CSC336

Numerical Methods

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2025

CONTENTS

Part I

Part 1

CHAPTER

Introduction 1

1.1 Motivation

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

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

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

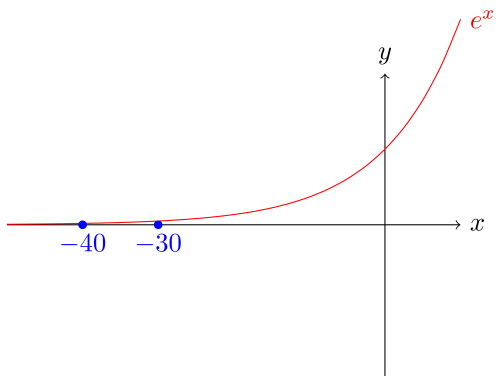
We could iterate over n until $|S_n - S_{n-1}| <$ tolerance.

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

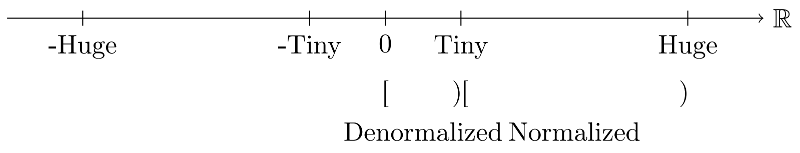
	Single Precision	Double Precision
C	`float`	`double`
Python		`float`
Rust	`f32`	`f64`

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),

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

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

Remark

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

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

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 $\in \{\texttt{+}, \texttt{-}, \texttt{*}, \texttt{/}\}$, 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

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

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,

$$\begin{aligned}
r_2 &= \frac{3.200\times10^2 - \sqrt{1.024\times10^5 - 6.400\times10^1}}{2.000\times10^0} \\
&\doteq \frac{3.200\times10^2 - \sqrt{1.023\times10^5}}{2.000\times10^0} && \text{1 round off error} \\
&\doteq \frac{3.200\times10^2 - 3.198\times10^2}{2.000\times10^0} \\
&= \frac{2.000\times10^{-1}}{2.000\times10^0} \\
&= 1.000\times10^{-1}
\end{aligned}$$

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

$$\varepsilon_{r_1} \doteq 1.6\times10^{-4} \le \varepsilon_{\text{machine}} = 5\times10^{-4} \qquad \varepsilon_{r_2} \doteq 1.0$$

$\diamondsuit$

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?

$$r_2 = \frac{3.200\times10^2 - 3.198\times10^2}{2.000\times10^0}$$

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

$$3.200\times10^2 - 3.198\text{xxxxxx}\times10^2$$

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 $x = 0$
- $r_2 = \frac{16}{r_1} = \frac{1.600\times10^1}{3{,}199\times10^2} = 5.002 \times 10^{-2} < \epsilon_{\text{machine}}$

◇

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

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

◇

Remark

Given expr1 and expr2, with all positive intermediate results,

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

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 $\doteq 8.74 \times 10^{-5} < \varepsilon_{\text{machine}}$

$\diamondsuit$

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

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

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.

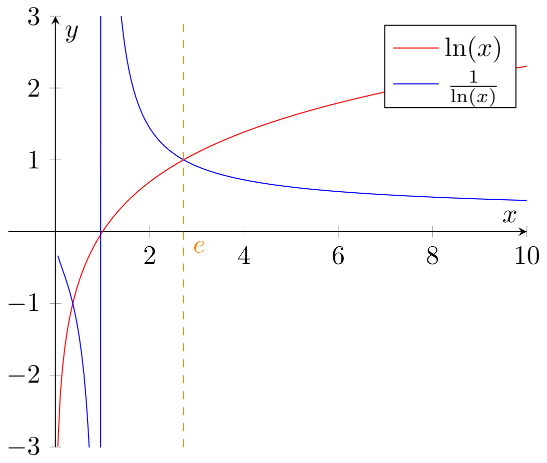
$$\begin{aligned}\kappa_{\ln}(x) &= \left|\frac{x\frac{d}{dx}\ln(x)}{\ln(x)}\right| \\ &= \left|\frac{x\frac{1}{x}}{\ln(x)}\right| \\ &= \frac{1}{\ln(x)}.\end{aligned}$$

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,

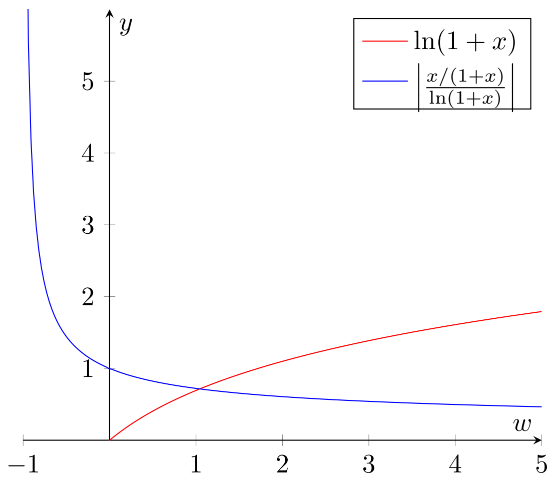
$$\ln(x) = \ln(1 + w)$$

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

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

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,

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



$\diamondsuit$

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

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

$\diamondsuit$

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
            $sum = sum + a_{ij} \cdot x_j$
        $x_i = (b_i - sum)/a_{ii}$
    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:      $n \leftarrow$ size($A$)
3:      $ms \leftarrow$ []                                    ▷ Multipliers
4:      FOR $i \leftarrow 1$ TO $n-1$ do                      ▷ Going down the diagonal
5:          FOR $j \leftarrow i+1$ TO $n$ do                  ▷ Below the diagonal
6:              $m \leftarrow A_{j,i}/A_{i,i}$
7:              $ms[j,i] \leftarrow m$
8:              FOR $k \leftarrow i+1$ TO $n$ do
9:                  $A_{j,k} \leftarrow A_{j,k} - m \cdot A_{i,k}$
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

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

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

$$M_1A = \begin{pmatrix} 1 & 0 & 0 & 0 \\ -2 & 1 & 0 & 0 \\ -4 & 0 & 1 & 0 \\ -3 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 2 & 1 & 1 & 0 \\ 4 & 3 & 3 & 1 \\ 8 & 7 & 9 & 5 \\ 6 & 7 & 9 & 8 \end{pmatrix} = \begin{pmatrix} 2 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ 0 & 3 & 5 & 5 \\ 0 & 4 & 6 & 8 \end{pmatrix}$$

- 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

$$M_2M_1A = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & -3 & 1 & 0 \\ 0 & -4 & 0 & 1 \end{pmatrix} \begin{pmatrix} 2 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ 0 & 3 & 5 & 5 \\ 0 & 4 & 6 & 8 \end{pmatrix} = \begin{pmatrix} 2 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ 0 & 0 & 2 & 2 \\ 0 & 0 & 2 & 4 \end{pmatrix}$$

- 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

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

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:

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

$\diamondsuit$

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
  $$\begin{pmatrix} x_{33} & x_{34} & x_{35} \\ x_{43} & x_{44} & x_{45} \\ x_{53} & x_{54} & x_{54} \end{pmatrix}$$
  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.

4.4 Gaussian Elimination with Pivoting

4.4.1 Instability of Gaussian Elimination

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

$$\begin{aligned} U &= M_2P_2M_1P_1A \\ &= M_2P_2M_1P_2P_2P_1A \\ &= M_2\hat{M}_1P_2P_1A && \text{where } \hat{M}_1 = P_2M_1P_2 \end{aligned}$$

◊

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}

$$\begin{aligned} P^{-1} &= (P_{n-1}P_{n-2}\cdots P_3P_2P_1)^{-1} \\ &= P_1^{-1}P_2^{-1}\cdots P_{n-2}^{-1}P_{n-1}^{-1} \\ &= P_1^\top P_2^\top\cdots P_{n-2}^\top P_{n-1}^\top \\ &= (P_{n-1}P_{n-2}\cdots P_3P_2P_1)^\top \\ &= P^\top \end{aligned}$$

2. How to store P?
   - Naïvely, we need n^2 entries to store P.
   - However, since $P = P^\top$, we only need n entries, storying one non-zero entry per row.

Define the n-vector $\underline{p}$, where $\underline{p}_i$ is the column index of the non-zero entry in row i. For example, we could store

$$\underline{p} = \begin{pmatrix} 1 \\ 3 \\ 2 \end{pmatrix} \qquad \text{for} \qquad P = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

In Gaussian Elimination, keep track of interchange using the pivot vector piv.

1. Start with the pivot vector $piv = \begin{pmatrix} 1 \\ 2 \\ \vdots \\ n \end{pmatrix}$ representing I

2. For $R_i \leftrightarrow R_j$, swap piv_i and piv_j

3. If at the end of GE, $piv = (4, 1, 3, 2)$, then we have

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

Note: Implementation Issue

Interchanging $R_i \leftrightarrow R_{r_i}$, we do not want to mechanically interchanging via

$$a_{i,j} \leftrightarrow a_{r_i,j}$$

Instead, we could do **indirect addressing** via the pivot vector piv.
Suppose we swap $piv(i)$ and $piv(j)$, then a reference to $a(i, j)$ becomes a reference to $a(piv(i), j)$.

A Note on Matrix Multiplication

Order of Multiplication Matters

Suppose we multiple $A \in \mathbb{R}^{m\times n}$ by $B \in \mathbb{R}^{n\times p}$ to get $C = AB$, we have $C \in \mathbb{R}^{m\times p}$ with

$$c_{i,j} = \sum_{k=1}^{n} a_{i,k} b_{k,j}$$

The operation count would be

$$2mnp \text{ FLOPs}$$

Now, suppose we compute

$$A_{n\times 1} = Q_{n\times n} R_{n\times n} S_{n\times 1}$$

- If we compute $(QR)S$, the operation count is

$$2n^3 + 2n^2 \text{ FLOPs}$$

- However, if we compute $Q(RS)$, the operation count is

$$4n^2 \text{ FLOPs}$$

  This is roughly half the cost of $(QR)S$.

Inverse is Costly

Suppose we have a non-singular M, and we want to compute

$$x = M^{-1}\underline{y} + \underline{z}$$

- Find M^{-1} by solving $MW = I$

  This step will cost $\frac{2}{3}n^3 + \Theta(n^2)$ FLOPs for factorization, and $n\left(2n^2 + \Theta(n)\right)$ FLOPs for solving. This requires a total of $\frac{8}{3}n^3 + \Theta(n^2)$ FLOPs.
- Compute $M^{-1}\underline{y}$, which requires $2n^2$ FLOPs.
- We add $\underline{z}$, which requires n FLOPs.

We could alternatively convert this problem into solving a linear system.
Let $\underline{c} = M^{-1}\underline{y}$, then

$$M\underline{c} = \underline{y}$$

We could find $\underline{c}$ with $\frac{2}{3}n^3 + \Theta(n^2) + 2n^2 + \Theta(n) = \frac{2}{3}n^3 + 3n^2 + \Theta(n)$ FLOPs.
This is about 4 times cheaper than the direct method.

Accessing the Accuracy of a Solution

Suppose we want to solve $A\underline{x} = \underline{b}$ with

$$A = \begin{pmatrix} 0.780 & 0.563 \\ 0.913 & 0.659 \end{pmatrix} \qquad \text{and} \qquad \underline{b} = \begin{pmatrix} 0.217 \\ 0.254 \end{pmatrix}$$

Suppose also we have two solutions

$$\underline{\hat{x}} = \begin{pmatrix} 0.341 \\ -0.087 \end{pmatrix} \qquad \text{and} \qquad \underline{\tilde{x}} = \begin{pmatrix} 0.999 \\ -1.001 \end{pmatrix}$$

Which answer is closer to the solution? We could compute the residual and compare the norms of the residuals.

Definition 4.4.1 Residual

The **residual** of a solution $\underline{x}$ to $A\underline{x} = \underline{b}$ is

$$\underline{r} = \underline{b} - A\underline{x}$$

It measures how much the solution does not satisfy the equation.

With the two solutions, we have

$$\underline{\hat{r}} = \underline{b} - A\underline{\hat{x}} = \begin{bmatrix} 0.000\,001 \\ 0 \end{bmatrix} \qquad \underline{\tilde{x}} = \underline{b} - A\underline{\tilde{x}} = \begin{bmatrix} 0.001\,343 \\ 0.001\,572 \end{bmatrix}$$

We conclude that $\hat{x}$ is a better solution.
However, if we take a look at the true solution

$$x^* = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

we have

$$\hat{e} = \hat{x} - x^* = \begin{bmatrix} -0.659 \\ 0.913 \end{bmatrix} \qquad \tilde{e} = \tilde{x} - x^* = \begin{bmatrix} -0.001 \\ 0.001 \end{bmatrix}$$

and we see that $\tilde{x}$ is a better solution.

Remark

A small residual need not imply an accurate solution.

We try to explain the phenomenon by looking at the condition number of the matrix A. Suppose we solve $A\underline{x} = \underline{b}$, the exact solution is $\underline{x}^*$, and we have an approximate solution $\underline{\bar{x}}$.

- Define $\underline{\bar{b}} = A\underline{\bar{x}}$ the right hand side for solving $A\underline{x} = \underline{b}$ that has solution $\underline{\bar{x}}$.
- Define $\underline{\bar{r}} = \underline{b} - \underline{\bar{b}}$ the residual for the approximate solution.

Since $A\underline{\bar{x}} = \underline{\bar{b}}$ and $A\underline{x}^* = \underline{b}$, we have

$$A(\underline{\bar{x}} - \underline{x}^*) = \underline{\bar{b}} - \underline{b} = -\underline{\bar{r}}$$

We are interested in the error

$$\underline{\bar{e}} = \underline{\bar{x}} - \underline{x}^*$$

We have

$$\begin{aligned} A\underline{\bar{e}} &= -\underline{\bar{r}} \\ \underline{\bar{e}} &= -A^{-1}\underline{\bar{r}} \end{aligned}$$

To convert the absolute error into a scalar quantity, we use the norm

$$\|\underline{\bar{e}}\| = \left\|-A^{-1}\underline{\bar{r}}\right\| \leq \left\|A^{-1}\right\| \cdot \|\underline{\bar{r}}\|$$

Moreover, we know that

$$\begin{aligned} A\underline{x}^* &= \underline{b} \\ \|A\underline{x}^*\| &= \|\underline{b}\| \end{aligned}$$

and so

$$\|A\| \cdot \|\underline{x}^*\| \geq \|\|A\underline{x}^*\|\| = \|\underline{b}\|$$

Thus, we have

$$\begin{aligned} \frac{\|\underline{\bar{x}} - \underline{x}^*\|}{\|A\| \cdot \|\underline{x}^*\|} &\leq \frac{\left\|A^{-1}\right\| \cdot \|\underline{\bar{r}}\|}{\|\underline{b}\|} \\ \frac{\|\underline{\bar{x}} - \underline{x}^*\|}{\|\underline{x}^*\|} &\leq \left(\|A\| \cdot \left\|A^{-1}\right\|\right) \frac{\|\underline{\bar{r}}\|}{\|\underline{b}\|} \\ &\leq \|A\|\|A^{-1}\| \end{aligned}$$

$\|A\|\|A^{-1}\|$ is the **normwise relative error** in computed solution, compared to the **nromwise relative residual** (relative to right hand side $\underline{b}$).

The quantity

$$\|A\|\|A^{-1}\|$$

is called the **condition number** of the matrix A.

Remark

If the relative residual in the computed solution is small, and the condition number of the matrix is small, then the relative error in the computed solution is small, and the solution is accurate.

Remark Vector Norme

$$\|\cdot\| : \mathbb{R}^n \to \mathbb{R}^{\geq 0}$$

- Positive semi-definite

  $\|\underline{x}\| \geq 0$ and $\|\underline{x}\| = 0$ if and only if $\underline{x} = \underline{0}$

- Homogeneous

  $\|\alpha\underline{x}\| = |\alpha|\|\underline{x}\|$ for all $\alpha \in \mathbb{R}$

- Triangle Inequality

  For all $\underline{x}, \underline{y} \in \mathbb{R}^n$, $\|\underline{x}+\underline{y}\| \leq \|\underline{x}\| + \|\underline{y}\|$

There are many norms, but we will focus on the p-norms.

- The Manhattan norm (1-norm)

$$\|\underline{x}\|_1 = \sum_{i=1}^{n} |x_i|$$

- The Euclidean norm (2-norm)

$$\|\underline{x}\|_2 = \sqrt{\sum_{i=1}^{n} x_i^2}$$

- The infinity norm

$$\|\underline{x}\|_\infty = \max_{1\leq i\leq n} |x_i|$$

Remark Matrix Norms

$$\|\cdot\| : \mathbb{R}^{n\times n} \to \mathbb{R}^{\geq 0}$$

- Positive semi-definite

  $\|A\| \geq 0$ and $\|A\| = 0$ if and only if $A = 0$

- Homogeneous

  $\|\alpha A\| = |\alpha|\|A\|$ for all $\alpha \in \mathbb{R}$

- Triangle Inequality

  For all $A, B \in \mathbb{R}^{n\times n}$, $\|A+B\| \leq \|A\| + \|B\|$

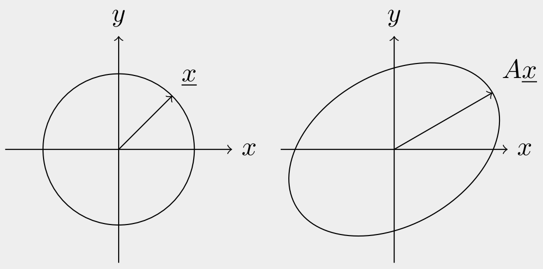
- Cauchy-Schwarz Inequality

  For all $A, B \in \mathbb{R}^{n\times n}$, $\|AB\| \leq \|A\|\|B\|$

We use induced norms for matrices, for example,

$$\|A\|_1 = \max_{\|\underline{x}\|=1} \|A\underline{x}\|$$

That is, consider all vectors in the unit circle and apply A to them. The maximum value of the norm of the resulting vectors is the induced matrix norm.



Induced norms are

- The 1-norm

$$\begin{aligned}\|A\|_1 &= \max_{\|\underline{x}\|_1=1} \|A\underline{x}\|_1 \\ &= \text{max absolute column sum} \\ &= \max_{i\le j\le n}\left(\sum_{i=1}^{n}|a_{i,j}|\right)\end{aligned}$$

- The 2-norm

$$\|A\|_2 = \sqrt{\lambda_{\max}(A^\top A)}$$

- The infinity norm

$$\begin{aligned}\|A\|_\infty &= \max_{\|\underline{x}\|_\infty=1} \|A\underline{x}\|_\infty \\ &= \text{max absolute row sum} \\ &= \max_{1\le i\le n}\left(\sum_{j=1}^{n}|a_{i,j}|\right)\end{aligned}$$

Another useful norm is the **Frobenius norm**

$$\|A\|_F = \sqrt{\sum_{i=1}^{n}\sum_{j=1}^{n} {a_{i,j}}^2}$$

Example. We revisit the example, where

$$A = \begin{pmatrix} 0.780 & 0.563 \\ 0.913 & 0.659 \end{pmatrix}$$

We have

$$\|A\|_\infty = 1.572$$

We have defined

$$\kappa(A) = \|A\|\|A^{-1}\|$$

but we did not define which norm to use. We could have different condition numbers for different norms.

$$\kappa_\infty(A) = \|A\|_\infty\|A^{-1}\|_\infty$$

From linear algebra, we know that **for a 2×2 matrix**

$$M = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

we have its inverse

$$M^{-1} = \frac{1}{ad - bc} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$$

Thus, we have

$$A^{-1} = \frac{1}{0.780 \cdot 0.659 - 0.563 \cdot 0.913} \begin{pmatrix} 0.659 & -0.563 \\ -0.913 & 0.780 \end{pmatrix}$$

so

$$\|A^{-1}\|_\infty \approx 1.693 \times 10^6$$

and hence the conditional number

$$\kappa_\infty(A) \approx 2.66 \times 10^6$$

This shows that solving the system is ill-conditioned.

The relative error in our compute solution is bounded above by

$$2.66 \times 10^6 \cdot \text{ relative residual in computed solution}$$

$\diamondsuit$

How small can the condition number be? There is a relation between condition number and near-singularity.

$$\begin{aligned} \kappa(A) &= \|A\| \cdot \|A^{-1}\| \\ &\geq \|AA^{-1}\| \\ &= \|I\| \\ &= 1 \end{aligned}$$

The condition number is bounded below by 1, and the closer it is to 1, the better conditioned the matrix is.

Example. We consider another system

$$A\underline{x} = \underline{b}$$

where

$$\begin{pmatrix} 1.0 \times 10^{-4} & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 1 \\ 2 \end{pmatrix}$$

The exact LU factorization yields

$$L = \begin{pmatrix} 1 & 0 \\ 1.0 \times 10^{-4} & 1 \end{pmatrix} \qquad \text{and} \qquad U = \begin{pmatrix} 1.0 \times 10^{-4} & 1 \\ 0 & -9.999 \end{pmatrix}$$

With forward solve,

$$\begin{aligned} L\underline{y} &= \underline{b} \\ y_1 &= 1 \\ y_2 &= -9.998 \end{aligned}$$

and then with backward solve,

$$\begin{aligned} U\underline{x} &= \underline{y} \\ x_2 &= \frac{9998}{9999} \\ x_1 &= \frac{1000}{9999} \end{aligned}$$

Now, suppose we get

$$\bar{L} = \begin{pmatrix} 1.00 \times 10^0 & 0 \\ 1.00 \times 10^4 & 1.00 \times 10^0 \end{pmatrix} \qquad \text{and} \qquad \bar{U} = \begin{pmatrix} 1.00 \times 10^{-4} & 1.00 \times 10^0 \\ 0 & 1.00 \times 10^4 \end{pmatrix}$$

and we compute

$$\begin{aligned} \bar{y}_1 &= 1.00 \times 10^1 \\ \bar{y}_2 &= fl\left(\frac{2 - 1.00 \times 10^4}{1.00 \times 10^0}\right) = -1.00 \times 10^4 \qquad \text{error} \end{aligned}$$

and then

$$\begin{aligned} \bar{x}_2 &= 1.00 \times 10^0 \\ \bar{x}_1 &= 0.00 \times 10^0 \end{aligned}$$

While $\bar{x}_2$ is accurate, $\bar{x}_1$ is not.

We first check if the matrix is ill-conditioned. We have

$$\|A\|_\infty = 2$$

and

$$\|A^{-1}\|_\infty = \left|\frac{1}{1.0 \times 10^{-4} - 1}\right| 2 = 2$$

so

$$\kappa_\infty(A) = 4$$

The large error is not due to ill-conditioning.

We observe that

$$x_1 = \frac{1.00 - 1.00}{1.0 \times 10{-}4}$$

and we see that we have catastrophic cancellation here.

We also observe that

$$A = LU$$

where

$$\kappa(L) \approx 1.0 \times 10^8 \qquad \text{and} \qquad \kappa(U) \approx 1.0 \times 10^8$$

so in fact we replaced a well conditioned problem with an ill-conditioned one. ♢

Note: Fact

Whenever multipliers are large (because diagonal elements are relatively small) a loss of accuracy can be observed.

4.4.2 Partial Pivoting

A solution to this issue is to try reordering the equations.

Example (Cont.). We perform row exchange $R_1 \leftrightarrow \mathbb{R}_2$,

$$\begin{pmatrix} 1 & 1 \\ 1 \times 10^{-4} & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 2 \\ 1 \end{pmatrix}$$

and we obtain

$$L = \begin{pmatrix} 1.00 & 0 \\ 1.00 \times 10^{-4} & 1.00 \end{pmatrix} \qquad \text{and} \qquad U = \begin{pmatrix} 1,00 & 1.00 \\ 0 & fl(1 - 1 \times 10^{-4}) = 1.00 \end{pmatrix}$$

so

$$\kappa(L) = 1 \qquad \text{and} \qquad \kappa(U) = 4$$

This way, we have a well-conditioned problem.
We now have

$$\begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = \begin{pmatrix} 2.00 \\ 1.00 \end{pmatrix} \qquad \text{and then} \qquad \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 1.00 \\ 1.00 \end{pmatrix}$$

which is the correct floating point representation of the exact solution. ◊

Definition 4.4.2 Pivot Position

The **pivot position** is the position in the matrix that is used to eliminate the other elements in the column.

Suppose we have a matrix

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

We interchange R_i, R_{r_i} using P_{i,r_i} to move small value off of diagonal.
Choose interchange rows r_i such that $\|a_{r_i,i}\| \geq \|a - j, i\|$ for all j from i to n.

- Guarantees multipliers are ≥ 1 in size
- Do rows interchanges to ensure multipliers are ≤ 1

Note: Fact

In practice, when row interchanges are used, the Gaussian Elimination algorithm is **stable**. and guarantees approximate solutions with relative errors $\frac{\|r\|}{\|b\|} \approx C_n \cdot \varepsilon_{\text{mach}}$ where C_n is a small constant dependent on n.
Thus,

$$\frac{\|\underline{x} - \underline{x}^*\|}{\|\underline{x}^*\|} \leq \kappa(A) \cdot \varepsilon_{\text{mach}} \approx \kappa(A) \cdot C_n \cdot \varepsilon_{\text{mach}}$$

Remark Rule of Thumb

Then number of bits of accuracy in the computed solution is approximately $P - \lceil \log_\beta \kappa(A) \rceil$, where P is the precision of the floating point system.

Remark Terms

Row interchanges, row pivoting, and partial pivoting are all the same thing.

4.4.3 Complete Pivoting

In row pivoting, we only search the columns, while in complete pivoting, we search the entire uneliminated submatrix

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

Suppose $|a_{s,t}| > |a_{i,j}|$ for al i, j, s, t in the un-eliminated submatrix.
In complete pivoting, we interchange to put $a_{s,t}$ in the pivot position.
Our factorization becomes

$$PAQ = LU$$

where

- P is a permutation matrix for row interchanges
- Q is a permutation matrix for column interchanges

$$\begin{aligned} A\underline{x} &= \underline{b} \\ PAQQ^\top \underline{x} &= P\underline{b} \\ LUQ^\top \underline{x} &= P\underline{b} \end{aligned}$$

Remark Considerations

Complete pivoting is not always necessary, is more computationally expensive than partial pivoting since we need to search in 2D space instead of 1D space.

Proof. WTS $\|A\|_\infty$ is the max absolute row sum of A.
Let $\underline{x}$ be a unit vector, then

$$\|A\|_\infty = \max_{\|\underline{x}\|=1} \|A\underline{x}\|_\infty$$

and

$$\|\underline{x}\|_\infty = \max_{1\le i\le n} |x_i|$$

Let $\underline{x}$ be such that $\|\underline{x}\| = 1$ and write $A = [\underline{a}_1, \underline{a}_2, \ldots, \underline{a}_n]$ where $\underline{a}_i$ is the i-th column of A.
Then,

$$A\underline{x} = x_1\underline{a}_1 + x_2\underline{a}_2 + \cdots + x_n\underline{a}_n = \sum_{j=1}^{n} x_j \underline{a}_j$$

and

$$(A\underline{x})_i = \sum_{j=1}^{n} x_j a_{i,j}$$

so

$$\|A\|_\infty = \max_{1\le i\le n} |(Ax)_i| = \max_{1\le i\le n} \left| \sum_{j=1}^{n} x_j a_{i,j} \right|$$

How to maximize for $\|\underline{x}\|_\infty = 1$?
For each $1 \le i \le n$, maximize by taking $x_j = 1 \cdot \text{sign}(a_{ij})$. Then,

$$x_j a_{ij} = |a_{ij}|$$

and so

$$\left| \sum_{j=1}^{n} x_j a_{ij} \right| = \sum_{j=1}^{n} |a_{ij}|$$

and so

$$\|A\|_\infty = \max_{1\le i\le n} \sum_{j=1}^{n} |a_{ij}|$$

which is the max absolute row sum of A. ■

CHAPTER

INTERPOLATION 5

5.1 Introduction

5.1.1 Definition

Example. Suppose we are given the following population data

year	1940	1950	1960	1970	1980	1990	2000	2010
Population (M)	132	151	179	203	226	249	281	308

We mey ask the question: what was the population in 1965? We can use **interpolation** to estimate the population in 1985.

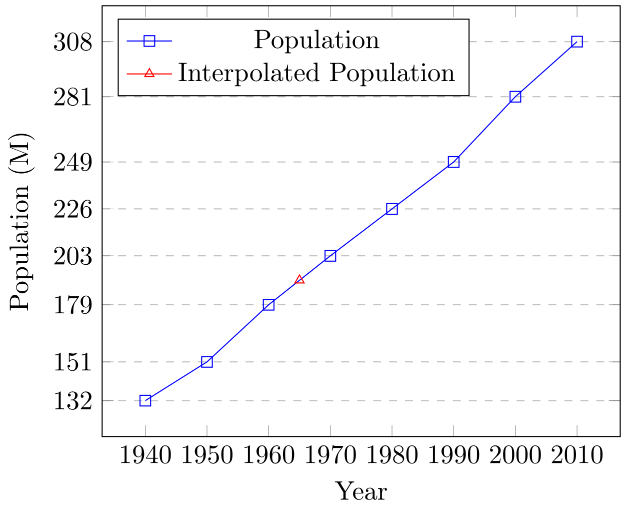


Figure 5.1: Population data and interpolated population in 1965

We may also ask the question: what will the population be in 2020? This will be an **extrapolation** problem. ♢

Definition 5.1.1

Given a set of m data points $\{(t_i, y_i)\}_{i=1}^m$ with $t_1 < t_2 < \cdots < t_m$, the **interpolation problem** is to find a function $g(t)$ from a specific class of functions that

$$g(t_i) = y_i \quad \text{for all } i = 1, 2, \ldots, m$$

Remark

Another use of interpolation is to approximate a function $f(t)$ by a simpler function $g(t)$ that is easier to work with.

Example. Suppose we have a function

$$\text{erf} = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2}\, dt$$

and we want to approximate it with a polynomial.

- Evaluate erf at m points, $\{(x_i, e_i)\}_{i=1}^m$
- Interpolate the points with a polynomial $p(x)$ such that $p(x_i) = e_i$ for all $i = 1, 2, \dots, m$
- Use the interpolant $p(x)$ in place of erf

◇

5.1.2 Design Goals for Interpolation

1. Easy to evaluate – quick, accurate
2. Gives accurate approximations for $t \neq t_i$
3. Can integrate and differentiate easily

Remark Caveats

Interpolations come with some caveats.

- Interpolations are not uniques.
- Not all interpolations have nice properties
- Interpolations does not always give the right solution choice

Note:

We assume **accurate data** has the form

$$\{(t_i, y_i)\}_{i=1}^m \qquad \text{or} \qquad \{t_i, f(t_i)\}_{i=1}^m$$

with

$$t_1 < t_2 < \cdots < t_m$$

5.1.3 Interpolation Problems

Example. Suppose we want to construct a linear fit for the data

$$\{(-1, 2), (1, 1)\}$$

Define $P_1(t) = b + mt$. We have $\begin{cases} P_1(-1) = 2 \\ P_1(1) = 1 \end{cases} \implies \begin{cases} b + m(-1) = 2 \\ b + m(1) = 1 \end{cases}$ which yields the solution

$$b = -\frac{1}{2} \qquad b = \frac{3}{3} \qquad \text{so} \qquad P_1(t) = \frac{3}{2} - \frac{1}{2}t$$

◇

Example. Suppose we want to construct a quadratic fit for the data

$$\{(-1,2),(1,1),(2,1)\}$$

Define $P_2(t) = a + bt + ct^2$. We have $\begin{cases} P_2(-1) = 2 \\ P_2(1) = 1 \\ P_2(2) = 1 \end{cases} \implies \begin{cases} a + b(-1) + c(-1)^2 = 2 \\ a + b(1) + c(1)^2 = 1 \\ a + b(2) + c(2)^2 = 1 \end{cases}$ which yields

$$P_2(t) = \frac{4}{3} - \frac{1}{2}t + \frac{1}{6}t^2$$

◊

Note:

We choose polynomial interpolants

$$P_{m-1}(t) = \sum_{i=1}^{m} c_i t^{i-1}$$

because they are easy to evaluate. The operation count is approximately

$$3n \text{ FLOPs}$$

Theorem 5.1.2 Horner's Rule
We can re-write our polynomial as

$$P_{m-1}(t) = c_1 + t(c_2 + t(c_3 + t(\cdots + t(c_{m-1} + c_m t))))$$

Note:

Horner's methods provide some advantages. The operation count reduces to

$$2m\text{FLOPs}$$

and it's easier to integrate and differentiate.

Theorem 5.1.3
For a set of points

$$\{(t_i, y_i)\}_{i=1}^m,$$

there exists a unique polynomial of degree at less than m that interpolates the data.

5.2 Solving Interpolation Problems

5.2.1 Monomial Basis

Given a set of points

$$S = \{(t_i, y_i)\}_{i=1}^m$$

we find the unique polynomial

$$P_{m-1}(t) = \sum_{i=1}^{m} c_i t^{i-1}$$

that interpolates the data.

Applying the interpolation conditions,

- $P_{m-1}(t_1) = y_1$
- $P_{m-1}(t_2) = y_2$
- $\vdots$
- $P_{m-1}(t_m) = y_m$

We have systems of equations

$$\begin{aligned} c_1 + c_2t_1 + c_3{t_1}^2 + \cdots + c_m{t_1}^{m-1} &= y_1 \\ c_1 + c_2t_2 + c_3{t_2}^2 + \cdots + c_m{t_2}^{m-1} &= y_2 \\ &\vdots \\ c_1 + c_2t_m + c_3{t_m}^2 + \cdots + c_m{t_m}^{m-1} &= y_m \end{aligned}$$

That is, a linear system

$$\begin{pmatrix} 1 & t_1 & t_1^2 & \cdots & {t_1}^{m-1} \\ 1 & t_2 & t_2^2 & \cdots & {t_2}^{m-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & t_m & t_m^2 & \cdots & {t_m}^{m-1} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_m \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{pmatrix}$$

The matrix V is called the **Vandermonde matrix**.

Lemma 5.2.1

If all the t_i are distinct, then the Vandermonde matrix is invertible.

Therefore, we can determine the poly coefficients $\underline{c}$.

```
import numpy as np

t = np.linspace(1.0, 2.0, 11)
# t = (1.0, 1.1, 1.2, ..., 2.0)

V = np.vander(t, increasing=True)
# V = [[1.0, 1.0, 1.0, ..., 1.0],
#      [1.0, 1.1, 1.21, ..., 2.0],
#      ...
#      [1.0, 2.0, 4.0, ..., 1024.0]]

np.linalg.cond(V)
# 6518493762298.583 ~ 6.52 * 10^12
```

Using IEEE double precision, solving $V\underline{c} = \underline{y}$ get $\underline{c}'s$ to approximately 4 significant digits of accuracy. It is difficult to determine interpolants accurately this way.

Originally, we are trying to find $P_{m-1}(t) \in \mathbb{P}_{m-1}$, write

$$P_{m-1}(t) = \sum_{i=1}^{m} c_i t^{i-1}$$

using monomial basis

$$\{1, t, t^2, \ldots, t^{m-1}\}$$

5.2.2 Lagrange Basis

Using a Different Basis

Suppose $\{b_i(t)\}_{i=1}^m$ is a basis for $\mathbb{P}_{m-1}$, then

$$P_{m-1}(t) = \sum_{i=1}^{m} \alpha_i b_i(t)$$

for some $\alpha_i \in \mathbb{R}$ to be determined.

We know that

$$P_{m-1}(t_i) = y_i$$

and using the new basis, we have

$$\begin{aligned} \alpha_1 b_1(t_1) + \alpha_2 b_2(t_1) + \cdots + \alpha_m b_m(t_1) &= y_1 \\ \alpha_1 b_1(t_2) + \alpha_2 b_2(t_2) + \cdots + \alpha_m b_m(t_2) &= y_2 \\ &\vdots \\ \alpha_1 b_1(t_m) + \alpha_2 b_2(t_m) + \cdots + \alpha_m b_m(t_m) &= y_m \end{aligned}$$

which yields the system of equations

$$\begin{pmatrix} b_1(t_1) & b_2(t_1) & \cdots & b_m(t_1) \\ b_1(t_2) & b_2(t_2) & \cdots & b_m(t_2) \\ \vdots & \vdots & \ddots & \vdots \\ b_1(t_m) & b_2(t_m) & \cdots & b_m(t_m) \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_m \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{pmatrix}$$

Remark

The choice of basis is important. We want to choose a basis that is easy to work with.

What if $B = I$? Then we $\kappa_I = 1$ and $\underline{\alpha} = \underline{y}$.

We choose a basis such that

$$b_i(t_j) = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}$$

Example. Consider $R = 1$, we want

- $b_1(t_2) = 0$
- $b_1(t_3) = 0$
- $\vdots$
- $b_1(t_m) = 0$

So if we were to construct a polynomial satisfying these conditions, we would include the factors

$$(t - t_2) \qquad (t - t_3) \qquad \cdots \qquad (t - t_m)$$

which suggests $b_1(t)$ takes the form

$$(t - t_2)(t - t_3) \cdots (t - t_m)$$

Note that this is of degree $m - 1$, and since our basis cannot have degree more than $m - 1$, we cannot add more factors.

Now we need to satisfy $b_1(t_1) = 1$, so we need to divide by a constant. We can choose

$$b_1(t) = \frac{(t - t_2)(t - t_3)\cdots(t - t_m)}{(t_1 - t_2)(t_1 - t_3)\cdots(t_1 - t_m)}$$

◊

In general,

$$b_k(t) = \frac{\prod_{j=1, j\neq k}^{m} (t - t_j)}{\prod_{j=1, j\neq k}^{m} (t_k - t_j)}$$

Lemma 5.2.2

The set of functions

$$\{b_k(t)\}_{k=1}^m$$

are linearly independent and form a basis for $\mathbb{P}_{m-1}$.

This basis is know as the **Lagrange basis**.

Definition 5.2.3 Lagrange Basis

The **Lagrange basis** is a set of functions

$$\{l_k(t)\}_{k=1}^m \qquad \text{where} \qquad l_k(t) = \prod_{j=1, j\neq k}^{m} \frac{t - t_j}{t_k - t_j}$$

Remark

The Lagrange basis has the property

$$l_k(t_j) = \begin{cases} 1 & \text{if } k = j \\ 0 & \text{if } k \neq j \end{cases}$$

The Lagrange form of the interpolating polynomial is

$$P_{m-1}(t) = \sum_{k=1}^{m} c_k l_k(t) \qquad \text{where } \underline{c} = \underline{y}$$

Example. We use the Lagrange basis to compute $P_2(t)$ that interpolates

$$\{(-1, 2), (1, 1), (2, 1)\}$$

We have the expressions for the Lagrange basis

$$\begin{aligned} l_1(t) &= \prod_{k=2,3} \frac{t - t_k}{t_1 - t_k} \\ &= \frac{t-1}{-1-1} \cdot \frac{t-2}{-1-2} \\ &= \frac{1}{6}(t-1)(t-2) \end{aligned} \qquad \begin{aligned} l_2(t) &= \prod_{k=1,3} \frac{t - t_k}{t_2 - t_k} \\ &= \frac{t+1}{1+1} \cdot \frac{t-2}{1-2} \\ &= -\frac{1}{2}(t+1)(t-2) \end{aligned} \qquad \begin{aligned} l_3(t) &= \prod_{k=1,2} \frac{t - t_k}{t_3 - t_k} \\ &= \frac{t+1}{2+1} \cdot \frac{t-1}{2-1} \\ &= \frac{1}{3}(t+1)(t-1) \end{aligned}$$

so

$$\begin{aligned} P_2(t) &= 2l_1(t) + 1l_2(t) + 1l_3(t) \\ &= 2 \cdot \frac{1}{6}(t-1)(t-2) - \frac{1}{2}(t+1)(t-2) + \frac{1}{3}(t+1)(t-1) \\ &= \frac{4}{3} - \frac{1}{2}t + \frac{1}{6}t^2 \end{aligned}$$

which is the same as the polynomial we found earlier. ◊

Remark Lagrange Basis are Expensive

For each $l_i(t)$, we require approximately $4m$ FLOPs.

- For the numerator, $m-1$ multiplications and $m-1$ subtractions
- For the denominator, $m-1$ multiplications and $m-1$ subtractions
- A finial division

so we require a total of

$$\Theta(m^2) \text{ FLOPs}$$

in total to compute the Lagrange basis.

5.2.3 Newton Basis

Recall for a general basis $\{b_i(t)\}_{i=1}^m$, we have

$$P_{m-1}(t) = \sum_{i=1}^{m} \alpha_i b_i(t)$$

and the interpolating conditions

$$P_{m-1}(t_i) = y_i$$

We solve the system of equations

$$B\underline{c} = \underline{y}$$

for $\underline{c}$, where

$$B = \begin{pmatrix} b_1(t_1) & b_2(t_1) & \cdots & b_m(t_1) \\ b_1(t_2) & b_2(t_2) & \cdots & b_m(t_2) \\ \vdots & \vdots & \ddots & \vdots \\ b_1(t_m) & b_2(t_m) & \cdots & b_m(t_m) \end{pmatrix}$$

We want a B that is easy to solve, but perhaps not as easy as the identity matrix. We explore a triangular system.

Lower Triangular System

We choose a basis $\{b_i(t)\}_{i=1}^m$ such that

$$B = \begin{pmatrix} b_1(t_1) & 0 & 0 & \cdots & 0 \\ b_1(t_2) & b_2(t_2) & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ b_1(t_{m-1}) & b_2(t_{m-1}) & \cdots & b_{m-1}(t_{m-1}) & 0 \\ b_1(t_m) & b_2(t_m) & \cdots & b_{m-1}(t_m) & b_m(t_m) \end{pmatrix}$$

For simplicity, take $b_1(t) = 1$.

- Row 1: $b_2(t_1) = 0, b_3(t_1) = 0, \ldots, b_m(t_1) = 0$
  We include $(t - t_1)$ as a factor of each $b_R(t)$ for $R = 2, 3, \ldots, m$.
- Row 2: $b_3(t_2) = 0, b_4(t_2) = 0, \ldots, b_m(t_2) = 0$
  We include $(t - t_2)$ as a factor of each $b_R(t)$ for $R = 3, 4, \ldots, m$.
- $\vdots$
- Row $m-1$: $b_m(t_{m-1}) = 0$
  We include $(t - t_{m-1})$ as a factor of $b_m(t)$.

which suggests

$$b_k(t) = \prod_{j=1}^{k-1}(t - t_j)$$

Remark

This is a basis because we have m linearly independent functions.

Definition 5.2.4 Newton Basis

The **Newton basis** is a set of functions

$$\{n_k(t)\}_{k=1}^{m} \qquad \text{where} \qquad n_k(t) = \prod_{j=1}^{k-1}(t - t_j)$$

The Newton form of the interpolating polynomial is

$$P_{m-1}(t) = \sum_{k=1}^{m} c_k \prod_{j=1}^{k-1}(t - t_j)$$

Remark Newton Basis are Cheaper

If we can remember the results $t - t_i$, then each new term added would only require 3 FLOPs. This is a significant improvement over the Lagrange basis. The total operation count is $\Theta(3m)$ FLOPs

Now, to determine the coefficients, we solve a lower triangular system $B\underline{c} = \underline{y}$ We know that

- $y_1 = P_{m-1}(t_1) = c_1$ so
$$c_1 = y_1$$
- $y_2 = P_{m-1}(t_2) = c_1 + c_2(t_2 - t_1)$ so
$$c_2 = \frac{y_2 - c_1}{t_2 - t_1}$$
- $\vdots$
- $y_m = P_{m-1}(t_m) = \sum_{k=1}^{m} c_k \prod_{j=1}^{k-1}(t_m - t_j)$ so

$$c_m = \frac{y_m - \sum_{j=1}^{m-1} c_j \prod_{k=1}^{j-1}(t_m - t_k)}{\prod_{k=1}^{m-1}(t_m - t_k)}$$

Example. Determine the Newton form of the degree 2 polynomial that interpolates

$$\{(-1,2),(1,1),(2,1)\}$$

We have the expressions for the Newton basis

- $c_1 = y_1 = 2$
- $$\begin{aligned} c_2 &= \frac{y_2 - c_1}{t_2 - t_1} \\ &= \frac{1-2}{1-(-1)} \\ &= -\frac{1}{2} \end{aligned}$$
- $$\begin{aligned} c_3 &= \frac{y_3 - [c_1 + c_2(t_3 - t_1)]}{(t_3-t_1)(t_3-t_2)} \\ &= \frac{1 - \left[2 - \frac{1}{2}(2-(-1))\right]}{(2-(-1))(2-1)} \\ &= \frac{1}{6} \end{aligned}$$

So the Newton form of the interpolating polynomial is

$$P_2(t) = 2 - \frac{1}{2}(t+1) + \frac{1}{6}(t+1)(t-1) = \frac{4}{3} - \frac{1}{2}t + \frac{1}{6}t^2$$

This is the same polynomial we found earlier with the monomial and Lagrange basis. ◇

5.2.4 Summary

	Monomial Basis	**Lagrange Basis**	**Newton Basis**
Evaluate $P_{m-1}(t)$	Easy	Difficult	Easy
Integrate/Differentiate	Easy	Difficult	Medium
Finding Coefficients	Can be Ill-conditioned	Very Easy	Easy
Add (t_{m+1}, g_{m+1})	All Coefficients Change	Just add $\frac{t-t_{m+1}}{t-t_m}$ to each $l_k(t)$	Add $c_m \prod_{j=1}^{m-1}(t-t_j)$ to previous interpolants

5.3 Error Analysis

What about accuracy? We know

$$P_{m-1}(t_i) = y_i \quad \text{for all } i = 1,2,\ldots,m$$

but how can we determine if $P_{m-1}(t)$ is a good approximation for $f(t)$ for $t \neq t_i$?

Theorem 5.3.1

Suppose the polynomial $P_{m-1}(t)$ interpolates the function $f(t)$ at distinct points $t_1 < t_2 < \cdots < t_m$. If f is m-times differentiable on the interval $[t_1, t_m]$, then for any point $t \in [t_1, t_m]$,

$$f(t) - p_{m-1}(t) = \frac{1}{m!} f^{(m)}(c_t)\omega_m(t)$$

where

- c_t is some point in $t_1, t_,$ that depends on t;
- $\omega_m(t) = (t-t_1)(t-t_2)\cdots(t-t_m) = \prod_{j=1}^{m}(t-t_j)$

We have

$$\max_{t\in[t_1,t_m]} |f(t) - P_{m-1}(t)| \leq \frac{1}{m!} \max_{t\in[t_1,t_m]} |f^{(m)}(t)| \max_{t\in[t_1,t_m]} |\omega_m(t)|$$

- m is the interpolation points we can control
- $f^{(m)}(t)$ is the m-th derivative of $f(t)$ which is the function we are trying to approximate
- depends on placement of t_i in the interval $[t_1, t_m]$
- We can show that

  $$\max_{t\in[t_1,t_m]} |\omega_m(t)| \leq \frac{h^m \cdot (m-1)!}{4}$$

  where

  $$h = \max_{i=1,\ldots,m-1} |t_{i+1} - t_i|$$

Thus,

$$\begin{aligned}\max_{t\in[t_1,t_m]} |f(t) - P_{m-1}(t)| &\leq \frac{1}{m!} \max_{t\in[t_1,t_m]} |f^{(m)}(t)| \frac{h^m \cdot (m-1)!}{4} \\ &\leq \frac{M \cdot h^m}{4m}\end{aligned}$$

where

$$M = \max_{t\in[t_1,t_m]} |f^{(m)}(t)|$$

If we add mode interpolation points (increasing m), while keeping $t_m - t_1$ fixed, will the error do down?

We know that

$$\text{error} \leq \frac{1}{4m} \cdot M \cdot h^m$$

and as we increase m,

- $\frac{1}{4m}$ decreases
- The behaviour of h^m depends on yhe function
- h^m decreases for $h < 1$

Example. Consider

$$f(t) = \sin(\pi t)$$

and we interpolate at equally spaced points on $[-1, 1]$.

- For $m = 4$, $t_i \in \{-1, -1/3, 1/3, 1\}$, and the interpolant is $P_3(t)$.
- For $m = 7$, $t_i \in \{-1, -2/3, -1/3, 0, 1/3, 2/3, 1\}$, and the interpolant is $P_3(t)$.
- For $m = 10$, $t_i \in \{-1, -7/9, \ldots, 7/9, 1\}$, and the interpolant is $P_10(t)$.

We have

$$\max_{t\in[-1,1]} |f^{(m)}(t)| = \pi^m$$

♢

Example. Consider the Rauge's function

$$f(t) = \frac{1}{1+25t^2}$$

and we interpolate at equally spaced points on $[-1, 1]$.

Consider $m = 4, m = 7, m = 10$, and $m = 13$.

We observe that in the middle area, the approximation gets better with increasing m. However, at the ends, the error is bigger and the approximation is less accurate. ♢

Remark

Degree $m-1$ polynomial interpolants does not necessarily converge to the function that they interpolate as m increases.

5.4 Piecewise Polynomial Interpolation

What should we do if we need to interpolate a large dataset?

5.4.1 Picecwise-Linear Interpolation

The idea is to split the data into smaller chunks and interpolate each chunk separately. We construct **piecewise polynomial interpolants**

$$\{P_{d,i}(t)\}$$

where

- d is the degree of the polynomial
- i is the interval number

Example (Piecewise-linear)**.** Given $\{(t_1, y_i)\}_{i=1}^m$, a piecewise-linear interpolant is

$$\{P_{1,i}(t)\}_{i=1}^{m-1}$$

We define the interpolant

$$L(t) = \{P_{1,i}(t) \text{ where } t \in [t_i, t_{i+1}]\}$$

The $\{t_i\}_{i=1}^m$ are called the **knots** of the piecewise-linear interpolant.

- If we consider Lagrange polynomials, we have

$$P_{1,i}(t) = y_i \frac{t - t_{i+1}}{t_i - t_{i+1}} + y_{i+1} \frac{t - t_i}{t_{i+1} - t_i}$$

- If we consider Newton polynomials, we have

$$P_{1,i}(t) = y_i + \frac{y_{i+1} - y_i}{t_{i+1} - t_i}(t - t_i)$$

♢

Remark

$L(t)$ is continuous. Indeed,

- Each piece is linear

- Connection at knots

$$P_{1,i}(t_{i+1}) = y_{i+1} = P_{1,i+1}(t_{i+1})$$

Remark

$$P_{1,i}{}'(t) = \frac{y_{i+1} - y_i}{t_{i+1} - t_i} \qquad P_{1,i+1}{}'(t) = \frac{y_{i+2} - y_{i+1}}{t_{i+2} - t_{i+1}}$$

Accuracy

Suppose $L(t)$ interpolates $f(x)$ at knots $\{t_i\}_{i=1}^{m}$. We have

$$f(t) - L(t) = f(t) - P_{1,i}(t) = \frac{1}{2!} f''(c_t)\Big[(t - t_i)(t - t_{i+1})\Big]$$

for some

$$c_t \in (t_i, t_{i+1})$$

Note that the second derative stays the same, and

$$\begin{aligned} \omega_2(t) &= (t - t_i)(t - t_{i+1}) \\ &= t^2 - (t_i + t_{i+1})t + t_i t_{i+1} \end{aligned}$$

We check the boundaries and the critical points

$$\omega'(t) = 2t - (t_i + t_{i+1})\omega_2(t_i) = 0 \qquad \text{and} \qquad \omega'(t) = 2t - (t_i + t_{i+1})\omega_2(t_{i+1}) = 0$$

ω_2 is part of a quadratic so the maximum of absolute values happens at the centre

$$\frac{t_i + t_{i+1}}{2}$$

For $t \in [t_1, t_m]$,

$$|L(t) - f(t)| \leq \frac{1}{2!} \cdot \frac{h^2}{4} \cdot \max_{t \in [t,t]} |f''(t)| = \frac{h^2}{8} \cdot \max_{t \in [t,t]} |f''(t)|$$

where $h = \max_i h_i$

For uniformly spaced t_i, increasing the number of interpolation points would reults in smaller h, leading to a lower error.

5.4.2 Piecewise-Cubit Interpolation

We observe that partial-linear interpolations struggles when there is curvatures.

Instead, we consider a piece-wise cubit interpolation.

For each $[t_i, t_{i+1}]$, we fit a cubit $P_{3,i}(t)$ where $t \in [t_i, t_{i+1}]$.

On each sub-interval, we need to determine

$$P_{3,i} = \alpha_i + \beta_i(t - t_i) + \gamma_i(t - t_i)^2 + \delta_i(t - t_i)^3$$

For $t = t_i$, we have

$$P_{3,i}(t_i) = \alpha_i = f(t_i)$$

and for $t = t_{i+1}$, we have

$$P_{3,i}(t_{i+1}) = \alpha_i + \beta_i h_i^1 + \gamma_i h_i^2 + \delta_i h_i^3$$

where $h_i = t_{i+1} - t_i$.

Remark

The algorithm requires the derivatives

$$P'_{3,i}(t) = \beta_i + 2\gamma_i(t-t_i) + 3\delta_i(t-t_i)^2$$

We have

$$P'_{3,i}(t_i) = \beta_i = f'(t_i) \qquad P'_{3,i}(t_{i+1}) = \beta_i + 2\gamma_i h_i + 3\delta_i h_i^2 = f'(t_{i+1})$$

We need to solve

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & h_i & h_i^2 & h_i^3 \\ 0 & 1 & 2h_i & 3h_i^2 \end{bmatrix} \begin{bmatrix} \alpha_i \\ \beta_i \\ \gamma_i \\ \delta_i \end{bmatrix} = \begin{bmatrix} f(t_i) \\ f'(t_i) \\ f(t_{i+1}) \\ f'(t_{i+1}) \end{bmatrix}$$

for each interval $[t_i, t_{i+1}]$. We get a **piecewise cubit Hermite interpolant** (PCHIP).

Remark Caveat

The PCHIP requires the derivatives of the function. This means that we need to know the function $f(t)$ in advance.

What happens if we are only given a set of points, and not the function itself? We construct a **cubit spline interpolation**.

Example. Suppose $m = 4$, and we are given

$$(t_1, y_1), (t_2, y_2), (t_3, y_3), (t_4, y_4)$$

Define $S(t) = \{S_i(t) \text{ if } t \in [t_1, t_{i+1}]\}$
Hence we are to determine

$$S_1(t), S_2(t), S_3(t)$$

Let $s_i(t) = a_i + b_i(t-t_i) + c_i(t-t_i)^2 + d_i(t-t_i)^3$ for $t \in [t_i, t_{i+1}]$.
There are 4 unknown coefficients per interval – in general, $4(m-1)$ unknown coefficients to determine.

- What do we know? We want $S(t)$ to interpolate data.

  The left end points

  - $S_1(t_1) = y_1$
  - $S_2(t_2) = y_2$.
  - $S_3(t_3) = y_3$.
  - $\vdots$
  - $S_{m-1}(t_{m-1}) = y_{m-1}$.

  The right end points

  - $S_1(t_2) = y_2$
  - $S_2(t_3) = y_3$.
  - $S_3(t_4) = y_4$.
  - $\vdots$
  - $S_{m-1}(t_m) = y_m$.
- We want $S(t)$ to be smooth.

- $S_i(t)$ is differentiable since it is a cubic polynomial.
- The issues happen at the knots t_i.

We require

$$s_i'(t+1) = s_{i+1}'(t_{i+1}) \qquad \text{for } i = 1, 2, \dots, m-2$$

and this proposes $m-2$ more constraints on the coefficients.

In total, we have $4(m-1)$ unknowns and

$$2(m-1) + (m-2) + (m-2) = 4m - 6$$

constraints.

The second $m-2$ comes from the constraints at the second derivatives. We require

$$S_1''(y_2) = S_2''(t_2) \qquad S_2''(t_3) = S_3''(t_3) \qquad \dots \qquad s_{m-2}''(t_{m-1}) = s_{m-1}''(t_{m-1})$$

◇

Remark

In SciPy, we could use the `scipy.interpolate.CubicSpline` function.

We realize that we are two constraints short. We could further impose constrains on the derivatives at the ends.

- $S_1''(t_1) = 0$, $S_{m-1}''(t_m) = 0$ are called **natural spline** boundary conditions.
- If y' are known at the ends, we have $s_1'(t_1) = y_1'$ and $s_{m-1}'(t_m) = y_m'$ which are called **clamped spline** boundary conditions.
- We force $S_1'''(t_2) = S_2'''(t_2)$ and $S_{m-2}'''(t_{m-1}) = S_{m-1}'''(t_{m-1})$ which are called **not-a-knot spline** boundary conditions.

5.4.3 Accuracies of the Cubic Slimes

Theorem 5.4.1

Let $f \in C^4[a,b]$.

If $S(t)$ is a natural or clamped or not-a-knot cubic spline that interpolates $f(t)$ at $a = t_1 < t_2 < \cdots < t_m = b$, then

$$\max_{t\in[a,b]} |S(t) - f(t)| \le C_{\text{method}} \cdot h^4 \cdot \max_{t\in[a,b]} |f^{(4)}(t)|$$

where

- C_{method} is a small constant dependent on the type of spline
  - $C_{\text{clamped}} = \frac{5}{384}$
  - $C_{\text{not-a-knot}} = \frac{5}{384}$
- $h = \max_i h_i = \max_i t_{i+1} - t_i$ is the maximum distance between knots

Suppose uniformally spaced knots,

$$h = \frac{b-a}{m-1}$$

If we double the amount of interpolation points, $h \to h/2$, and the error goes down by a factor of $2^4 = 16$.

Remark

For derivative approximations,

$$\max_{t\in[a,b]} |f^{(p)}(t) - S^{(p)}(t)| \leq C_{\text{method}} \cdot h^{4-p} \cdot \max_{t\in[a,b]} |f^{(4)}(t)|$$

for $p = 0, 1, 2$.

Part II

Appendices

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