CSC336

Numerical Methods

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2025

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Part I

Part 1

CHAPTER

1 Introduction

1.1 Motivation

$$\text{Math Textbook} + \text{Laptop} + \text{Coding} \stackrel{?}{\Longrightarrow} \text{Compute Accurate Solution}$$

Consider the McLaurin series expansion of the function $f(x) = e^x$:

$$\begin{aligned} e^x &= 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots \\ &= \sum_{n=0}^{\infty} \frac{x^n}{n!} \end{aligned}$$

The issue is that we cannot compute to infinity. We need to introduce partial sums

$$S_n = \sum_{i=0}^{n} \frac{x^i}{i!}$$

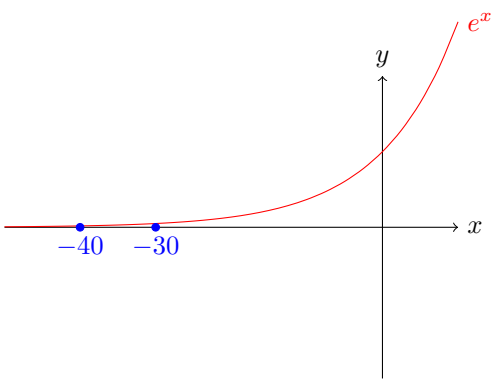
We could iterate over n until $|S_n - S_{n-1}| <$ tolerance.

x	0	1	10	20	40
Num Terms to "Converge"	2	13	42	69	104

We observe that the running time is dependent on the value of x. We need to find a better way to compute the sum – with more consistent running time.

Using the python program,

- When $x = -30$, convergence happened after 97 terms, to -6.0×10^{-5}.
- When $x = -40$, convergence happened after 124 terms, to approximately -5.9×10^{0}.



Clearly, we have inaccuracy when $x = -40$, as $0 < e^x < 1$ for all $x < 0$. The math textbooks' s techniques does not always provide good computational algorithms.

Course goal:

Show computational algorithms and discuss why they are good.

Example (e^x Better Algorithm)**.** A better algorithm is as follows

- Find k such that $r = \frac{x}{k}$ exactly with $\|r\| < 1$.
- Compute $e^r = e^{x/k}$ using the McLaurin series.
- Then, $e^x = (e^r)^k$.

♢

Remark Error due to Catasrophic Cancellation

When we subtract two numbers that are very close to each other, we lose precision.

1.2 Topics

- Computer Arithmetic and Computational Errors (Chap. 1)
  - Floating Point Arithmetic
  - Two Concepts
    - The conditioning of a math problem
    - the numerical stability of an algorithm
- Solving Systems of Linear Equations (Chap. 2)
  - Solve $Ax = b$ for x
- Solving Non-linear Equations (Chap. 5)

  Fine x s.t. $f(x) = 0$ or $g(x) = 0$ or $f(x) = g(x)$.
- Interpolation (Chap. 7)
  - Given the set of data

    $$\{(t_i, y_i)\}_{i=0}^n \qquad \text{or} \qquad \{(t_i, f(t_i))\}_{i=0}^n$$

    come up with a function $g(t)$ that approximates the data.

CHAPTER

Computer Arithmetic and Computational Errors 2

2.1 Numerical Stability

There is only finite space in computer. How would we store π, an irrational number? We can't. We can only store an approximation of π. How does introduction of approximations affect the accuracy of our computations?

Example. Suppose we want to compute the value for the sequence of integrals

$$y_n = \int_0^1 \frac{x^n}{x+5}\,dx$$

for $n = 0, 1, 2, \ldots, 8$, with 3 decimal digits of accuracy.

There are several properties that I can claim:

- $y_n > 0$ for all n, since the integrand $\frac{x^n}{x+5} > 0$ for all $x \in (0,1)$.
- $y_{n+1} < y_n$ for all n, since the integrand $\frac{x^{n+1}}{x+5} = x \cdot \frac{x^n}{x+5} < \frac{x^n}{x+5}$ for all $x \in (0,1)$.

There is not closed-form solution to this problem.

$$\begin{aligned}
x^n &= x^n \cdot \frac{x+5}{x+5} && \text{for } x \in (0,1)\\
x^n &= \frac{x^{n+1}}{x+5} + \frac{5x^n}{x+5}\\
\int_0^1 x^n\,dx &= \int_0^1 \frac{x^{n+1}}{x+5}\,dx + 5\int_0^1 \frac{x^n}{x+5}\,dx\\
\frac{1}{n+1}x^{n+1}\Big|_0^1 &= y_{n+1} + 5y_n\\
y_{n+1} &= \frac{1}{n+1} - 5y_n
\end{aligned}$$

Fortunately,

$$\begin{aligned}
y_0 &= \int_0^1 \frac{1}{x+5}\,dx\\
&= \ln(x+5)\Big|_0^1\\
&= \ln 6 - \ln 5\\
&= \ln\frac{6}{5} \doteq 0.182
\end{aligned}$$

By the recurrence,

$$\begin{aligned} y_1 &= \frac{1}{1} - 5y_0 \doteq 1 - 5(0.182) = 0.0900 \\ y_2 &= \frac{1}{2} - 5y_1 \doteq 0.5 - 5(0.0900) = 0.0500 \\ y_3 &= \frac{1}{3} - 5y_2 \doteq 0.333 - 5(0.0500) = 0.0830 \\ y_4 &= \frac{1}{4} - 5y_3 \doteq 0.25 - 5(0.0830) = -0.165 \end{aligned}$$

Clearly, something went wrong. We have a negative value for y_4, which is impossible. We also have $y_3 > y_2$. The problem is that we are using floating point arithmetic, which is not exact. We are losing precision in our calculations.

What if we leave y_0 as an unevaluated term?

$$\begin{aligned} y_1 &= 1 - 5y_0 \\ y_2 &= \frac{1}{2} - 5y_1 \\ &= -\frac{9}{2} + 25y_0 \\ y_3 &= \frac{1}{3} - 5y_2 \\ &= \frac{137}{6} - 125y_0 \\ y_4 &= \frac{1}{4} - 5y_3 \\ &= -\frac{1367}{12} + 625y_0 \end{aligned}$$

We approximated $y_0 = \ln \frac{6}{5} \approx 0.182$. We know that the true value of $y_0 \in [0.1815, 0.1825]$. Another way to express y_0 is $y_0 = 0.182 + E$, where $|E| \leq 0.0005 = 5 \times 10^{-4}$ is the error in our approximation.

Substituting this into the formula for y_4, we get

$$\begin{aligned} y_4 &= -\frac{1367}{12} + 625(0.182 + E) \\ &= -113.91\dot{6} + 113.75 + 625E \\ &= -0.1\dot{6} + 625E \end{aligned}$$

where

$$625E \leq 625 \times 5 \times 10^{-4} = 0.3125$$

and

$$y_4 < y_0 \doteq 0.182$$

so our propagated error is greater than the quantity to compute. ♢

A lesson learned from the previous example is that the math textbook algorithms does not necessarily produce good computational algorithms. This algorithms for computing y_n is said to be an **numerically unstable algorithm**, since a small error was magnified by the algorithm. We want the algorithms to be **numerically stable**.

Definition 2.1.1 Numerically Unstable

An algorithm is said to be **numerically unstable** if the error in the output is not bounded by the error in the input.

Remark

In the previous example, a small error E is magnified by 5 each step.

Example (Cont.). We can re-arrange the recurrent relation

$$\begin{aligned} y_{n+1} &= \frac{1}{n-1} - 5y_n \\ 5y_n &= \frac{1}{n+1} - y_{n+1} \\ y_{n+1} &= \frac{1}{5}\left(\frac{1}{n+1} - y_{n+1}\right) \end{aligned}$$

We have bounded the error in the output by the error in the input, but we are at a disadvantage since we are computing backwards. How can we start this recurrent relation?

Recall that

$$y_{100} < y_{99} < \cdots < y_0 \doteq 0.182$$

We start by approximating $y_{100} \doteq 0$. We know the exact value is $y_{100} = 0 + \varepsilon$, where $0 < \epsilon < 0.182$. Then,

$$\begin{aligned} y_{99} &= \frac{1}{5}\left(\frac{1}{100} - y_{100}\right) \\ &= \frac{1}{5}\left(\frac{1}{100} - (0+\varepsilon)\right) \\ &= \frac{1}{500} - \frac{\varepsilon}{5} \end{aligned} \qquad \begin{aligned} y_{98} &= \frac{1}{5}\left(\frac{1}{100} - y_{99}\right) \\ &= \frac{1}{5}\left(\frac{1}{100} - \left(\frac{1}{500} + \frac{\varepsilon}{5}\right)\right) \\ &= \cdots + \frac{\varepsilon}{25} \end{aligned}$$

We observe that the effect of the error is ε is diminished by a factor of $\frac{1}{5}$ each step. This is a numerically stable algorithm. By the time we get to y_8, we can expect an accurate result. ♢

Definition 2.1.2 Numerical Stability

An algorithm is said to be **numerically stable** if the error in the output is bounded by the error in the input.

2.2 Floating Point Arithmetic

2.2.1 Floating Point Representation

We only have finite space in the computer. This means we cannot store all real numbers, only an approximation of them. We use the **floating point representation** to store real numbers.

Definition 2.2.1 Floating Point Representation

A real number x is represented in the form

$$fl(x) = \pm d_0.d_1d_2\ldots d_{p-1} \times \beta^e \qquad d_0 \neq 0$$

where m is the **significant** or **mantissa**, β is the **base**, and e is the **exponent**.

Note:

- d_i's are bounded by
$$0 \leq d_i < \beta.$$
- p is the precision of the accuracy.
- E is also bounded by
$$L \leq E \leq U$$

With the floating point representation, we have a finite set of floating point numbers

$$F(\beta, p, L, U) = \{\pm d_0.d_1 d_2 \dots d_{p-1} \times \beta^E : 0 \leq d_i < \beta, L \leq E \leq U\}.$$

Remark $d_0 \neq 0$

We observe that this representation is not unique. Consider a system

$$F(\beta = 10, p = 5, L = -10, U = 10)$$

and the number 1.23, we have the representation

$$+1.2300 \times 10^0 \in F(10, 5, -10, 10)$$

but also

$$+0.1230 \times 10^1 \in F(10, 5, -10, 10)$$

and

$$+0.0123 \times 10^2 \in F(10, 5, -10, 10)$$

Thus, we need to choose a unique representation for each number. We can add a rule that **the first digit is not zero**, which normalizes the floating point representation, and makes representations unique.

Remark Representating Zero

Since $d_0 \neq 0$, how can we represent zero? We define another rule

$$fl(0) = 0.000 \dots 0 \times \beta^{L-1}$$

where **an exponent of $L - 1$ is used to indicate the value is denormalized**.

In the early days of computing, different manufacturers used different floating point representations. This made it difficult to write portable code. The IEEE 754 standard [2] was introduced to standardize floating point representations.

	Single Precision	Double Precision
β	2	2
p	24	53
L	-126	-1022
U	127	1023

Note:

For single precision, we have
$$E \in \{-126, -125, \dots, 127\}$$
with a cardinality of 254. If we use 8 bits to represent the exponent, we have $2^8 = 256$ possible

values. We have 2 special values: $E = L - 1 = -127$ for denormalized numbers, and $E = U + 1 = 128$ for infinity and NaN (Not a Number).

Remark Memory Requirements

For single precision, we need $1 + 24 + 8 = 33$ bits to represent a number. This is a very weird number of bits. We don't know any computer that uses 33 bits to represent a number.

Turns out we only need 23 bits for the significant, since the first digit in a normalized system is always 1. We can drop the first digit, and use 23 bits for the significant, 8 bits for the exponent, and 1 bit for the sign. This gives us 32 bits, which is a more common number of bits.

Note: Types in Different Languages

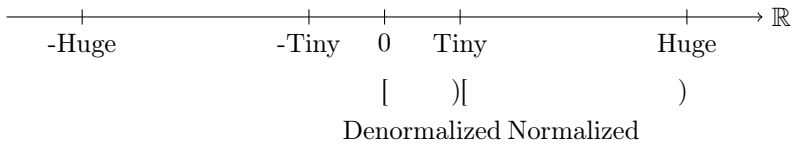
	Single Precision	Double Precision
C	`float`	`double`
Python		`float`
Rust	`f32`	`f64`

Note: Extended Precision and Reduced Precision

For accurate engineering, we may need more precision, called **extended precision** (Quad Precision). This is not part of the IEEE 754 standard, but is available in some systems.

In machine learning systems, we want the opposite – we want to use less precision to save memory and computation time. This is called **reduced precision**, and we often use 16 or 8 bits. This is a topic of active discussion, and the IEEE committee is working on a standard for reduced precision for ML.

Note that the distribution of floating point numbers is not uniform. There are more floating point numbers near zero than near $\pm\infty$. This is because the exponent is distributed uniformly, but the significant is not.



	Single	Double
HUGE	$+1.11\ldots1 \times 2^{127} \approx 3.4 \times 10^{38}$	$+1.11\ldots1 \times 2^{1023} \approx 1.8 \times 10^{308}$
TINY	$+1.00\ldots0 \times 2^{-126} \approx 1.2 \times 10^{-38}$	$+1.00\ldots0 \times 2^{-1022} \approx 2.2 \times 10^{-308}$

Remark

What about $x \in \mathbb{R}$, $x >$ HUGE? In this case, we have an overflow, and the computer will return $fl(x) = +\infty = 1.00\ldots0 \times \beta^{u+1}$.

Remark

What happens if we have $(+\infty) - (+\infty)$? In this case, we have an indeterminate form, and the

computer will return NaN (Not a Number),

$$1.xx\ldots x \times \beta^{u+1}$$

where at least one of the x's is not zero.

Remark

For $0 \leq x \leq$ TINY, take

$$fl(x) = \begin{cases} 0.00d_i d_{i+1} \ldots d_{p-1} \times \beta^{L-1} \\ 0 \qquad\qquad\qquad\qquad\qquad \text{eventually} \end{cases}$$

Example. Suppose we have

$$F(\beta, p, L, U) = F(10, 3, -10, 10)$$

and

$$x = 3.00 \times 10^5, y = 3.00 \times 10^5, \qquad x, y \in \mathbb{R}$$

Computing

$$z = x^2 + y^2$$

would give

$$z = 1.60 \times 10^{11} + 9.00 \times 10^{10} \notin F(10, 3, -10, 10)$$

and hence $fl(z) = +\text{Inf}$.

What if we instead want to compute

$$z = \sqrt{x^2 + y^2}?$$

Using the standard algorithm, we get +Inf inside the square root, and the computer will return NaN. We need to repair our algorithm.

$$h = \max(|x|, |y|) \times \sqrt{1 + \left(\frac{\min(|x|, |y|)}{\max(|x|, |y|)}\right)^2}$$

♢

Remark

The `libm` library in C and the `math` module in python both have a function called `hypot` that computes the Euclidean distance. This is a numerically stable algorithm that avoids overflow and underflow.

Note: Inf Could Have Meanings

Suppose you are computing the slope of a line, and you get infinity. This would indicate that the line is parallel to the y-axis. This is a meaningful result, and not an error.

Note: Sometimes, Underflow is OK

Recall the McLaurin series for

$$y = 1 + x + \frac{x^2}{2}$$

Suppose we are computing in $F(10, 3, -10, 10)$.

$$y = 1.00 \times 10^0 + 1.00 \times 10^{-5} + 5.00 \times 10^{-11}$$

The last term would underflow, but that's OK. We can ignore it, since it is negligible.

2.3 Computational Errors

2.3.1 Intuition

Example. We know that $\sqrt{255} = 15.9687194227\ldots$, but how should we represent this in our floating point system $F(\beta, p, L, U) = F(10, 3, -10, 10)$?

The easiest solution is **chopping** / **truncation**, where we only keep the first p digits. This gives us

$$fl(\sqrt{255}) = 1.59 \times 10^1$$

Another approach is **round to nearest**, which gives us

$$fl(\sqrt{255}) = 1.60 \times 10^1$$

♢

Remark

Heath called $x \in \mathbb{R} \to fl(x) \in F$ **rounding**. This is why we use **round-to-nearest** to disambiguate.

Note:

We can also round to +Inf or to −Inf

Note: Banker's Rounding

Banker's rounding is a method of rounding that rounds the last digit to the nearest even number, if it is exactly halfway between two numbers. This is the default rounding method in IEEE 754. This method is also known as **round to even**.

Example (Cont.). After rounding, we have error

$$fl(\sqrt{255}) - \sqrt{255} \doteq \begin{cases} -0.0687 & \text{chop} \\ 0.0313 & \text{round-to-nearest} \end{cases}$$

♢

Definition 2.3.1 Absolute and Relative Error

If $\tilde{x}$ is an approximation to x, the **absolute error in the approximation** is

$$|\tilde{x} - x|$$

and the **relative error** is

$$\frac{|\tilde{x} - x|}{|x|} \qquad x \neq 0$$

Example. The relative error of the approximation of $\sqrt{255}$ is

$$\doteq \begin{cases} 4.3 \times 10^{-3} & \text{chop} \\ 1.96 \times 10^{-3} & \text{round-to-nearest} \end{cases}$$

♢

> **Remark**
> Absolute error is not sensitive to scale, while relative error is.

Example. Let $x, y \in \mathbb{R}$, and they are approximated by $\tilde{x}, \tilde{y} \in F$.

Consider $x = 100.001, y = 0.112, \tilde{x} = 100., \tilde{y} = 0.113$. The absolute error is

$$|\tilde{x} - x| = 0.001, \quad |\tilde{y} - y| = 0.001$$

They absolute errors are the same, but this does not meas the two approximations are equally good. The relative error is

$$\frac{|\tilde{x} - x|}{|x|} \doteq 1.0 \times 10^{-5}, \quad \frac{|\tilde{y} - y|}{|y|} \doteq 9.0$$

The relative error for y is much larger than for x, so the approximation for y is worse. ♢

2.3.2 Machine Epsilon

If $x \in \mathbb{R}$ is approximated by $fl(x) \in F$, how large can the relative error be?

Example. Consider $F(10, 3, L, U), a \in \mathbb{R}$ with $a = w.xyz \times 10^E$ with $0 < w \leq 9$, $0 \leq x, y, z \leq 9$, and $L \leq E \leq U$.

Assume we determine $fl(a)$ using round to nearest,

$$|fl(a) - a| \leq 0.005 \times 10^E$$

The maximum relative error is

$$\begin{aligned} \max \frac{|fl(a) - a|}{|a|} &\leq \frac{\max |fl(a) - a|}{\min |a|} \\ &= \frac{0.005 \times 10^E}{1.000 \times 10^E} \\ &= 0.005 = \frac{1}{2} \times 10^{-2} \end{aligned}$$

♢

In general, for $x \in \mathbb{R}$ and $fl(x) \in F(\beta, p, L, U)$ with round to nearest, we have

$$\frac{|fl(x) - x|}{|x|} \leq \frac{1}{2} \times \beta^{1-p}$$

assuming x is representable.

This quantity is called the **relative round-off error bound**.

> **Definition 2.3.2** Machine Epsilon
> The **round-off error bound** or **machine epsilon** is the maximum relative error that can occur when approximating a number,
>
> $$\varepsilon_{\text{machine}} = \frac{1}{2} \times \beta^{1-p}$$

Remark

In IEEE 754, we have

$$\varepsilon_{\text{machine}} = \begin{cases} 2^{-24} \doteq 5.96 \times 10^{-8} & \text{Single Precision} \\ 2^{-53} \doteq 1.1 \times 10^{-16} & \text{Double Precision} \end{cases}$$

Example. Suppose we have $F(10, 3, -10, 10)$, $x = 1.51 \times 10^8$, and $y = 3.71 \times 10^6$, $x, y \in \mathbb{R}$, $fl(x) = x, fl(y) = y$.

We want to compute $z = x + y$. We have

$$z = 1.51 \times 10^8 + 3.71 \times 10^6 = 1.5471 \times 10^8 \notin F.$$

♢

Remark

Mathematically, addition is not closed in F.

Note:

In the CPU, there is extended precision in the floating point unit. This means that the CPU can store more digits than the standard floating point representation. This is useful for intermediate calculations, for example, the 0.0371×10^8 in the previous example, but the final result is rounded to the standard representation.

Example (Cont.).

$$fl(z) = \begin{cases} 1.54 \times 10^8 & \text{chop} \\ 1.55 \times 10^8 & \text{round-to-nearest} \end{cases}$$

We have the relative error

$$\frac{|fl(x+y) - (x+y)|}{|x+y|} = \begin{cases} 0.00459 & \text{chop} \\ 0.00187 & \text{round-to-nearest} \end{cases} \leq \varepsilon_{\text{machine}} = \begin{cases} 0.01 & \text{chop} \\ 0.005 & \text{round-to-nearest} \end{cases}$$

♢

Remark

For IEEE arithemetic, for $x, y \in F$ and operation op $\in \{+, -, *, /\}$, we must have

$$\frac{|fl(x \text{ op } y) - (x \text{ op } y)|}{|x \text{ op } y|} \leq \varepsilon_{\text{machine}}$$

and the square root of x

$$\frac{|fl(\text{sqrt}(x)) - \sqrt{x}|}{|\sqrt{x}|} \leq \varepsilon_{\text{machine}}$$

How does the error accumulates as we perform more operations?

Example.

- $\text{expr1} = \text{sqrt}(2.0) + \log(42.0)$
- $\text{expr1} = \exp(7.0) + \sin(45.0)$

We have

$$\varepsilon_{\text{expr1}} = \frac{|\text{expr1} - (\sqrt{2} + \ln(42))|}{|\sqrt{2} + \ln(42)|}$$

and

$$\varepsilon_{\text{expr2}} = \frac{|\text{expr2} - (e^7 + \sin(45))|}{|e^7 + \sin(45)|}$$

Suppose we compute

$$\text{expr1} + \text{expr2} \qquad \text{expr1} \times \text{expr2} \qquad \text{expr1} \div \text{expr2}$$

We know that

- $\varepsilon_{\text{expr1}+\text{expr2}} \leq \max(\varepsilon_{\text{expr1}}, \varepsilon_{\text{expr2}}) + |\epsilon_A|$
- $\varepsilon_{\text{expr1}\times\text{expr2}} \leq \varepsilon_{\text{expr1}} + \varepsilon_{\text{expr2}} + |\epsilon_B|$
- $\varepsilon_{\text{expr1}\div\text{expr2}} \leq \varepsilon_{\text{expr1}} + \varepsilon_{\text{expr2}} + |\epsilon_C|$

The first terms are error due to in exact operands. The last terms are due to the representing the result in floating point, and since they are representation errors, they need to be smaller than the machine epsilon,

$$|\epsilon_A|, |\epsilon_B|, |\epsilon_C| \leq \varepsilon_{\text{machine}}$$

♢

> **Remark**
> Error does not grow too quickly, but it does grow. This is why we need to be careful when performing many operations.

What about subtraction? That is a whole different story.

2.3.3 Catastrophic Cancellation

Example. Suppose we want to find the roots of

$$x^2 + (-320x) + 16 = 0.$$

From math textbooks, we know the quadratic formula

$$r_{1,2} = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

Using $F(10, 4, L, U)$, we have

$$\begin{aligned}
r_1 &= \frac{3.200 \times 10^2 + \sqrt{1.024 \times 10^5 - 6.400 \times 10^1}}{2.000 \times 10^0} \\
&\doteq \frac{3.200 \times 10^2 + \sqrt{1.023 \times 10^5}}{2.000 \times 10^0} && \text{1 round off error} \\
&\doteq \frac{3.200 \times 10^2 + 3.198 \times 10^2}{2.000 \times 10^0} \\
&= \frac{6.398 \times 10^2}{2.000 \times 10^0} \\
&= 3.199 \times 10^2
\end{aligned}$$

Similarly,

$$\begin{aligned} r_2 &= \frac{3.200 \times 10^2 - \sqrt{1.024 \times 10^5 - 6.400 \times 10^1}}{2.000 \times 10^0} \\ &\doteq \frac{3.200 \times 10^2 - \sqrt{1.023 \times 10^5}}{2.000 \times 10^0} && \text{1 round off error} \\ &\doteq \frac{3.200 \times 10^2 - 3.198 \times 10^2}{2.000 \times 10^0} \\ &= \frac{2.000 \times 10^{-1}}{2.000 \times 10^0} \\ &= 1.000 \times 10^{-1} \end{aligned}$$

You can show that the exact roots are

$$r_1^* \doteq 319.950 \quad r_2^* \doteq 0.050 \qquad r_2^* = 0.05001$$

So the relative errors

$$\varepsilon_{r_1} \doteq 1.6 \times 10^{-4} \leq \varepsilon_{\text{machine}} = 5 \times 10^{-4} \qquad \varepsilon_{r_2} \doteq 1.0$$

♢

> **Remark**
> A machine epsilon of 1 tells us that the result is completely wrong. There is no digits of accuracy in the result.

Why would this happen?

$$r_2 = \frac{3.200 \times 10^2 - 3.198 \times 10^2}{2.000 \times 10^0}$$

We know that

- 3.200×10^2 is exact
- 3.198×10^2 has 2 rounding errors, $fl(\sqrt{fl(102400 - 64)})$
- 2.000×10^0 is exact

We wanted to subtract

$$3.200 \times 10^2 - 3.198\texttt{xxxxxx} \times 10^2$$

We see that the leading terms cancel out, and `xxxxxx` are insignificant in the intermediate result, but they are significant in the final result. This is know as the **catastrophic cancellation**.

> **Definition 2.3.3** Catastrophic Cancellation
> **Catastrophic Cancellation** is the loss of significance in the result in subtracting two possibly inexact quantities close in value.

> **Remark**
> To avoid catastrophic cancellation, avoid subtracting nearly equal inexact quantities.

Example (Cont.). So how to determine r_2 accurately?

We know that

$$(1x^2 - 320x + 16) = 1 \cdot (x - r_1)(x - r_2)$$

so

- $1 \cdot r_1 r_2 = 16$ when $x = 0$
- $r_2 = \dfrac{16}{r_1} = \frac{1.600 \times 10^1}{3{,}199 \times 10^2} = 5.002 \times 10^{-2} < \epsilon_{\text{machine}}$

♢

Remark

A better algorithm to compute roots of

$$ax^2 + bx + c = 0$$

is

$$r_1 = \frac{-b - \text{sign}(b)\sqrt{b^2 - 4ac}}{2a} \qquad r_2 = \frac{c}{ar_1}$$

Why there is no catastrophic cancellation in $b^2 - 4ac$?

If there is cancellation, we must have $b^2 \approx 4ac$, which means their difference would be a small number, and the square root would be a small number. We later adds it with a much bigger number b, so the small number is insignificant, and the inaccuracy here does not affect the final result.

Example. Consider $F(10, 4, L, U)$, $x = 1,23 \times 10^1$, and $y = 2.3xx \times 10^{-2}$.

We have

$$\begin{aligned} x + y &= 12.34 + 0.023\texttt{xx} \\ &= 12.363\texttt{xx} \xrightarrow{\text{round}} fl(x + y) = 1.236 \times 10^1 \end{aligned}$$

♢

Remark

Given expr1 and expr2, with all positive intermediate results,

$$\varepsilon_{\text{expr1}-\text{expr2}} \leq \left|\frac{\text{expr1}}{\text{expr1} - \text{expr2}}\right| \varepsilon_{\text{expr1}} + \left|\frac{\text{expr2}}{\text{expr1} - \text{expr2}}\right| \varepsilon_{\text{expr2}} + \varepsilon_D$$

where $\varepsilon_D < \varepsilon_{\text{machine}}$ is the representation error.

Remark

Software try to avoid the subtraction of 2 nearly equal inexact values.

Example. Give an accurate algorithm for computing the value of

$$f(x) = \sqrt{1 + x} - 1$$

for $x > 0$.

The naïve approach would be to compute

```
f = math.sqrt(1 + x) - 1
```

but this would lead to catastrophic cancellation when x is small. The significant of any error in `math.sqrt(1+x)` is revealed by the subtraction.

A work around is to compute

$$\begin{aligned} f(x) &= (\sqrt{1+x} - 1) \cdot \frac{\sqrt{1+x}+1}{\sqrt{1+x}+1} \\ &= \frac{(1+x)-1}{\sqrt{1+x}+1} \\ &= \frac{x}{\sqrt{1+x}+1} \end{aligned}$$

and since $x > 0$, there is no catastrophic cancellation. A trade off, however, is that this approach is slower than the naïve approach as we have 1 more operation.

FUNCTION F(x)
  IF $x \geq 3$ **then**
    $f =$ `math.sqrt(1+x) - 1`
  ELSE
    $f =$ `x / (math.sqrt(1+x) + 1)`

♢

Definition 2.3.4 Numerically Stable Algorithm

An algorithm is said to be **numerically stable** if the result it produces is the exact result of a "nearby" problem.

Example. Recall computing the root for

$$1 \cdot x^2 + (-320)x + 16 = 0$$

Recall also

$$ax^2 + bx + c = 0 \qquad a(x - r_1)(x - r_2) = 0$$

are two ways to express the quadratic.
The quadratic formula gives

$$r_1\ 3.199 \times 19^2 \quad r_2 = 1.000 \times 10^{-1}$$

For which quadratic equation is this the exact solution?

$$1(x - 3.199 \times 10^2)(x - 1.000 \times 10^{-1}) = 0$$

which is the same as

$$x^2 - 320x + 31.99 = 0$$

We got the exact roots of a very different problem, $16 \to 31.99$ with a relative increment ≈ 1.

The later modifier algorithm gave us

$$r_1 = 3.199 \times 10^2 \quad r_2 = 5.002 \times 10^{-2}$$

Fir which quadratic equation is this the exact solution?

$$1(x - 3.199 \times 10^2)(x - 5.002 \times 10^{-2}) = 0$$

which is the same as

$$x^2 - 319.95002x + 16.001398 = 0$$

The difference

- $\Delta a = 0$
- $\Delta b = 0.04998$ with relative change $\doteq 1.56 \times 16^4 < \varepsilon_{\text{machine}}$
- $\Delta c = 0.01398$ with relative change $\doteq 8.74 \times 10^{-5} < \varepsilon_{\text{machine}}$

CHAPTER

Mathematically Conditioning 3

3.1 Introduction

3.1.1 Problem Statement

Suppose we want to compute $f(x)$ at $x = \bar{x}$. Suppose we do not know $\bar{x}$ exactly, but only an approximation of it, $\hat{x}$ to $\bar{x}$ where $\hat{x} \doteq \bar{x}$.

Definition 3.1.1 Signed Relative Error

The **signed relative error** in approximation of $\bar{x}$ by $\hat{x}$ is defined as

$$\delta x = \frac{\hat{x} - \bar{x}}{\bar{x}}.$$

We want to compute $f(\bar{x})$, but what we get is $f(\hat{x})$ – a slightly different problem.

$$\begin{aligned} f(\hat{x}) &= f(\bar{x}(1+\delta x)) \\ &= f(\bar{x} + \bar{x}\delta x) \\ &= f(\bar{x}) + (\bar{x}\delta x) f'(\bar{x}) + \dots && \text{Taylor series expansion} \\ &\doteq f(\bar{x}) + (\bar{x}\delta x) f'(\bar{x}) \\ &= f(\bar{x}) \left(1 + \frac{\bar{x} f'(\bar{x})}{f(\bar{x})} \delta x\right) \end{aligned}$$

The relative error in approximating $f(\bar{x})$ by $f(\hat{x})$ is

$$\frac{|f(\hat{x}) - f(\bar{x})|}{|f(\bar{x})|} = \left|\frac{\bar{x} f'(\bar{x})}{f(\bar{x})}\right| |\delta x|.$$

An accurate estimation is when $\left|\frac{\bar{x} f'(\bar{x})}{f(\bar{x})}\right|$ is small. This is known as the **condition number** of the problem.

Definition 3.1.2 Condition Number

The condition number of evaluating $f(x)$ is defined as

$$\kappa_f(x) = \left|\frac{x f'(x)}{f(x)}\right|.$$

Remark

Note we nave not written any algorithm. The condition number is a pure mathematical concept.

Remark

When $\kappa_f(x)$ is small, the problem is **well-conditioned**. When $\kappa_f(x)$ is large, the problem is **ill-conditioned**.

Remark Rule of Thumb

You loose approximately

$$\log_2 \kappa_f(x)$$

bits of accuracy when you approximate $f(\bar{x})$ by $f(\hat{x})$.

Example. Consider $f(x) = \sqrt{x}$. Let $\hat{x} \doteq \bar{x}$.

How well does $f(\hat{x})$ approximate $f(\bar{x})$?

Let's look at the conditional number for this function,

$$\begin{aligned}
\kappa_{\sqrt{}}(x) &= \left| \frac{x \frac{d}{dx}\sqrt{x}}{\sqrt{x}} \right| \\
&= \left| \frac{x \cdot \frac{1}{2} \cdot \frac{1}{\sqrt{x}}}{\sqrt{x}} \right| \\
&= \frac{1}{2}.
\end{aligned}$$

Since $\kappa_{\sqrt{}}(x) < 1$, $\sqrt{\hat{x}}$ is a good approximation to $\sqrt{\bar{x}}$. Any error δx in $\hat{x}$ becomes $\frac{1}{2}\delta x$ in $f(\hat{x})$ in the relative sense.

We draw the conclusion that evaluating square roots is a well-conditioned problem. If we have an numerically stable algorithm to compute square roots, we should get an accurate result. ♢

Remark

If we use a numerically stable algorithm on a well-conditioned problem, we should get an accurate result.

The contra positive is also true: if we get an inaccurate result, then either the problem is ill-conditioned or the algorithm is not numerically stable.

Example. Consider $f(x) = \ln(x)$. Let $\hat{x} \doteq \bar{x}$.

Suppose we want to evaluate $\ln(0.999)$, where 0.999 is an intermediate result with some error. We will get $\ln(0.999) \doteq -1.0005 \times 10^{-3}$.

Consider a 0.01% relative change to argument,

$$\ln(0.999(1 + 0.00001)) = -9.0049 \times 10^{-4} = -1.0005 \times 10^{-3}(1 + 0.09996)$$

We see that the relative error in the result is 9.996%. A small change in the argument results in a large change in the result. This tells us that evaluating logarithms must be an ill-conditioned problem.

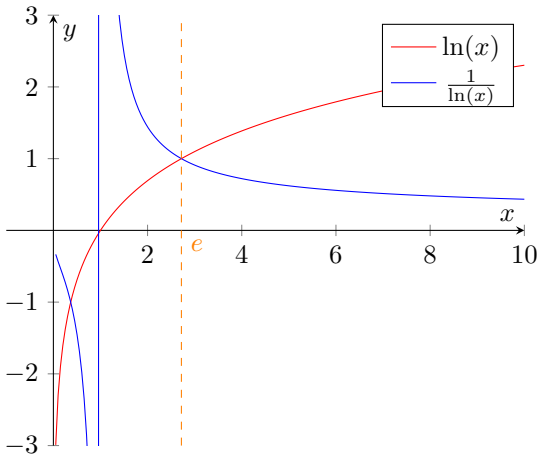
$$\begin{aligned}
\kappa_{\ln}(x) &= \left| \frac{x \frac{d}{dx}\ln(x)}{\ln(x)} \right| \\
&= \left| \frac{x \frac{1}{x}}{\ln(x)} \right| \\
&= \frac{1}{\ln(x)}.
\end{aligned}$$

At $x = 0.999$, we have

$$\kappa_{\ln}(0.999) = \frac{1}{\ln(0.999)} \doteq 999.5.$$

For x near 0.999, the effect of a small error is magnified by approximately 1000. ♢

Example. Is $f(x) = \ln(x)$ always ill-conditioned? No.



We see that $\kappa_{\ln}(x)$ is small for x near 0 and $x > e$.
What about x near 1? We introduce a new argument w,

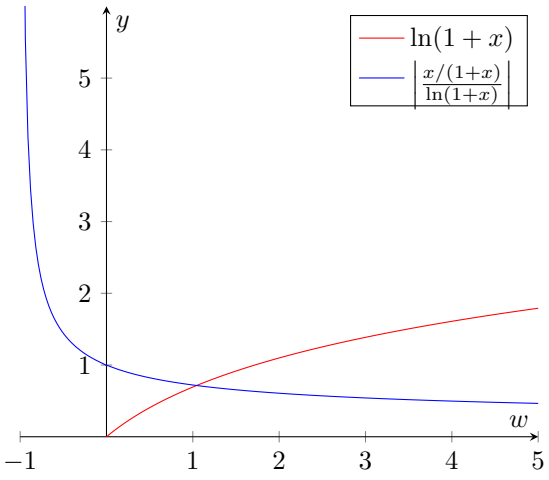
$$\ln(x) = \ln(1 + w)$$

Consider $g(w) = \ln(1 + w)$.

$$\kappa_g(w) = \left| \frac{w \frac{d}{dw} \ln(1 + w)}{\ln(1 + w)} \right|$$
$$= \left| \frac{w \cdot \frac{1}{1+w}}{\ln(1 + w)} \right|$$

We know that $f(x)$ is ill-conditioned for $x \to 1, w \to 0$. What is $\kappa_g(w)$ for $w \to 0$?
Using L'Hôpital's Rule,

$$\lim_{w \to 0} \left| \frac{w \cdot \frac{1}{1+w}}{\ln(1 + w)} \right| = 1.$$



♢

> **Remark**
>
> In `libm`, the C standard math library, the function `log1p` is used to compute $\ln(1+x)$ for small x. This function is numerically stable for small x.

Example. How to accurately evaluate

$$f(x) = x = \sqrt{x^2 - 1} \qquad \text{for } |x| > 1$$

♢

CHAPTER

Linear systems 4

4.1 Introduction

Definition 4.1.1 Non-Singular Matrix

A coefficient matrix A is **non-singular** if and only if

$$\exists A^{-1} \text{ such that } AA^{-1} = A^{-1}A = I$$

Remark

Some facts

- $A\underline{x} = \underline{b}$ has a **unique** solution if and only if A is non-singular.
- A is non-singular if and only if $\det(A) \neq 0$.

In the contrast, a singular matrix is one that is not invertible.

Proposition 4.1.2

If $\exists z \neq 0$ such that $Az = 0$, then A is singular.

Remark

Suppose exists y such that $A\underline{y} = \underline{b}$, then $y + \alpha z$ solves $A\underline{x} = \underline{b}$ may not be a solution.
For example,

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

has no solution.

We will stick to the case where A is non-singular.

4.1.1 Cramer's Rule

Definition 4.1.3 Cramer's Rule

For a linear system $A\underline{x} = \underline{b}$, the solution is

$$x_i = \frac{\det(A_i)}{\det(A)}$$

where A_i is the matrix obtained by replacing the ith column of A with b.

Remark

Cramer's Rule is not practical for large systems, as it requires $n+1$ determinants.

4.2 Gaussian Elimination

Alternatively, we can compute A^{-1} and then $x = A^{-1}b$.

To solve for A^{-1}, we solve for $AY = I$, then $x = Yb$.

For $i = 1$ to n: use some method to solve $Ay_i = e_i = \begin{pmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix}$.

4.2.1 Intuition

Case I

Suppose A is non-singular diagonal matrix,

$$A = \begin{pmatrix} a_1 & 0 & \cdots & 0 \\ 0 & a_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & a_n \end{pmatrix}$$

We must have $\begin{cases} a_{ij} \neq 0 & \text{if } i = j \\ a_{ij} = 0 & \text{if } i \neq j \end{cases}$

Indeed, since A non-singular, $\det(A) \neq 0$, and since A diagonal, $\det(A) = a_1 a_2 \cdots a_n \neq 0$. None of the diagonal elements can be zero.

Then, for $Ax = b$, we have $x_i = b_i / a_{i,i}$. We can solve this within a single loop.

FOR $i = 1$ to n **do**
  $x_i = b_i / a_{i,i}$

To count the number of operations, we define a new unit of operation, the **flop**.

Definition 4.2.1 FLOP

A **FLOP** is a **F**loating-point **L**inear **O**peration. This is a single arithmetic operation on floating-point numbers.

Example. For the above algorithm, each iteration require 1 FLOP – a division. Thus, we require n FLOPs to solve the system. ♢

Case II

Suppose A is non-singular lower-triangular,

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

We must have $\begin{cases} a_{ij} = 0 & \text{if } i < j \\ a_{ii} \neq 0 & \text{since } A \text{ non-singular} \end{cases}$

- $x_1 = b_1/a_{1,1}$
- $x_2 = (b_2 - a_{2,1}x_1)/a_{2,2}$
- $x_3 = (b_3 - a_{3,1}x_1 - a_{3,2}x_2)/a_{3,3}$
- $\vdots$
- $x_i = \left(b_i - \sum_{j=1}^{i-1} a_{ij}x_j\right)/a_{ii}$

This algorithm is called **forward substitution**.

```
FUNCTION FORWARDSUBSTITUTION(A, b)
    FOR i = 1 TO n do
        sum = 0
        FOR j = 1 TO i − 1 do
            sum = sum + a_ij · x_j
        x_i = (b_i − sum)/a_ii
    RETURN x
```

We have the operation count

$$\sum_{i=1}^{n}\left[\left(\sum_{j=1}^{i-1} 2\right) + 2\right] = n^2 + \Theta(n) \text{ FLOPs.}$$

Case III

Suppose A is non-singular upper-triangular,

$$A = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ 0 & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & a_{nn} \end{pmatrix}$$

We must have $\begin{cases} a_{ij} = 0 & \text{if } i > j \\ a_{ii} \neq 0 & \text{since } A \text{ non-singular} \end{cases}$

- $x_n = b_n/a_{n,n}$
- $x_{n-1} = (b_{n-1} - a_{n-1,n}x_n)/a_{n-1,n-1}$
- $x_{n-2} = (b_{n-2} - a_{n-2,n}x_n - a_{n-2,n-1}x_{n-1})/a_{n-2,n-2}$
- $\vdots$
- $x_i = \left(b_i - \sum_{j=i+1}^{n} a_{ij}x_j\right)/a_{ii}$

This algorithm is called **backward substitution**.

FUNCTION BACKWARDSUBSTITUTION(A, b)
  FOR $i = n$ DOWNTO 1 **do**
    $sum = 0$
    FOR $j = i + 1$ TO n **do**
      $sum = sum + a_{ij} \cdot x_j$
    $x_i = (b_i - sum)/a_{ii}$
  RETURN x

The operation count will be the same as for forward substitution,

$$n^2 + \Theta(n) \text{ FLOPs.}$$

Case IV

What if A is dense? We can use Gaussian elimination to reduce A to a triangular form.

4.2.2 Gaussian Elimination

Example. Suppose we want to solve the linear system

$$\begin{pmatrix} 2 & 1 & 1 & 0 \\ 4 & 3 & 3 & 1 \\ 8 & 7 & 9 & 5 \\ 6 & 7 & 9 & 8 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ -1 \\ 3 \end{pmatrix}$$

Recall from linear algebra that elementary operations do not change the solution to the system. We can use the elementary row operation

$$R_j = R_j - m \cdot R_i$$

to convert A to an upper-triangular form.

1. $R_2 = R_2 - 2 \cdot R_1 \qquad R_3 = R_3 - 4 \cdot R_1 \qquad R_4 = R_4 - 3 \cdot R_1$

$$\begin{pmatrix} 2 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ 0 & 3 & 5 & 5 \\ 0 & 4 & 6 & 8 \end{pmatrix} \underline{x} = \begin{pmatrix} 1 \\ -1 \\ -5 \\ -6 \end{pmatrix}$$

2. $R_3 = R_3 - 3 \cdot R_2 \qquad R_4 = R_4 - 4 \cdot R_2$

$$\begin{pmatrix} 2 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ 0 & 0 & 2 & 2 \\ 0 & 0 & 2 & 4 \end{pmatrix} \underline{x} = \begin{pmatrix} 1 \\ -1 \\ -2 \\ -2 \end{pmatrix}$$

3. $R_4 = R_4 - R_3$

$$\begin{pmatrix} 2 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ 0 & 0 & 2 & 2 \\ 0 & 0 & 0 & 2 \end{pmatrix} \underline{x} = \begin{pmatrix} 1 \\ -1 \\ -2 \\ 0 \end{pmatrix}$$

We now have a triangular system. We can use backward substitution to solve for x.

$$\underline{x} = \begin{pmatrix} 1 \\ 0 \\ -1 \\ 0 \end{pmatrix}$$

How could we program this algorithm? ♢

```
1: Function GaussianElimination(A, b)
2:     n ← size(A)
3:     ms ← []                                          ▷ Multipliers
4:     For i ← 1 To n − 1 do                            ▷ Going down the diagonal
5:         For j ← i + 1 To n do                        ▷ Below the diagonal
6:             m ← A_{j,i}/A_{i,i}
7:             ms[j, i] ← m
8:             For k ← i + 1 To n do
9:                 A_{j,k} ← A_{j,k} − m · A_{i,k}
10:    Return A, ms
```

Remark

The reason not to update b, but rather to store the multipliers, is that often in practice we have multiple right-hand sides. We can then use the same multipliers to solve for all right-hand sides.

What is the operation count for Gaussian elimination? We consider only the operations on A, since the operations on b are negligible.

- The inner most operation occurs on line 9, with 2 FLOPs.
- They are repeated for $k = i + 1$ to n, $\sum_{k=i+1}^{n} 2$ FLOPs.
- There is one more operation on line 6, with 1 FLOP.
- The j loop is repeated for $j = i + 1$ to n, $\sum_{j=i+1}^{n} \left(1 + \sum_{k=i+1}^{n} 2\right)$ FLOPs.
- The outer loop is repeated for $i = 1$ to $n - 1$, $\sum_{i=1}^{n-1} \left(1 + \sum_{j=i+1}^{n} \left(1 + \sum_{k=i+1}^{n} 2\right)\right)$ FLOPs.

We then simplify

$$\begin{aligned} \text{FLOP} &= \sum_{i=1}^{n-1} \left(1 + \sum_{j=i+1}^{n} \left(1 + \sum_{k=i+1}^{n} 2\right)\right) \\ &= \sum_{i=1}^{n-1} \left(1 + \sum_{j=i+1}^{n} (1 + 2(n-i))\right) \\ &= \sum_{i=1}^{n-1} [(n-i)(1 + 2(n-i))] \end{aligned}$$

Taking $m = n - i$, we have

$$\begin{aligned}\text{FLOP} &= \sum_{m=1}^{n-1} m(1+2m) \\ &= \left(\sum_{m=1}^{n-1} m\right) + 2\left(\sum_{m=1}^{n-1} m^2\right) \\ &= \frac{n(n-1)}{2} + 2 \cdot \frac{2n^3 - 3n^2 + n}{6} \\ &= \frac{2n^3}{3} - \frac{n^2}{2} - \frac{n}{6} \\ &= \frac{2}{3}n^3 + \Theta(n^2) \text{ FLOPs}\end{aligned}$$

4.2.3 Gauss Transforms

Definition 4.2.2 Gauss Transformation Matrix

A $n \times n$ **Gauss transformation matrix** m_R is defined as

$$m_R = I - \underline{m}_r \cdot \underline{e}_r^\top$$

where $m_R \in \mathbb{R}^n$ and

$$\underline{m}_r = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ m_{r+1,r} \\ m_{r+2,r} \\ \vdots \\ m_{n,r} \end{pmatrix} \quad \text{and} \quad \underline{e}_r = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \; r\text{th row} \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

Remark

$$\begin{aligned} M_r &= I - m_r e_r^\top \\ &= I - \begin{pmatrix} 0 & & & & \\ & \ddots & & & \\ & & 0 & & \\ & & m_{r+1,r} & 0 & \\ & & m_{r+2,r} & 0 & 0 \\ & & \vdots & & \ddots \\ & & m_{n,r} & & 0 \end{pmatrix} = \begin{pmatrix} 1 & & & & \\ & \ddots & & & \\ & & 1 & & \\ & & -m_{r+1,r} & 1 & \\ & & -m_{r+2,r} & 0 & 1 \\ & & \vdots & & \ddots \\ & & -m_{n,r} & & 1 \end{pmatrix} \end{aligned}$$

Note: Properties of Gauss Transforms

Gauss transforms have nice properties:

1. For indices $r \leq s$,

$$M_r M_s = I - \underline{m}_r \underline{e}_r^\top - \underline{m}_s \underline{e}_s^\top$$

(not a Gauss transform)

2. $$M_r^{-1} = I + \underline{m}_r \underline{e}_r^\top$$

(is a Gauss transform)

3. For any $n-$vector $\underline{v} = [v_1, v_2, \ldots, v_n]^\top$,

$$\begin{aligned} M_r \underline{v} &= (I - \underline{m}_r \underline{e}_r^\top)\underline{v} \\ &= \underline{v} - \underline{m}_r (\underline{e}_r^\top \underline{v}) \\ &= \underline{v} - v_r \underline{m}_r \\ &= \begin{pmatrix} v_1 \\ \vdots \\ v_r \\ v_{r+1} - v_r m_{r+1,r} \\ \vdots \\ v_n - v_r m_{n,r} \end{pmatrix} \end{aligned}$$

Example. Suppose

$$A = \begin{pmatrix} 2 & 1 & 1 & 0 \\ 4 & 3 & 3 & 1 \\ 8 & 7 & 9 & 5 \\ 6 & 7 & 9 & 8 \end{pmatrix}$$

- Choose

$$m_1 = \begin{pmatrix} 0 \\ 2 \\ 4 \\ 3 \end{pmatrix} \implies M_1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ -2 & 1 & 0 & 0 \\ -4 & 0 & 1 & 0 \\ -3 & 0 & 0 & 1 \end{pmatrix}$$

We have

$$M_1 A = \begin{pmatrix} 1 & 0 & 0 & 0 \\ -2 & 1 & 0 & 0 \\ -4 & 0 & 1 & 0 \\ -3 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 2 & 1 & 1 & 0 \\ 4 & 3 & 3 & 1 \\ 8 & 7 & 9 & 5 \\ 6 & 7 & 9 & 8 \end{pmatrix} = \begin{pmatrix} 2 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ 0 & 3 & 5 & 5 \\ 0 & 4 & 6 & 8 \end{pmatrix}$$

- Choose

$$m_2 = \begin{pmatrix} 0 \\ 0 \\ 3 \\ 4 \end{pmatrix} \implies M_2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & -3 & 1 & 0 \\ 0 & -4 & 0 & 1 \end{pmatrix}$$

We have

$$M_2 M_1 A = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & -3 & 1 & 0 \\ 0 & -4 & 0 & 1 \end{pmatrix} \begin{pmatrix} 2 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ 0 & 3 & 5 & 5 \\ 0 & 4 & 6 & 8 \end{pmatrix} = \begin{pmatrix} 2 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ 0 & 0 & 2 & 2 \\ 0 & 0 & 2 & 4 \end{pmatrix}$$

- Choose

$$m_3 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \implies M_3 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & -1 & 1 \end{pmatrix}$$

We have

$$M_3M_2M_1A = \begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&-1&1\end{pmatrix}\begin{pmatrix}2&1&1&0\\0&1&1&1\\0&0&2&2\\0&0&2&4\end{pmatrix} = \begin{pmatrix}2&1&1&0\\0&1&1&1\\0&0&2&2\\0&0&0&2\end{pmatrix}$$

We end up with an upper-triangular matrix

$$U = M_3M_3M_1A = \begin{pmatrix}2&1&1&0\\0&1&1&1\\0&0&2&2\\0&0&0&2\end{pmatrix}$$

This also implies

$$\begin{aligned}A = (M_3M_2M_1)^{-1}U &= M_1^{-1}M_2^{-1}M_3^{-1}U\\ &= (I+\underline{m}_1\underline{e}_1^\top)(I+\underline{m}_2\underline{e}_2^\top)(I+\underline{m}_3\underline{e}_3^\top)U \qquad \text{by property 2}\\ &= \begin{pmatrix}1&0&0&0\\2&1&0&0\\4&3&1&0\\3&4&1&1\end{pmatrix}U\end{aligned}$$

and we have an anti lower-triangular matrix

$$L = \begin{pmatrix}1&0&0&0\\2&1&0&0\\4&0&1&0\\3&0&0&1\end{pmatrix}$$

We can think of Gaussian Elimination as factoring A into LU, where L is lower-triangular and U is upper-triangular.

Verify:

$$LU = \begin{pmatrix}1&0&0&0\\2&1&0&0\\4&3&1&0\\3&4&1&1\end{pmatrix}\begin{pmatrix}2&1&1&0\\0&1&1&1\\0&0&2&2\\0&0&0&2\end{pmatrix} = \begin{pmatrix}2&1&1&0\\4&3&3&1\\8&7&9&5\\6&7&9&8\end{pmatrix}$$

♢

4.3 Solving System of Linear Equations

4.3.1 LU Factorization

How to solve $A\underline{x} = \underline{b}$?

1. Factor $A = LU$

   The operation cont is

   $$\frac{2}{3}n^3 + \Theta(n^2) \text{ FLOPs}$$

   Then, we have

   $$L(U\underline{x}) = \underline{b}$$

   Let $\underline{y} = U\underline{x}$, we have an triangular system

   $$L\underline{y} = \underline{b}$$

2. Solve $L\underline{y} = \underline{b}$ for $\underline{y}$ using forward substitution.
   The operation count is
   $$n^2 + \Theta(n) \text{ FLOPs}$$
   Then, we have
   $$U\underline{x} = \underline{y}$$

3. Solve $U\underline{x} = \underline{y}$ for $\underline{x}$ using backward substitution.
   The operation count is
   $$n^2 + \Theta(n) \text{ FLOPs}$$
   The total operation count is
   $$n^2 + \Theta(n) \text{ FLOPs}$$

4. The total cost is
   $$\frac{2}{3}n^3 + \Theta(n^2) \text{ FLOPs}$$

Remark

Now, suppose we are given a new problem

$$A\underline{z} = \underline{c} \qquad \text{for } \underline{z}$$

where A is the same as before, but $\underline{c}$ is different.

Note that the output from step 1 depends solely on A, and we do not need to recompute it. We *skip the most expensive step*, and use the same L and U to solve for $\underline{z}$ using forward and backward substitution.

- Solve $L\underline{d} = \underline{c}$ for $\underline{d}$ using forward substitution
- Solve $U\underline{z} = \underline{d}$ for $\underline{z}$ using backward substitution

The total new cost is
$$2n^2 + \Theta(n) \text{ FLOPs}$$

Remark

How to reduce memory usage?
Note that

- L is unit lower triangular (diagonal is all 1s)
- U is upper triangular, and
- A is dense.

We can store L and U in a single matrix, for example,

$$\begin{pmatrix} 2 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 \\ 4 & 3 & 2 & 2 \\ 3 & 4 & 1 & 2 \end{pmatrix}$$

where

$$L = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 2 & 1 & 0 & 0 \\ 4 & 3 & 1 & 0 \\ 3 & 4 & 1 & 1 \end{pmatrix} \quad \text{and} \quad U = \begin{pmatrix} 2 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ 0 & 0 & 2 & 2 \\ 0 & 0 & 0 & 2 \end{pmatrix}$$

Edge-case

Example. Suppose we want to compute the LU factorization of

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

The algorithm fails from 0 division

$$m_{1,1} = \frac{1}{0}$$

However, we could perform a row exchange $R_1 \leftrightarrow R_2$ to get

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

which is now solvable.

♢

We can use permutation matrix to keep track row exchanges. The permutation matrix for the i-th permutation interchanging rows i, r_i is the identity matrix with rows i, r_i swapped.

Remark

This is also the identity with **columns** i, r_i interchanged.

Example. Consider 3×3 matrices.

$$P_{2,3} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

is the permutation matrix that swaps rows 2 and 3.

We verify that

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

What if we perform right-multiplication, i.e. $AP_{2,3}$?

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

which swaps columns 2 and 3. ♢

Remark

We can use permutation matrices to keep track of row exchanges in LU factorization.
Suppose we have a permutation matrix P_{i,r_i} and a matrix A.

- $P_{i,r_i}A$ swaps *rows* i, r_i in A.
- AP_{i,r_i} swaps *columns* i, r_i in A.

Note: Facts

Note that

$$P_{i,r_i}^{-1} = P_{i,r_i}^{\top} = P_{r_i,i}.$$

Example. Suppose after two steps of gaussian elimination, we have

$$\begin{pmatrix} x_{11} & x_{12} & x_{13} & x_{14} & x_{15} \\ 0 & x_{22} & x_{23} & x_{24} & x_{25} \\ 0 & 0 & x_{33} & x_{34} & x_{35} \\ 0 & 0 & x_{43} & x_{44} & x_{45} \\ 0 & 0 & x_{53} & x_{54} & x_{55} \end{pmatrix}$$

- If $x_{33} \neq 0$, no interchanging is required, and $P_{i,r_i} = I$.
- However, if $x_{33} = 0$, we need to get the zero off the diagonal
  We only consider the submatrix
  $$\begin{pmatrix} x_{33} & x_{34} & x_{35} \\ x_{43} & x_{44} & x_{45} \\ x_{53} & x_{54} & x_{55} \end{pmatrix}$$
  since the rest of the matrix is already in upper-triangular form.

♢

The gaussian elimination factorization becomes

$$M_{n-1}P_{n-1,r_{n-1}} \cdots M_2 P_{2,r_2} M_1 P_{1,r_1} A = U$$

we can re-arrange to isolate the permutations from the eliminations.

Example. Consider a 3×3 case

$$M_2 P_2 M_1 P_1 A = U$$

with

$$P_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \quad \text{and} \quad M_1 = \begin{pmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 3 & 0 & 1 \end{pmatrix}$$

We have

$$P_2 M_1 = \begin{pmatrix} 1 & 0 & 0 \\ 3 & 0 & 1 \\ 2 & 1 & 0 \end{pmatrix}$$

which is not a permutation matrix.

We can then write

$$P_2 M_1 P_2 = \begin{pmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 3 & 0 & 1 \end{pmatrix}$$

Since $P_2^{-1} = P_2$, we have

$$P_2 M_1 P_2 P_2 = P_2 M_1$$

This allows us to re-write the factorization as

$$\begin{aligned} U &= M_2 P_2 M_1 P_1 A \\ &= M_2 P_2 M_1 P_2 P_2 P_1 A \\ &= M_2 \hat{M}_1 P_2 P_1 A \qquad \text{where } \hat{M}_1 = P_2 M_1 P_2 \end{aligned}$$

♢

For larger systems, we generalize

$$\begin{aligned} U &= M_{n-1}P_{n-1}M_{n-2}P_{n-2}\cdots P_3M_2P_2M_1P_1A \\ &= M_{n-1}P_{n-1}M_{n-2}P_{n-2}\cdots P_3M_2\hat{M}_1P_2P_1A && \text{where } \hat{M}_1 = P_2M_1P_2 \\ &= M_{n-1}P_{n-1}M_{n-2}P_{n-2}\cdots P_3\hat{M}_2P_2P_1A && \text{where } \hat{M}_2 = P_3M_2\hat{M}_1P_3 \\ &\vdots \\ &= \hat{M}_{n-1}P_{n-1}P_{n-2}\cdots P_3P_2P_1A \end{aligned}$$

We re-label as

$$L^{-1}PA = U$$

where

- $L^{-1} = \hat{M}_{n-1}$
- $P = P_{n-1}P_{n-2}\cdots P_3P_2P_1$

Our algorithm now becomes

1. Find P, L, U such that $PA = LU$
2. Since $A\underline{x} = \underline{b}$, $PA\underline{x} = P\underline{b}$
3. Solve $LU\underline{x} = P\underline{b}$ for $\underline{x}$
   a. Solve $L\underline{y} = P\underline{b}$ for $\underline{y}$ using forward substitution
   b. Solve $U\underline{x} = \underline{y}$ for $\underline{x}$ using backward substitution

> **Remark**
>
> We ask the following questions
>
> 1. How to deduce a simple expression for P^{-1}
> 2. How to store P?

Part II

Appendices

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