We also care about how efficient an algorithm is. This is to count how many flops are needed in a computer. Each flop is one of the following operations: $+, -, \times, \div$. For example, the inner product $x^T y$ requires n multiplications and $n-1$ summations, given both vectors have n coordinates. So $x^T y$ needs $2n-1$ flops.

- Matrix-Vector multiplication: Given $A \in \mathbb{R}^{m\times n}, x \in \mathbb{R}^n$, Ax is computing m inner products, so needs $m(2n-1)$ flops.
- Matrix-Matrix multiplication: Given $A \in \mathbb{R}^{m\times n}, B \in \mathbb{R}^{n\times p}$, AB is computing p matrix-vector multiplications. So the calculation of AB requires $pm(2n-1)$ flops. In particular, if both A and B are square matrices, then AB needs $2n^3 - n^2 \approx 2n^3$ flops.

3.1 Gaussian Elimination and LU factorization

Gaussian elimination is a core material in linear algebra and is the procedure one performs when finding key features like linear dependence, rank, null space, basis, dimension, etc. Gauss elimination is the simplest way to solve linear systems of equations by hand, and also the standard method for solving them on computers.

The following notations are standard:

$$Ax = b \Longleftrightarrow \begin{array}{cccccc} a_{11}x_1 & +a_{12}x_2 & +\cdots & +a_{1n}x_n & = b_1 \\ a_{21}x_1 & +a_{22}x_2 & +\cdots & +a_{2n}x_n & = b_2 \\ \vdots & \vdots & & \vdots & \vdots \\ a_{m1}x_1 & +a_{m2}x_2 & +\cdots & +a_{mn}x_n & = b_m \end{array} \Longleftrightarrow [A|b].$$

The matrix A is called the coefficient matrix and the matrix $[A|b]$ is called the augmented matrix.

Gaussian elimination is suitable for systems of all sizes, but **in this section our examples and analysis will focus on $Ax = b$ where A is invertible.** When solving $Ax = b$, the Gaussian elimination consists of two procedures: forward elimination and backward substitution.

Example 3.1. Solve $\left[\begin{array}{ccc|c} 1 & 2 & 2 & 1 \\ 2 & 7 & 7 & 5 \\ 2 & 7 & 9 & 5 \end{array}\right]$.

Forward Elimination:
$\left[\begin{array}{ccc|c} 1 & 2 & 2 & 1 \\ 2 & 7 & 7 & 5 \\ 2 & 7 & 9 & 5 \end{array}\right] \xrightarrow{\rho 1(-2)+\rho 2} \left[\begin{array}{ccc|c} 1 & 2 & 2 & 1 \\ 0 & 3 & 3 & 3 \\ 2 & 7 & 9 & 5 \end{array}\right] \xrightarrow{\rho 1(-2)+\rho 3} \left[\begin{array}{ccc|c} 1 & 2 & 2 & 1 \\ 0 & 3 & 3 & 3 \\ 0 & 3 & 5 & 3 \end{array}\right] \xrightarrow{\rho 2(-1)+\rho 3} \left[\begin{array}{ccc|c} 1 & 2 & 2 & 1 \\ 0 & 3 & 3 & 3 \\ 0 & 0 & 2 & 0 \end{array}\right]$.

Backward substitution:
(1) Equation form:

$$2x_3 = 0 \Rightarrow x_3 = 0$$
$$3x_2 + 3 * 0 = 3 \Rightarrow x_2 = 1$$
$$x_1 + 2 * 1 + 2 * 0 = 1 \Rightarrow x_1 = -1$$

(2) Matrix form:
$\left[\begin{array}{ccc|c} 1 & 2 & 2 & 1 \\ 0 & 3 & 3 & 3 \\ 0 & 0 & 2 & 0 \end{array}\right] \xrightarrow{\rho 3/2} \left[\begin{array}{ccc|c} 1 & 2 & 2 & 1 \\ 0 & 3 & 3 & 3 \\ 0 & 0 & 1 & 0 \end{array}\right] \xrightarrow[\rho 3(-2)+\rho 1]{\rho 3(-3)+\rho 2} \left[\begin{array}{ccc|c} 1 & 2 & 0 & 1 \\ 0 & 3 & 0 & 3 \\ 0 & 0 & 1 & 0 \end{array}\right] \xrightarrow{\rho 2/(3)} \left[\begin{array}{ccc|c} 1 & 2 & 0 & 1 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{array}\right]$
$\xrightarrow{\rho 2(-2)+\rho 1} \left[\begin{array}{ccc|c} 1 & 0 & 0 & -1 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{array}\right]$.

As seen in Example 3.1, the Gaussian elimination consists of two procedures: Forward elimination and backward substitution. Next, we will describe them generally and also count the flops used in each procedure.

The following two formula will be useful:

$$\sum_{i=1}^{n} i = \frac{n(n+1)}{2}, \qquad \sum_{i=1}^{n} i^2 = \frac{n(n+1)(2n+1)}{6}.$$

Forward elimination of Gaussian elimination: This is to get to an upper triangular matrix with row operations.

Column 1

We eliminate all entries below a_{11}.

$$\left[\begin{array}{cccc|c} a_{11} & a_{12} & \cdots & a_{1n} & b_1 \\ a_{21} & a_{22} & \cdots & a_{2n} & b_2 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} & b_n \end{array}\right] \longrightarrow \left[\begin{array}{cccc|c} a_{11} & a_{12} & \cdots & a_{1n} & b_1 \\ 0 & a'_{22} & \cdots & a'_{2n} & b'_2 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & a'_{n2} & \cdots & a'_{nn} & b'_n \end{array}\right] \tag{3.1}$$

At each row, we need $n+1$ multiplications and n additions. [for example, to obtain the new row 2, we first compute $-\frac{a_{21}}{a_{11}}$, which takes one multiplication/division. Then we add $-\frac{a_{21}}{a_{11}}$ copy of row 1 to row 2.] There are $n-1$ rows to perform, so a total of $(n-1)\cdot(2n+1) = 2n^2 - n - 1$ flops are needed to get to the right hand side of (3.1).

Column 2: Now we use a'_{22} to eliminate all entries below. This is the same work except we have an $(n-1)\times(n-1)$ system now, so we need $2(n-1)^2 - (n-1) - 1$ flops.

Total: We keep doing this until the coefficient matrix becomes upper triangular, so there are a total of $\sum_{i=1}^{n}(2i^2 - i - 1) = \frac{n(n+1)(2n+1)}{3} - \frac{n(n+1)}{2} - n = \frac{2}{3}n^3 + \frac{1}{2}n^2 - \frac{7}{6}n \approx \frac{2}{3}n^3$ flops.

Backward substitution of Gaussian Elimination: After forward elimination, we obtain an upper triangular system

$$\left[\begin{array}{cccc|c} c_{11} & c_{12} & \cdots & c_{1n} & y_1 \\ 0 & c_{22} & \cdots & c_{2n} & y_2 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & c_{nn} & y_n \end{array}\right]. \tag{3.2}$$

The backward substitution can be done in either the equation form or the matrix form, both of which are illustrated in Example 3.1. We will use the equation form in our operation counts here. We will start with last row and work our way up.

Row n: $c_{nn}x_n = y_n$. Takes 1 division to solve x_n

Row $n-1$: $c_{n-1,n-1}x_{n-1} + c_{n-1,n}x_n = y_{n-1}$. Takes 1 multiplication, 1 addition, 1 division to solve x_{n-1}.

Row $n-2$: $c_{n-2,n-2}x_{n-2} + c_{n-2,n-1}x_{n-1} + c_{n-2,n}x_n = y_{n-2}$. Takes 2 multiplication, 2 addition, 1 division to solve x_{n-2}.

...

Row 1: $c_{11}x_1 + c_{12}x_2 + \cdots + c_{1n}x_n = y_1$. Takes $n-1$ multiplications, $n-1$ additions, 1 division to solve x_1.

Add up all counts, we have

$\sum_{i=1}^{n}[(i-1) + (i-1) + 1] = n^2$.

Gaussian elimination operation counts:

$$\underbrace{\frac{2}{3}n^3 + \frac{1}{2}n^2 - \frac{7}{6}n}_{forward\ elim.} + \underbrace{n^2}_{backward\ sub.} = \frac{2}{3}n^3 + \frac{3}{2}n^2 - \frac{7}{6}n \approx \frac{2}{3}n^3.$$

3.1.1 Forward elimination = LU factorization

Each row operation corresponds to a matrix (often called an elementary row operation matrix). In the forward elimination process of Example 3.1, let $A = \begin{bmatrix} 1 & 2 & 2 \\ 2 & 7 & 7 \\ 2 & 7 & 9 \end{bmatrix}$, then $L_1 A = \begin{bmatrix} 1 & 2 & 2 \\ 0 & 3 & 3 \\ 2 & 7 & 9 \end{bmatrix}$, where L_1 represents the first row operation. To figure out L_1, we perform the very row operation on the identity matrix: $\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \xrightarrow{\rho 1(-2)+\rho_2} \begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = L_1$. For the rest two row operations, we can compute in the same fashion that $L_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -2 & 0 & 1 \end{bmatrix}, L_3 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -1 & 1 \end{bmatrix}$.

The forward elimination process of Example 3.1 can be written as

$$L_3L_2L_1A = U = \begin{bmatrix} 1 & 2 & 2 \\ 0 & 3 & 3 \\ 0 & 0 & 2 \end{bmatrix}.$$

So

$$A = (L_3L_2L_1)^{-1}U = L_1^{-1}L_2^{-1}L_3^{-1}U := LU.$$

L_1, L_2, L_3 are very special matrices, and their inverses and L can be figured out easily:

$$L_1^{-1} = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, L_2^{-1} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 2 & 0 & 1 \end{bmatrix}, L_3^{-1} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 1 \end{bmatrix}, L = L_1^{-1}L_2^{-1}L_3^{-1} = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 2 & 1 & 1 \end{bmatrix}.$$

So we can decompose/factor A as

$$A = \begin{bmatrix} 1 & 2 & 2 \\ 2 & 7 & 7 \\ 2 & 7 & 9 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 2 & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 2 & 2 \\ 0 & 3 & 3 \\ 0 & 0 & 2 \end{bmatrix} = LU.$$

In general, if there is no row exchange involved in forward elimination, then A can always be written as the product of a lower triangular matrix and an upper triangular matrix. This is called the LU factorization of A. It requires $\frac{2}{3}n^3$ flops as well because it is done through forward elimination. In fact, the operation counts is slightly less because we don't need to consider the right hand side b, but it is still on the order of $\frac{2}{3}n^3$.

3.1.2 A 'second way' to solve $Ax = b$

If the LU factorization of A is already done, then it is very easy to solve $LUx = b$. We set $Ux = y$. We first solve y from $Ly = b$, which is very straightforward as we will see in Example 3.2. Then we solve x from $Ux = y$. We will use the same example to illustrate.

Example 3.2. Suppose we are given $\begin{bmatrix} 1 & 2 & 2 \\ 2 & 7 & 7 \\ 2 & 7 & 9 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 2 & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 2 & 2 \\ 0 & 3 & 3 \\ 0 & 0 & 2 \end{bmatrix}$. In order to solve

$$\begin{bmatrix} 1 & 2 & 2 \\ 2 & 7 & 7 \\ 2 & 7 & 9 \end{bmatrix} x = \begin{bmatrix} 1 \\ 5 \\ 5 \end{bmatrix},$$

(1) We first solve $\begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 2 & 1 & 1 \end{bmatrix} y = \begin{bmatrix} 1 \\ 5 \\ 5 \end{bmatrix}$ $(Ly = b)$.

$$\begin{aligned} y_1 &= 1 \\ 2 * 1 + y_2 = 5 &\Rightarrow y_2 = 3 \\ 2 * 1 + 1 * 3 + y_3 = 5 &\Rightarrow y_3 = 0 \end{aligned}$$

(2) Then we solve $Ux = y$, which is already done in the backward substitution of Example 3.1. It is not a coincidence that the y we solved in (1) is the same as the right hand side of the system after forward elimination.

It is obvious that solving $Ly = b$ and $Ux = y$ cost the same number of operations because the only difference is that $Ly = b$ is solved forwardly, and $Ux = y$ is solved backwardly.

Solve $Ax = b$ via LU decomposition		
Step 1:	$A = LU$. (Now equation becomes $LUx = b$.)	$\frac{2}{3}n^3$ flops
Step 2:	Solve $Ly = b$. (y will equal to Ux.)	n^2 flops
Step 3:	Solve $Ux = y$.	n^2 flops

LU decomposition approach is better when we need to solve multiple systems with the same coefficient matrix A.

We compare the flop counts of these two approaches for solving m systems:

$$Ax = b_1, Ax = b_2, \cdots, Ax = b_m.$$

Regular Gauss Elimination:	$\frac{2}{3}n^3 m$ flops
LU approach:	$\frac{2}{3}n^3 + 2mn^2$ flops

If $m = n$, then regular GE approach takes around $\frac{2}{3}n^4$ operations, whereas LU approach operation count is $\frac{8}{3}n^3$, still on the order of n^3. This makes a huge difference when the system is large (i.e. big n).

Chapter 3 Exercises

1. Write out the full matrix $A = [a_{ij}]_{3\times 4}$ where $a_{ij} = i^{j-1}$.
2. Let $A = \begin{bmatrix} 3 & 0 \\ -1 & 2 \\ 1 & 1 \end{bmatrix}, B = \begin{bmatrix} 1 & 5 & 2 \\ -1 & 0 & 1 \\ 3 & 2 & 4 \end{bmatrix}, C = \begin{bmatrix} 1 & 4 & 2 \\ 3 & 1 & 5 \end{bmatrix}$. Compute the following (write undefined if operation is not legal).
   (a) $2A^T + C$ (b) CBB (c) BA
3. Compute $x^T Ax$, where $x = (x_1, x_2, x_3)$, and $A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{12} & a_{22} & a_{23} \\ a_{13} & a_{23} & a_{33} \end{bmatrix}$ (A is symmetric.)
4. Perform forward elimination.
   (a) $\left[\begin{array}{ccc|c} 2 & 2 & 2 & 0 \\ -2 & 5 & 2 & 1 \\ 8 & 1 & 4 & -1 \end{array}\right]$ (b) $\left[\begin{array}{ccc|c} 0 & -2 & 3 & 1 \\ 3 & 6 & -3 & -2 \\ 6 & 6 & 3 & 5 \end{array}\right]$
5. Find scalars c_i for which the equation $c_1(-1, 0, 2) + c_2(2, 2, -2) + c_3(1, -2, 1) = (-6, 12, 4)$ holds.
6. How many **exact** flops are needed for the following computations?
   (a) x dot product y, where x, y are vectors in $\mathbb{R}^9$.
   (b) $A + B$, where A, B are both $m \times n$.

(c) ABC, where A, B, C are 5×5 matrices.

(d) Ux, where U is $n \times n$ upper triangular matrix and x is a vector in $\mathbb{R}^n$.

(e) ABC, where A is 10×100, B is 100×100, C is 100×100.

(f) LU, where L is $n \times n$ lower triangular, U is $n \times n$ upper triangular.

7. Find the 4×4 elementary row matrices that correspond to

   (a) $\rho 2(3) + \rho 3$ (b) $\rho 1(-3) + \rho 4$

8. Find the inverse of the matrix in 7(a). What row operation does this inverse correspond to?

9. Find the inverse of $\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$.

10. Is $\begin{bmatrix} 1 & 1 & 1 \\ 1 & 2 & 1 \\ 2 & 3 & 2 \end{bmatrix}$ invertible?

11. Find the LU decomposition of the coefficient matrix in 4(a).

12. Does the system in 4(b) solvable? Is the matrix $A = \begin{bmatrix} 0 & -2 & 3 \\ 3 & 6 & -3 \\ 6 & 6 & 3 \end{bmatrix}$ invertible?

13. Given $\begin{bmatrix} 3 & -6 & -3 \\ 2 & 0 & 6 \\ -4 & 7 & 4 \end{bmatrix} = \begin{bmatrix} 3 & 0 & 0 \\ 2 & 4 & 0 \\ -4 & -1 & 2 \end{bmatrix} \begin{bmatrix} 1 & -2 & -1 \\ 0 & 1 & 2 \\ 0 & 0 & 1 \end{bmatrix}$, solve the system

$$\begin{array}{llll} 3x_1 & -6x_2 & -3x_3 & = -3 \\ 2x_1 & & +6x_3 & = -22 \\ -4x_1 & +7x_2 & +4x_3 & = 3 \end{array} .$$

14. Solve $\begin{bmatrix} 2 & 6 & 2 \\ -3 & -8 & 0 \\ 4 & 9 & 2 \end{bmatrix} x = \begin{bmatrix} 2 \\ 2 \\ 3 \end{bmatrix}$ $(Ax = b)$ by

   (a) First find the LU factorization of A.

   (b) Second solve $Ly = b$.

   (c) Third solve $Ux = y$.

Chapter 4

Preliminaries

4.1 Calculus

Theorem 4.1 (Intermediate Value Theorem)**.** *If $f(x)$ is continuous on $[a, b]$, then for any m that is in between $f(a)$ and $f(b)$, there exists a number $c \in [a, b]$ such that $f(c) = m$.*

Theorem 4.2 (Taylor's Theorem)**.** *Suppose $f \in C^n[a, b]$ and $f^{(n+1)}$ exists on [a,b]. Let $x_0 \in [a, b]$. For every $x \in [a, b]$, there exists a number ξ between x_0 and x such that*

$$f(x) = f(x_0)+f'(x_0)(x-x_0)+\frac{f''(x_0)}{2!}(x-x_0)^2+\cdots+\frac{f^{(n)}(x_0)}{n!}(x-x_0)^n+\frac{f^{(n+1)}(\xi)}{(n+1)!}(x-x_0)^{n+1}. \quad (4.1)$$

Theorem 4.3 (Mean Value Theorem)**.** *If $f \in C[a, b]$ and f is differentiable on (a, b), then a number c in (a, b) exists such that*

$$f'(c) = \frac{f(b) - f(a)}{b - a}.$$

MVT is often in the form of $f(b) - f(a) = f'(c)(b-a)$, which can be rewritten as $\int_a^b f'(x)dx = f'(c)(b - a)$. This becomes the MVT for integrals:

$$\int_a^b h(x)dx = h(c)(b - a),$$

but we will present a more general version below.

Theorem 4.4 (Mean Value Theorem for Integrals)**.** *If $f \in C[a, b]$, g is integrable on [a,b] and $g(x)$ does not change sign on [a,b], then there exists a number c in (a,b) such that*

$$\int_a^b f(x)g(x)dx = f(c)\int_a^b g(x)dx.$$

4.2 Linear Algebra

4.2.1 Vector/Matrix algebra

The notation for a matrix will be a capital letter, such as A, with its corresponding lower letter (with double subscripts), such as a_{ij} to refer to ith row, jth column entry; that is

$$A = [a_{ij}] = [a_{ij}]_{m\times n} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix}$$

is an $m \times n$ matrix. The *transpose* of A is

$$A^T = [a_{ji}]_{n\times m} = \begin{bmatrix} a_{11} & a_{21} & \cdots & a_{m1} \\ a_{12} & a_{22} & \cdots & a_{m2} \\ \vdots & \vdots & \vdots & \vdots \\ a_{1n} & a_{2n} & \cdots & a_{mn} \end{bmatrix}.$$

The letters towards the end of the alphabet, like x, y, z, usually indicate vectors. **They are considered as column vectors unless otherwise stated.** For a vector x, x_i will denote its ith coordinate. The square brackets $[\cdot]$ is for matrices. Since vectors are a special kind of matrices, we have

- $x = [x_1, x_2, \cdots, x_n]$ is a row vector.
- $x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$ is a column vector.
- $x = [x_1, x_2 \cdots, x_n]^T$ is a column vector.
- $x = (x_1, x_2 \cdots, x_n)$ is a column vector. Yes, if we use parenthesis, it is a column vector!

In consideration of saving space, you will see the last two expressions often.

Given $x = (x_1, x_2 \cdots, x_n), y = (y_1, y_2, \cdots, y_n)$, and a scalar $a \in \mathbb{R}$.

$$x + ay = (x_1 + ay_1, x_2 + ay_2, \cdots, x_n + ay_n).$$

Let A be an $m \times n$ matrix and $x = (x_1, x_2 \cdots, x_n)$. There are two equivalent ways to compute Ax (a matrix times a vector). First we write

$$A = [a_{ij}]_{m\times n} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix} = \begin{bmatrix} r_1^T \\ r_2^T \\ \vdots \\ r_m^T \end{bmatrix} = [c_1, c_2, \cdots, c_n],$$

where r_i^T is the ith row of this matrix and c_j is the jth column of this matrix.

1. $Ax = \begin{bmatrix} r_1^T \\ r_2^T \\ \vdots \\ r_m^T \end{bmatrix} x = \begin{bmatrix} r_1^T x \\ r_2^T x \\ \vdots \\ r_m^T x \end{bmatrix} = \begin{bmatrix} a_{11}x_1 + a_{12}x_2 + a_{1n}x_n \\ a_{21}x_1 + a_{22}x_2 + a_{2n}x_n \\ \vdots \\ a_{m1}x_1 + a_{m2}x_2 + a_{mn}x_n \end{bmatrix}$.

2. $Ax = [c_1, c_2, \cdots, c_n] \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \sum_{i=1}^{n} x_i c_i$. Ax is a linear combination of columns of A.

A very important special case is when A is reduced to a $1 \times n$ matrix (a row vector). Given $y = (y_1, y_2, \cdots, y_n)$,

$$y^T x = [y_1, y_2, \cdots, y_n] \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \sum_{i=1}^{n} x_i y_i = x^T y = x \cdot y = \langle x, y \rangle. \tag{4.2}$$

The number in (4.2) is called the *inner product or dot product* of x and y.

For two general matrices $A = [a_{ij}]_{m \times n}, B = [b_{ij}]_{n \times p}$, their product AB is $m \times p$, and is defined as

$$(AB)_{ij} = \sum_{k=1}^{m} a_{ik} b_{kj} = a_{i1} b_{1j} + a_{i2} b_{2j} + \cdots + a_{im} b_{mj}.$$

For example, given $y = (y_1, y_2, \cdots, y_n), z = (z_1, z_2, \cdots, z_m)$. y can be viewed as $n \times 1$ matrix and z^T is $1 \times m$, then yz^T is $n \times m$ and

$$yz^T = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} [z_1, z_2, \cdots, z_m] = [y_i z_j]_{n \times m} = \begin{bmatrix} y_1 z_1 & y_1 z_2 & \cdots & y_1 z_n \\ y_2 z_1 & y_2 z_2 & \cdots & y_2 z_n \\ \vdots & \vdots & \vdots & \vdots \\ y_n z_1 & y_n z_2 & \cdots & y_n z_m \end{bmatrix}$$

For more examples, please refer to [3, Section 1.2].

A matrix $U = [u_{ij}]$ is called *upper (lower) triangular* if $u_{ij} = 0$ for $i > j$ ($i < j$). A matrix $D = [d_{ij}]$ is *diagonal* if $d_{ij} = 0$ for $i \neq j$. The *identity* matrix of order n, $I_n = [\delta_{ij}]$, is an $n \times n$ diagonal matrix with entries $\delta_{ii} = 1$. Moreover, the columns of I_n are often denoted e_i, that is $I_n = [e_1, e_2, \cdots, e_n]$.

A square matrix A is called *symmetric* if $A = A^T$. Visually, it appears that the entries of such matrices are symmetric about the diagonal.

4.2.2 Matrix Inversion

An $n \times n$ matrix A is *invertible* if there exists B such that $AB = I_n$ or $BA = I_n$.[1] The matrix B is called the *inverse* of A, denoted by A^{-1}. A matrix is called *singular* if it is not invertible; an invertible matrix is also called *nonsingular*.

Gaussian Elimination is the standard way to find out whether a matrix is invertible, and to compute its inverse when invertible. **If we only need to decide invertibility, we stop at the**

[1]The common definite requires $AB = BA = I_n$, but it can be shown that either $AB = I$ or $BA = I$ is sufficient.

end of forward elimination. If number of pivots equals n, then it's invertible; if number of pivots is less than n, then it's singular. Taking $A = \begin{bmatrix} 1 & 2 & 2 \\ 2 & 7 & 7 \\ 2 & 7 & 9 \end{bmatrix}$ for example, we already know from Example 3.1 that it's invertible because there are 3 pivots. To find its inverse, we want to find a matrix $B = [b_1, b_2, b_3]$ such that $AB = I_3$, which is $[Ab_1, Ab_2, Ab_3] = [e_1, e_2, e_3]$. This is solving three linear systems with the same coefficient matrix, so the row operations can be done in parallel, i.e., perform Gaussian elimination on $[A|e_1, e_2, e_3]$. We recycle all the row operations done in Example 3.1:

$$\left[\begin{array}{ccc|ccc} 1 & 2 & 2 & 1 & 0 & 0 \\ 2 & 7 & 7 & 0 & 1 & 0 \\ 2 & 7 & 9 & 0 & 0 & 1 \end{array}\right] \xrightarrow[\rho 1(-2)+\rho 3]{\rho 1(-2)+\rho 2} \left[\begin{array}{ccc|ccc} 1 & 2 & 2 & 1 & 0 & 0 \\ 0 & 3 & 3 & -2 & 1 & 0 \\ 0 & 3 & 5 & -2 & 0 & 1 \end{array}\right] \xrightarrow{\rho 2(-1)+\rho 3} \left[\begin{array}{ccc|ccc} 1 & 2 & 2 & 1 & 0 & 0 \\ 0 & 3 & 3 & -2 & 1 & 0 \\ 0 & 0 & 2 & 0 & -1 & 1 \end{array}\right]$$

$$\xrightarrow[\rho 2/3]{\rho 3/2} \left[\begin{array}{ccc|ccc} 1 & 2 & 2 & 1 & 0 & 0 \\ 0 & 1 & 1 & -\frac{2}{3} & \frac{1}{3} & 0 \\ 0 & 0 & 1 & 0 & -\frac{1}{2} & \frac{1}{2} \end{array}\right] \xrightarrow[\rho 3(-2)+\rho 1]{\rho 3(-1)+\rho 2} \left[\begin{array}{ccc|ccc} 1 & 2 & 0 & 1 & 1 & -1 \\ 0 & 1 & 0 & -\frac{2}{3} & \frac{5}{6} & -\frac{1}{2} \\ 0 & 0 & 1 & 0 & -\frac{1}{2} & \frac{1}{2} \end{array}\right] \xrightarrow{\rho 2(-2)+\rho 1} \left[\begin{array}{ccc|ccc} 1 & 0 & 0 & \frac{7}{3} & -\frac{2}{3} & 0 \\ 0 & 1 & 0 & -\frac{2}{3} & \frac{5}{6} & -\frac{1}{2} \\ 0 & 0 & 1 & -1 & -\frac{1}{2} & \frac{1}{2} \end{array}\right].$$

Remark 4.5. Cancellation DOES NOT hold for matrix algebra, that is $AB = AC$ DOES NOT imply $B = C$. What is true in matrix multiplication is that we can cancel invertible matrices: if A is invertible and $AB = AC$, then we can apply A^{-1} on both sides to get $B = C$.

If A, B are both invertible, then AB is also invertible and

$$(AB)^{-1} = B^{-1}A^{-1}.$$

4.2.3 Determinant

The determinant is a number associated to a square matrix and can be intuitively understood as a signed area/volume of the parallelepiped associated with the matrix. For our purpose, we need to know

- The best way (for humans or computers) to compute determinant is to use forward elimination. In Example 3.1, the determinant of the original coefficient matrix is the same as the determinant of $\begin{bmatrix} 1 & 2 & 2 \\ 0 & 3 & 3 \\ 0 & 0 & 2 \end{bmatrix}$, which is just the product of the pivots, which is 6. Scaling changes the determinant and row exchange makes the determinant the opposite.
- $\det \begin{bmatrix} a & b \\ c & d \end{bmatrix} = ad - bc$.
- Determinant of a 3×3 matrix can be found by row/column expansion. For example, if we expand along first row, then

$$\begin{vmatrix} a & b & c \\ d & e & f \\ g & h & i \end{vmatrix} = a \begin{vmatrix} e & f \\ h & i \end{vmatrix} - b \begin{vmatrix} d & f \\ g & i \end{vmatrix} + c \begin{vmatrix} d & e \\ g & h \end{vmatrix}.$$

4.2.4 Linear Independence and span

Given vectors $v_1, v_2, \cdots, v_n$ and let $A = [v_1, v_2, \cdots, v_n]$, the following are equivalent:

1. $v_1, v_2, \cdots, v_n$ are linearly independent;
2. The solution of $Ax = 0$ is unique (only $x = 0$: the trivial solution).
3. rank$A$ = number of pivots after doing forward elimination = n.

If in addition that A is square, then there are 2 additional equivalent conditions:

4. A is invertible.
5. $\det A \neq 0$.

Given a set of vectors $\{v_1, v_2, \cdots, v_m\} \subset \mathbb{R}^n$,

$\text{span}\{v_1, v_2, \cdots, v_m\}$ = all linear combinations of $v_1, \cdots, v_n = \{c_1 v_1 + \cdots + c_n v_n : c_i \in \mathbb{R}\}$

4.2.5 Eigenvalues

Given $A \in \mathbb{R}^{n \times n}$, if $Ax = \lambda x$ for some $x \neq 0$, then x is an eigenvector of A, and λ is the corresponding eigenvalue. For example, we have $\begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = 3 \begin{bmatrix} 1 \\ 1 \end{bmatrix}$, which means that $[x, 1]^T$ is an eigenvector of $A = \begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix}$, with the corresponding eigenvalue 3.

To figure out all the eigenvalues and its corresponding eigenvectors of A, we need to first find roots of $\det(A - \lambda I)$, and second solve $(A - \lambda I)x = 0$ for each root λ.

Example 4.6. Find eigenvalues and eigenvectors of $A = \begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix}$.

$\det \begin{bmatrix} 1-\lambda & 2 \\ 2 & 1-\lambda \end{bmatrix} = (1-\lambda)^2 - 4 = (1-\lambda-2)(1-\lambda+2) = (-1-\lambda)(3-\lambda)$.

$\lambda_1 = -1$, solve $\begin{bmatrix} 2 & 2 \\ 2 & 2 \end{bmatrix} x = 0$, $u_1 = [1, -1]^T$.

$\lambda_2 = 3$, solve $\begin{bmatrix} -2 & 2 \\ 2 & -2 \end{bmatrix} x = 0, u_2 = [1, 1]^T$.

4.2.6 Norm

Let $x \in \mathbb{R}^n$, then its (Euclidean) *norm* is defined as

$$\|x\| := \left(\sum_{i=1}^{n} x_i^2 \right)^{1/2} = \sqrt{x_1^2 + x_2^2 + \cdots x_n^2}. \tag{4.3}$$

Note that $x^T x = \langle x, x \rangle = \|x\|^2$. x is called a unit (norm) vector if $\|x\| = 1$.

Given an arbitrary vector x, $\dfrac{x}{\|x\|}$ is a unit vector that has the same direction as x. This is called normalization of x.

4.3 Complexity

Big O notation is frequently used in mathematics and computer science.

Let $f(x), g(x)$ be both real functions. We write

$$f(x) = O(g(x)) \text{ as } x \to \infty$$

if and only if there exist M and x_0 such that $|f(x)| \leq Mg(x)$ for all $x \geq x_0$.

This notation is used a lot in algorithm analysis. For example, for a polynomial, we have $\sum_{k=1}^{M} a_k x^k = O(x^M)$.

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