CP315: Introduction to Scientific Computing

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1 Introduction

CP315 is a set of methods for solving mathematical problems with computers; fair enough - we will be using Maple and MatLab. Fundamental operations that are used: addition and multiplication. These are needed to evaluate a <u>polynomial</u> at a specific value. As we know, polynomials are basic objects in scientific computing $\rightsquigarrow$ efficient evaluation.

1.1 Polynomial Evaluation

Consider a general, fourth-degree polynomial:

$$P(x) = c_0 + c_1 x + c_2 x^2 + c_3 x^3 + c_4 x^4$$

i. Find $P\left(\frac{1}{2}\right)$ naively requires substituting $\frac{1}{2}$ into $P(x) \rightsquigarrow 10$ multiplications and 4 additions comes to a total of 14 operations.

ii. Store powers of $\frac{1}{2}$ progressively $\rightsquigarrow 3$ multiplications (from the powers) + 4 multiplications (from the coefficients) and 4 additions. The new total is 11 operations.

iii. *Horner's Method*: Rewrite $P(x)$ "backwards":

$$P(x) = c_0 + x(c_1 + x(c_2 + x(c_3 + x(c_4))))$$

This brings it down to 8 total operations.

Fact: A degree d polynomial can be a evaluated in d multiplications and d additions.

Portfolio Part 1: Implement Horner's Method in Maple and/or MatLab.

1.1.1 Variation on the Theme

Evaluate:

$$\begin{aligned} P(x) &= x^5 + x^8 + x^{11} + x^{14} \\ &= x^5(1 + x^3 + x^6 + x^9) \\ &= x^5(1 + x^3(1 + x^3 + x^6)) \\ &= x^5(1 + x^3(1 + x^3(1 + x^3))) \end{aligned}$$

We get a total of 6 multiplications by 3 additions, thus 9 operations.

Overview of Calculus

Theorem 1. *Intermediate Value Theorem*

If $f(x)$ is continuous in $[a, b]$ then $\forall$ y, such that, $f(a) \leq y \leq f(b)$ $\exists$ c, such that $a \leq c \leq b$ and $f(c) = y$.

Corollary 2. If $f(a), f(b) < 0$, then $\exists$ c, such that $f(c) = 0$. Where c is a root of $f(x) = 0$.

Theorem 3. *Mean Value Theorem*

If $f(x)$ is differentiable in $[a, b]$ then $\exists$ c, such that $f'(c) = \frac{f(a) - f(b)}{b - a}$. Thus, there is a point where we will be able to calculate the slope at c.

Corollary 4. *Rolle's Theorem*

If $f(x)$ is differentialable at $[a, b]$ then $\exists$ c, such that $a \leq c \leq b$ and $f'(c) = 0$.

Theorem 5. *Taylor's Theorem*

If $f(x)$ is $(k + 1)$-differentiable in $[x_0, x]$, $\exists$ c, such that:

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{f''(x_0)}{2!}(x - x_0)^2 + ... + \frac{f^{k+1}(x_0)}{(k+1)!}(x - x_0)^{k+1} + R$$

where $R = \frac{f^{(k+1)}(c)}{(k+1)!}(x - x_0)^{k+1}$, is the remainder. If we know $f(x_0)$, then we can find nearby values $f(x)$ as a polynomial of degree k.

Example 6. $f(x) = \sin(x)$. Find a degree-4 Taylor polynomial (approximation) about $x_0 = 0$.

$$P_4(x) = x - \frac{x^3}{6}$$

with a remainder is $R = \frac{x^5}{120}\cos(c)$. Now, we need to estimate the size of the remainder term:

$$|R| \leq \frac{|x|^5}{120}$$

If $|x| \leq 10^{-4}$ then $|R| \leq \frac{10^{-20}}{120}$. This tells us that for all numbers $\leq 10^{-4}$, R is close to zero and thus the Taylor approximation is accurate.

Theorem 7. *Mean Value Theorem for Integrals*

If f is continuous in $[a, b]$ and g is integrable in $[a, b]$ and does not change sign in $[a, b]$ then, $\exists$ c such that $a \leq c \leq b$ and

$$\int_a^b f(x)g(x)\mathrm{dx} = f(c)\int_a^b g(x)\mathrm{dx}$$

Note: *This helps because this result gives us a way to evaluate $\int f(x)g(x)$ - as there is no defined way to do this.*

2 Floating Point Representation of Real Numbers ($\mathbb{R}$)

IEEE 754 is a standard to model floating point arithmetic on a computer. The problem is that we have finite-precision memory locations to represent infinite-precision numbers, YIKES.

IEEE 754 is a set of **binary** representations of real numbers.

A floating point, or real, number has three parts:

1. Sign ($\pm$) - s

2. Mantissa (AKA significant digits) - m

3. Exponent - e

These three parts are stored in a word. There are three common precision types:

1. Single: 32 bits, (s: 1, m: 8, e: 23)

2. Double: 64 bits (s: 1, m: 11, e: 52)

3. Long-double: 80 bits, (s: 1, m: 15, e: 64)

Definition 8. *A normalized IEEE 754* **floating point number** *is the following:*

$$\pm 1.b_1 b_2 ... b_N \times 2^p$$

where p is an M-bit binary number; where

$$b_i \in \{0, 1\}, i = 1, ..., N$$

Example 9. 9 decimal and we want to convert to an IEEE FLP number.

$$
\begin{aligned}
9 &\rightarrow 1001 \,(\text{binary}) \\
+1 \quad . \quad &001 \times 2^3 \\
N &= 3 \\
P &= 3
\end{aligned}
$$

Multiplication by power of $2 \equiv$ a shift.

Typical double precision parameters in C/MatLab: $M = 11$, $N = 52$.

Example 10. We want to represent 1.

$$
\begin{aligned}
1 &\rightsquigarrow 0001 \\
+1 \quad . \quad &0...0_{52} \times 2^0 \,(52 \,\text{zeroes})
\end{aligned}
$$

What is the "next" number we can represent? The answer is: $+1.0...0_{51}1 \times 2^0 \rightsquigarrow 1 + 2^{-52}$, this is 51 zeroes.

Definition 11. *Machine epsilon,* $\mathrm{E_{mach}}$, *is the distance between 1 and the smallest FLP number greater than 1.*

Remark 12. *For IEEE 754, double precision, we have* $\mathrm{E_{mach}} = 2^{52}$.

2.1 IEEE Nearest Rounding Rule

Example 13. 9.4 in decimal $\rightarrow 1001.\overline{0110}$

The binary representation of $0.4 \approx \frac{1}{2^2} + \frac{1}{2^3} + \frac{1}{2^6} + \frac{1}{2^7} + ... = \sum_{k=1}^{\infty} \left(\frac{1}{2^{4k+2}} + \frac{1}{2^{4k+3}} \right)$

We need to fit this precision number in 52 bits.

$$1.\underline{001}011001100110...0110\,\underline{0} \times 2^3$$

We have the three bits in the beginning following by 12 sets of 0110:

$$3\,\text{bits} + 12 \times 4\,\text{bits} = 51\,\text{bits}$$

RMR: Look at the 53rd bit to the right of the radix point: $\begin{cases} 1 \to \text{add 1 to bit 52} \\ 0 \to \text{do nothing} \end{cases}$

So in our example: 53rd bit is 1, so we add 1 to 52.

Thus, 9.4 is represented as:

$$+1.0010\underline{0110}\,\mathbf{1} \times 2^3$$

which is actually $9.4 + 0.2 \times 2^{-49}$ in decimal.

Remark 14. The IEEE double precision number associated with 9.4 using RNR is:

$$fl(9.4) = 9.4 + 0.2 \times 2^{-49}$$

where 0.2×2^{-49} is the error.

Definition 15.

$$
\begin{aligned}
x_c &= \text{computed value of } x \\
\text{absolute error} &= |x_c - x| \\
\text{relative error} &= \frac{|x_c - x|}{|x|}
\end{aligned}
$$

Remark **16.** *Relative error in IEEE 754 is bounded by:*

$$\frac{|fl(x) - x|}{|x|} \leq \frac{1}{2} E_{\text{mach}}$$

2.2 Loss of Significant Digits

Example 17. $E_1 = \frac{1 - \cos(x)}{\sin^2(x)}$ and $E_2 = \frac{1}{1 + \cos(x)}$. $\therefore E_1 = E_2$ in exact arithmetic. Evaluate E_1 and E_2 numerically for $x = 1.000...$, $x = 0.100...$, $x = 0.010...$.

Remark 18. For values of $x < 10^{-5}$, E_1 losses signifcant digits. For $x < 10^{-8}$, E_1 has no correct significant digits. Well, we are subtracting numbers that are nearly equal.

Example 19. $x^2 + 9^{12}x - 3 = 0$, with $a = 1$, $b = 9^{12}$, $c = -3$.

$$
\begin{aligned}
\Delta &= \sqrt{b^2 - 4ac} \\
x &= \frac{-b \pm \Delta}{2a} \\
\oplus \rightsquigarrow \quad x &= \frac{-b + b}{2a} = 0
\end{aligned}
$$

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But how?! We need to restructure the formula, using the conjugate quantity:

$$\frac{-b+\sqrt{\Delta}}{2a} \times \left(\frac{-b+\sqrt{\Delta}}{-b+\sqrt{\Delta}}\right)$$

$$= \frac{\Delta - b^2}{2a\left(b+\sqrt{\Delta}\right)^2}$$

$$= \frac{-4ac}{2a\left(b+\sqrt{\Delta}\right)}$$

$$= \frac{-2c}{b+\sqrt{\Delta}}$$

Note: This formula only applies for degree-2 polynomials.

3 Equation Solving

- We will explore iterative methods to locate solutions of $f(x)=0$

- Convergence, complexity

We are also going to look at three different methods of solving equations:

1. Bisection

2. Fixed-point

3. Newtons's method

3.1 Bisection Method

- We are looking to solve $f(x)=0$

- Means find r, st $f(r)=0$

- Existence of r: IVT

Steps:

1. Find $[a,b]$ st $f(a) \times f(b) < 0$

2. Then, $\exists r: a < r < b$ st $f(r)=0$

Example 20. $f(x)=x^3+x-1$, we know $f(0)=-1$, $f(1)=1$ and thus:

$$\rightsquigarrow \exists r \in [0,1] \text{ st } f(r)=0$$

Also:

$$f\left(\frac{1}{2}\right)<0 \rightsquigarrow f\left(\frac{1}{2}\right) \times f(1) < 0 \rightsquigarrow r \in \left[\frac{1}{2},1\right]$$

Next step in the interation:

$$f\left(\frac{1}{2}\right)>0 \rightsquigarrow f(0) \times f\left(\frac{1}{2}\right) < 0 \rightsquigarrow r \in \left[0,\frac{1}{2}\right]$$

And thus we know:

$$f\left(\frac{1}{2}\right) < 0$$

We now know that $\frac{1}{2} < f\left(\frac{1}{2}\right) < 1$. We know can check the midpoint of $\left[\frac{1}{2}, 1\right]$ which is $\frac{3}{4}$. Next interation:

$$f\left(\frac{3}{4}\right) > 0 \rightsquigarrow r \in \left[\frac{1}{2}, \frac{3}{4}\right]$$

Portfolio Part 2: Implement Bisection Method in Maple and/or MatLab.

Algorithm 1

Bisection Method
Input: `f`, `a`, `b` st. $f(a) \times f(b) < 0$; tolerance (ϵ) - `e`
Output: approximate root `r`, in $[a, b]$, $f(r) = 0$

```
while (b-a)/2 > e do
     r=(a+b)/2
     if f(r)=0 then return r
     if f(a)*f(r) < 0
          b=r
          else
                a=r
     return (a+b)/2
```

Example 16 cont.

ϵ	#`while` step	approx `r`
10^{-4}	13	0.6823
10^{-5}	16	0.6823
10^{-6}	19	0.68232
10^{-7}	23	0.68232780

Definition 21. *An approximate solution is correct to* <u>*p decimal places*</u> *if the error*

$$|x_c - r| < \frac{1}{2}10^{-p}$$

3.1.1 Error Analysis

- Start $[a, b]$

- After n bisection steps $[a_n, b_n]$

$$x_c = \frac{a_n + b_n}{2} \rightsquigarrow |x_c - r| < \frac{b - a}{2^{n+1}}$$

Question 22. *How many bisection steps are needed to compute a solution correct to 6 decimal places?*

Answer. *Error after n bisection steps:* $\frac{1}{2^{n+1}}$ *and thus*

$$
\begin{aligned}
\frac{1}{2^{n+1}} &< \frac{1}{2}10^{-6} \\
10^6 &< 2^n \\
\log(10^6) &< \log(2^n) \\
6 \times \log(10) &< n \times \log(2) \\
6 &< n \times \log(2) \\
19.9 &< n
\end{aligned}
$$

And thus we need 20 steps to compute 0.739085.

3.2 Fixed-Point Iteration

Definition 23. *r is a fixed point (fp) of a function $g(x)$, iff $g(r) = r$.*

Example 24. $g(x) = x^3$. *We have three fixed points: $0, \pm 1$.*

Observation. Finding a fp of $g(x) \Leftrightarrow$ solving the equation: $g(x) - x = 0$ where we can define $g(x) - x$ as $f(x)$.

Algorithm 2

FPI
Input: $f(x) = g(x) - x$, initial guess, x_0
Output: approximate solution of $f(x) = 0$, (ie. a fp of $g(x)$)

```
for i = 0..k
    x_{i+1}=g(x_i)
```

If the sequence x_0, x_1, x_2, ... <u>converges</u> to a value, r, then r is a fp of $g(x)$. For some j: $|x_{j+1} - x_j| < \text{E}$.

Question 25. *Can any fct, $f(x)$ be written as $g(x) - x$?*

Answer. *Yes, and often in more ways than one.*

Example 26. $x^2 + x - 1 = 0$

$$x = 1 - x^3 \tag{1}$$

$$x = (1 - x)^{\frac{1}{2}} \tag{2}$$

$$x = \frac{1 + 2x^3}{1 + 3x^2} \tag{3}$$

Use fp iterations with $x_0 = 0.5$.

1. The interates flip-flop from 0 to 1, **no convergence**

2. The iterates converge to 0.6823 in 25 iterations

Explanation: $|g'(r) > 1, < 1|$

Example 27.

$$g_1(x) = -\frac{3}{2}x + \frac{5}{2} \quad \text{with } r = 1 \text{ and } |g_1'(1)| = \frac{3}{2} > 1$$
$$g_2(x) = -\frac{1}{2}x + \frac{3}{2} \quad \text{with } r = 1 \text{ and } |g_2'(1)| = \frac{1}{2} < 1$$

Thus, we have $x_{i+1} = g_1(x_i)$. Consider $g(x) \rightsquigarrow$

$$x_{i+1} - 1 = -\frac{3}{2}(x_i - 1)$$

denote by $e_i = |1 - x_i|$ then $e_{i+1} = \frac{3}{2}e_i \rightsquigarrow$ error increases, divergent.

Consider $g_2(x)$ with $x_{i+1} = g_2(x_i) \rightsquigarrow$

$$x_{i+1} - 1 = -\frac{1}{2}(x_i - 1)$$

then $e_{i+1} = \frac{1}{2}e_i$. 1

Definition 28. *Denote by e_i, the error at step i, of an iterative method.*

$$e_i = |r - x_i|$$

*The method **converges linearly** with rate, S, if:*

$$\lim_{i \to \infty} \frac{e_{i+1}}{e_i} = S$$

and $S < 1$.

Observation. *f-p iteration for $g_2(x)$ converges linearly with rate $S = \frac{1}{2}$.*

Theorem 29. *Assume g is differentiable.*

$$g(r) = \quad r \quad \text{and } r \text{ is an fp of } g$$
$$|g'(r)| = \quad S < 1$$

Then, the fp iteration for g, coverges linearly with rate, S to r. For initial guesses, x_0, sufficiently close to r.

Example 30. $f(x) = x^3 + x - 1$ in the form of $g(x) = x$.

1. $g_1(x) = 1 - x^3$, now $|g_1'(x)| = 3x^2 \longrightarrow x = 0.6823 \longrightarrow > 1$

2. $g_2(x) = (1-x)^{\frac{1}{3}}$, now $|g_2'(x)| = \frac{1}{3}(1-x)^{-\frac{2}{3}} + 1 \longrightarrow x = ... \longrightarrow < 1 \quad \therefore \text{ converges}$

3. $g_3(x) = \frac{1 + 2x^3}{1 + 3x^2}$, now $|g_3'(x)| = \frac{(6x^2)(1 + 3x^2) + (6x)(1 + 2x^3)}{(1 + 3x^2)^2} \longrightarrow x = ... \longrightarrow 0 < 1 \quad$ We have a linear convergence with rate, $S = 0$

3.2.1 Stopping Criteria for FPI

Where do we need to stop the iteration?

1. Bounded absolute error:

$$|x_{i+1} - x_i| < \text{E}$$

2. Bounded relative error:

$$\frac{|x_{i+1} - x_i|}{|x_{i+1}|} < \mathrm{E}$$

Example 31. $\begin{cases} g(x) = \frac{x + \frac{2}{x}}{2} \\ x_0 = 1 \end{cases}$. Set up FPI as $g(x) = x$.

$$g(\sqrt{2}) = \frac{\sqrt{2} + \frac{2}{\sqrt{2}}}{2} = \sqrt{2}$$

3.2.2 Forward and Backward Error

Example 32. $f(x) = x^3 - 2x^2 + \frac{4}{3}x - \frac{8}{27}$. Use the bisection method to compute a root with 6 correct significant digits. We have $f(0)\, f(1) < 0$ and $f(\frac{2}{3}) = 0$.

Observation. 16 steps $\rightsquigarrow$ 0.6666641. We cannot get the 6$^{\text{th}}$ digit correct.

IEEE double precision, there are many float point numbers within 10^{-5} of the correct root $r = \frac{2}{3}$.

Definition 33. *Suppose a function, f, with root r and $f(r) = 0$. Also, x_a is an approximation to r computed by a root-finding method.*

Backwards error (BE): $|f(x_a)|$

Forward error (FE): $|r - x_a|$

BE amount by which we need to change $f(x)$ so that x_a is a solution. FE amount by which we need to change the approximate solution to make it correct.

***Remark* 34.** *The problem we encountered with the previous example is that the BE is near* $\mathrm{E}_{\text{mach}} = 10^{-16}$ *and the FE* $\approx 10^{-5}$.

Definition 35. *Multiple Roots*

f, a differentiable function, with root r and $f(r) = 0$ if

$$o = f(r) = f'(r) = f''(r) = \dots = f^{(m-1)}(r)$$

and $f^{(m)}(r) \neq 0$. Then, f, has a root of multiplicity m, at r; where r is a multiple root of order m of f.

$$\begin{cases} m = 1; r \text{ single root} \\ m = 2; r \text{ double root} \\ m = 3; r \text{ triple root} \end{cases}$$
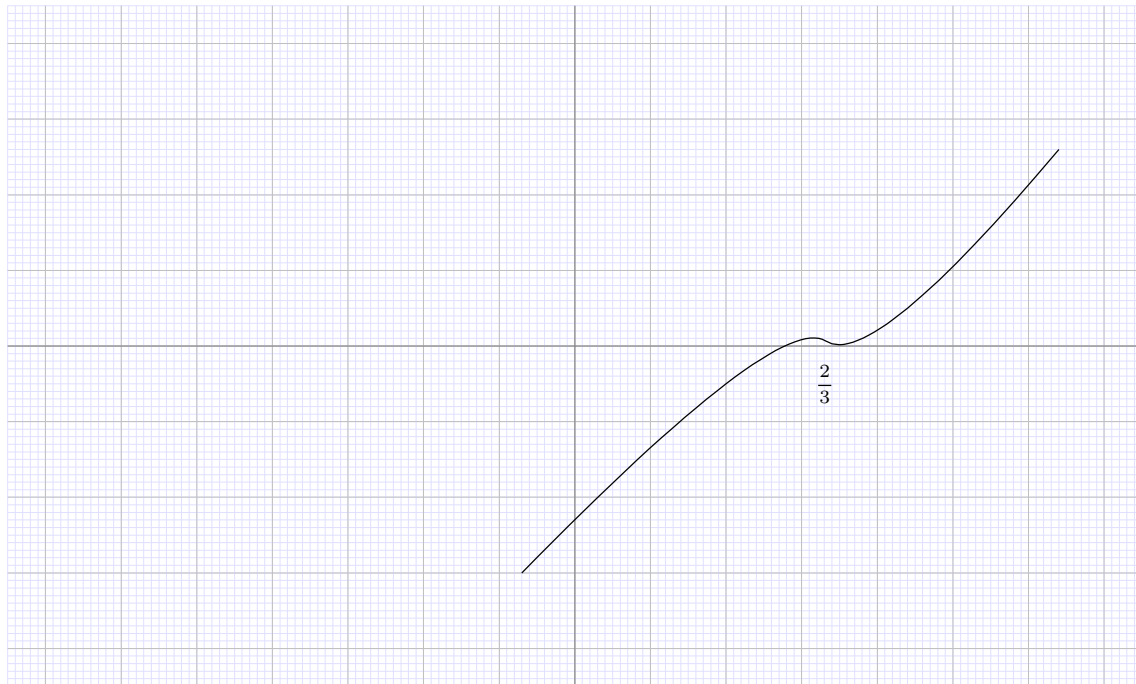
Example 36. $f(x) = x^2$, has a double root at $x = 0$.

$$\begin{array}{rcl} f(0) & = & 0 \\ f'(0) & 2x|_{x=0} & = 0 \\ f''(0) & = & 2 \neq 0 \end{array}$$

Also, $f(x) = x^3$ has a triple root at $x = 0$.

Geometric Intuition.

Graph of $f(x) = \left(x - \frac{2}{3}\right)^3$.

$\frac{2}{3}$ is a triple root. The graph is [supposed to be] flat around the triple root.

Consequence. Large disparity between BE and FE.

$$\text{BE} \ll \text{FE}$$

where BE is the vertical dimension and FE is the horizantal dimension.

Example 37. $f(x) = \sin(x) - x$ has a triple root at $r = 0$ and $x_a = 0.001$ is the approx. root. Compute BE and FE.

$$
\begin{aligned}
\text{BE: } |f(x_a)| &= \ 10^{-3} \\
\text{FE: } |r - x_a| &= \ |\sin(0.001) - 0.001| \\
&\approx \ \ 1.6667 \times 10^{-10}
\end{aligned}
$$

Stopping Criteria. Either make FE small or make BE small.

$$\text{Bisection: } \begin{cases} \text{BE: known} \\ \text{FE: } < \frac{b - a}{2} \end{cases}$$

```
> if abs(f(xₐ)) < E then ...
> if abs(b − a/2) < E then ...
```

$$\text{Fixed point: } \begin{cases} \text{BE: known} \\ \text{FE: not known} \end{cases}$$

3.2.3 Wilkinson Polynomial

$$
\begin{aligned}
W(x) &= (x - 1)(x - 2)...(x - 20) \\
&= \prod_{i=1}^{20} (x - i)
\end{aligned}
$$

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It has 20 (simple) roots, $x = 1, ..., 20$. To compute numerical approximations to the roots of the expanded $W(x)$ is very hard. $W(x) = x^{20} \pm ...$

3.2.4 Sensitivity of Root Finding

A problem is called sensitive if small errors in the input (the eq. we are solving). This leads to large errors in the output (solution).

We need to measure how far a root is moved when the eq. is changed (perturbed).

Proposition 38. *Supposed, we change $f(x) \to f(x) + \epsilon\, g(x)$.*

Let Δ_r be the corresponding change to the root r.

$$f(r + \Delta_r) + \epsilon\, g(r + \Delta_r) = 0$$

D-d-d-d-d-drop the Taylor and neglect the higher order terms (H.O.T).

$$\Delta_r \approx -\frac{\epsilon\, g(r)}{f'(r)}$$

for $\epsilon \ll f'(r)$.

Example 39. Estimate the largest root of

$$P(x) = \left(\prod_{i=1}^{6} (x - i) \right) - 10^{-6} x^7$$

Get all emotional and used the sensitivity formula.

$$\begin{aligned} \epsilon &= -10^{-6} \\ g(x) &= x^7 \\ f(x) &= P(x) \end{aligned}$$

Now:

$$\Delta_r \approx \frac{\epsilon\, 6^7}{5!} = -2332.8\,\epsilon$$

and thus:

$$6 + \Delta_r = 6.0023$$

3.3 Newton's Method

Problem. Find a root of a fn, $f(x) = 0$.

The first thing we need to do is start with an initial guess of x_0. Draw the tangent line to f at x_0 and identify the point where the tangent intersects with the x-axis.

We can get the equation of the tangent line at $(x_0, f(x_0))$.

$$y - f(x_0) = f'(x_0)\, (x - x_0)$$

where $f'(x_0)$ is the slope. The intersection of the above equation and the x-axis $\leadsto y = 0$, we obtain:

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

Algorithm 3

    Input: $f(x)$, x_0 (initial guess)
    Ouput: approximation to root r st $f(r) = 0$
    The way it would iterate:

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$$

    where $i = 0, 1, 2, ...$

Example 40. $f(x) = x^3 + x - 1$.

First compute $f'(x) = 3x^2 + 1$. Newton iteration is:

$$
\begin{aligned}
x - \frac{f(x)}{f'(x)} &= x - \frac{x^3 + x - 1}{3x^2 + 1} \\
&= \frac{2x^3 + 1}{3x^2 + 1}
\end{aligned}
$$

Thus we have a generalized form: $x_{i+1} = \frac{2x_i^3 + 1}{3x_i^2 + 1}$ with $x_0 = 0.1$.

We can perform 6 iterations to give you the root with the correct 8 significant digits: 0.68232780.

Definition 41. *Denote e, as the error at step i:* $|r - x_i|$.

The iterative method converges quadratically $\iff$

$$\lim_{i \to \infty} \frac{e_{i+2}}{e_i^2} = M$$

Remark 42. *If $f(r) = 0$, and $f'(r) = 0$, then Newton's method converges quadratically to r and thus, $M = \frac{f''(r)}{2\,f'(r)}$, where **M** denotes the rate of convergence.*

Example 40 Continued. We then have $f''(x) = 6x$ with $r = 0.6823$ and $M \approx 0.85$.

Example 43. $f(x) = x^2$, with $r = 0$ being a double root.

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)} = x_i - \frac{x_i^2}{2x_i} = \frac{x_i}{2}$$

We can make an educated guess for $x_0 = 1$.

i	x_i	$e_i \longrightarrow \dfrac{e_i}{e_{i-1}}$		
0	1.000	1.000	$\longrightarrow$	—
1	0.500	0.500	$\longrightarrow$	0.500
2	0.250	0.250	$\longrightarrow$	0.500
3	0.125	0.125	$\longrightarrow$	0.500

Remark 44. If f has a root with multiplicity, m, then Newton's method is locally convergent to r, with rate: $\frac{m-1}{m}$:

$$\frac{e_{i+1}}{e_i} \approx \frac{m-1}{m}$$

Example 45.

1. $f(x) = \sin(x) + x^2 \cos(x) - x^2 - x \longrightarrow$ find the mult. of root $r = 0$

   - First check that $f(0) = 0$, $f'(0) = 0$, ... We have computed the multiplicity when $f^{(n)}(0) \neq 0$. In this case, $f''(0) \neq 0 \ldots f'''(0) \neq 0$. Thus, we have a triple root $\to$ with a convergence rate of $\frac{2}{3}$. The error decreases by $\frac{2}{3}$ at each iteration.

2. Estimate the number of Newton iterations to converge with 6 significant digits

   - Suppose that we choose $x_0 = 1$. The estimate is $\left(\frac{2}{3}\right)^n < \frac{1}{2} 10^{-6} \longrightarrow n > 35$

3.3.1 Modified Newton's Method

If $f(x)$ has a root of mult. m, then:

$$x_{i+1} = x_i - m \frac{f(x_i)}{f'(x_i)}$$

converges quadratically to r.

3.3.2 Alternative Derivation to Newton's Method

Assume $f(x) = 0$, x_0. The Taylor series expansion about x_0 is:

$$
\begin{aligned}
f(x) &= f(x_0) + (x - x_0)\, f'(x_0) + \underline{\text{HOT}} \rightsquigarrow \\
x &= x_0 - \frac{f(x_0)}{f'(x_0)}
\end{aligned}
$$

where the *HOT* are neglected.

Example 46. Solve $f(x) = x^2 + 1 \rightsquigarrow r = \pm i$. Now, $x_0 = 0.1 \pm i$. This converges to i in 4 iterations.

3.3.3 Newton's Method Can Fail

Example 47. $f(x) = 4x^4 - 6x^2 - \frac{11}{4} = 0$ with $x_0 = \frac{1}{2}$ (bi-quadratic equation). We then have the Newton iteration being:

$$x_{i+1} = x_i - \frac{f(x_i)}{16x_i^3 - 12x_i}$$

$$
\begin{aligned}
x_1 &= -\frac{1}{2} \\
x_2 &= \frac{1}{2} \\
x_3 &= \frac{1}{2} \\
x_4 &= -\frac{1}{2} \\
&\vdots
\end{aligned}
$$

There is no convergence. Roots are ± 1.3667. We have an even function st $f(x) = f(-x)$ and thus

$$f\left(\frac{1}{2}\right) = f\left(-\frac{1}{2}\right) = -4$$

The tangent lines at $\left(\frac{1}{2}, 4\right)$ and $\left(-\frac{1}{2}, 4\right)$ will intersect at the x-axis at $-\frac{1}{2}, \frac{1}{2}$.

Example 48. $f(x) = \sin(2x)$, with $x_0 = 0.75$. Newton's method converges to the root -2π. We convrege to and missed the closer root, 0.

Why? This occurs, if $f(x_i)$ is very small, then the tangent line is almost horizantal.

Example 49. $f(x) = x\, e^x$. Newton iteration with $x_0 = 2$. The Newton iteration is:

$$x_{i+1} = x_i - \frac{x_i\, e^{-x_i}}{e^{x_i} - x_i\, e^{-x_i}} = \frac{x_i^2}{x_i - 1}$$

$$
\begin{aligned}
x_1 &= 4 \\
x_2 &= \frac{16}{3} \\
x_3 &= \ldots \\
&\vdots \\
&\to \infty
\end{aligned}
$$

This converges to infinity and thus fails.

3.3.4 Multivariate Newton's Method

Example 50. $f_1(x_1, x_2) = x_1^2 + x_2^2 - 8x_1 - 4x_2 + 11 = 0$ and $f_2(x_1, x_2) = x_1^2 + x_2^2 - 20x_1 + 75 = 0$.

These equations give us two circles. We need to solve the system $\begin{cases} f_1(x_1, x_2) = 0 \\ f_2(x_1, x_2) = 0 \end{cases}$. The solution of the system will give us the two points where the circles intersect (twice).

Let's start with the initial condition $(x_1^\circ = 2, x_2^\circ = 4)$. First step: compute 4 partial derivatives.

$$
\begin{aligned}
\frac{\delta f_1}{\delta x_1} &= 2x_1 - 8 \\
\frac{\delta f_2}{\delta x_1} &= 2x_2 + 20
\end{aligned}
$$

And then:

$$
\begin{aligned}
\frac{\delta f_1}{\delta x_2} &= 2x_2 - 4 \\
\frac{\delta f_2}{\delta x_2} &= 2x_2
\end{aligned}
$$

This gives us: $f_1(x_1^\circ, x_2^\circ) = -1$ and $f_2(x_1^\circ, x_2^\circ) = 55$. We can then put these values in a Jacobian matrix: $J(x_1, x_2) = (f_1, f_2) =$

$$
\begin{pmatrix}
2x_1 - 8 & 2x_2 - 4 \\
2x_1 - 20 & 2x_2
\end{pmatrix}
$$

We need compute it's value at $(2, 4)$. This gives us:

$$
J_{(f_1, f_2)}(2, 4) = \begin{pmatrix} -4 & 4 \\ -16 & 8 \end{pmatrix}
$$

To compute the next iterate (x_1^1, x_2^1). To do this, we compute:

$$
\begin{aligned}
x_1^1 &= x_1^\circ + \Delta x_1 \\
x_2^1 &= x_2^\circ + \Delta x_2
\end{aligned}
$$

Now solve:

$$\begin{pmatrix} -4 & 4 \\ -16 & 8 \end{pmatrix} \begin{pmatrix} \Delta x_1 \\ \Delta x_2 \end{pmatrix} = \begin{pmatrix} 1 \\ -55 \end{pmatrix}$$

Using the values of $\Delta x_1 = 7.125$ and $\Delta x_2 = 7.375$. This gives us:

$$\begin{aligned} x_1^1 &= 2 + 7.125 = 9.125 \\ x_2^1 &= 4 + 7.375 = 11.375 \end{aligned}$$

This converges in 8 iterations.

Algorithm 4

Input: $f_1(x_1, ..., x_n) = 0$ (square system of non-linear equations)
$\vdots$
$f_n(x_1, ..., x_n) = 0$
ϵ, initial point $(x_1^\circ, ..., x_n^\circ)$
Output: Approx. solution $\vec{r} = (r_1, ..., r_n)$ st $f_1\left(\vec{r}\right) = ... = f_n\left(\vec{r}\right) = 0$

```
i = 1
while (|f_j(r)| >= eps, j = 1) do
    i = i+1
    solve system of linear eqs
```

$$J_{(f_1 ::: f_n)}(x_1^i ; :::; x_n^i) \begin{pmatrix} \Delta x_1 \\ \Delta x_2 \end{pmatrix} = \begin{pmatrix} -f_1\left(\vec{x^i}\right) \\ \vdots \\ -f_n\left(\vec{x^i}\right) \end{pmatrix}$$

```
x_j^(i) = x_j^(i-1) + Δx_j, j=1..n
```

Let's talk Jacobian dude.

Jacobian $n \times n$ Matrix

$$J_{(f_1, ..., f_n)}(x_1, ..., x_n) = \begin{pmatrix} \dfrac{\delta f_1\left(\vec{x}\right)}{\delta x_1} & \cdots & \dfrac{\delta f_1\left(\vec{x}\right)}{\delta x_n} \\ \vdots & \ddots & \vdots \\ \dfrac{\delta f_n\left(\vec{x}\right)}{\delta x_1} & \cdots & \dfrac{\delta f_n\left(\vec{x}\right)}{\delta x_n} \end{pmatrix}$$

3.4 Secant Method (root-finding without derivatives)

We want to replace the tangent with the *secant* line:

$$f'(x_i) = \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}}$$

So we replace the tangent line with a discrete approximation.

Algorithm 5

Input: $f(x)$, x_0, x_1, ϵ (two initial guesses)
Output: approximation to the root, r

$$x_{i+1} = x_i - f(x_i) \frac{x_i - x_{i-1}}{f(x_i) - f(x_{i-1})} = x_i - f(x_i) \frac{1}{f'(x_i)}$$

Where $i = 1, 2, 3, ...$
Error Analysis:

If $f'(r) \neq 0$ (simple root), and the secant method converges, then $e_{i+1} \approx c\, e_i^\phi$. This is called *superlinear convergence*.

We have the golden ratio, $\phi = \frac{1 + \sqrt{5}}{2} \approx 1.6$

4 Systems of Linear Equations

$$\begin{cases} a_{11}x_1 + a_{12}x_2 + ... + a_{1n}x_n = b_1 \\ a_{21}x_1 + a_{22}x_2 + ... + a_{2n}x_n = b_2 \\ \vdots \\ a_{n1}x_1 + a_{n2}x_2 + ... + a_{nn}x_n = b_n \end{cases}$$

In an $n \times n$ system, there are n equations and n variables. The <u>matrix form</u> of a system:

$$\begin{pmatrix} a_{11} & a_{12} & ... & a_{1n} \\ a_{21} & a_{22} & ... & a_{2n} \\ & & \vdots & \\ a_{n1} & a_{n2} & ... & a_{nn} \end{pmatrix} \times \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}$$

<u>Solution methods:</u>

Direct methods:

- Gauss elimination

- Gauss-Jordan

- LU decomposition

Iterative methods:

- Jacobi

- Gauss-Seidel

- Relaxtion

4.1 Vector, Matrix Norms

If we have $\vec{x} = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}$, we need to measure the size of $\vec{x}$ by the *Euclidean* norm:

$$\left\| \vec{x} \right\| = \sqrt{x_1^2 + ... x_n^2}$$

Then we have the L_p norm:

$$\left\| \vec{x} \right\| = \sqrt[p]{|x_1|^p + ... + |x_n|^p}$$

The following results occur:

$$\begin{aligned} p = 1 \ &\rightsquigarrow \ \text{sum of absolute values of the elements of } \vec{x} \\ p = 2 \ &\rightsquigarrow \ L_p = \text{Euclidean norm} \\ p = \infty \ &\rightsquigarrow \ \max |x_i| \end{aligned}$$

We can denote $A = (\, a_{ij} \,)$, where A is an $m \times n$ matrix (rows $\times$ columns).

We have the *Frobenius* norm:

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

where the $\|A\|_F$ has $m \times n$ terms.

p-norms:

$$\|A\|_p = \max \left\| A \vec{x} \right\|_p$$

where $\left\| \vec{x} \right\| = 1$.

Next, we look at 4 square matrices $n \times n$:

$$\|A\|_2 = \max \lambda_i$$

where $i = 1, ..., n$. λ_i are the eigenvalues of A.

Next, the *spectral* norm:

$$\|A\|_1 = \max_{1 \leq j \leq n} \left(\sum_{i=1}^{n} |a_{ij}| \right)$$

$$\|A\|_\infty = \max_{1 \leq i \leq n} \left(\sum_{j=1}^{m} |a_{ij}| \right)$$

4.1.1 Norm Inequalities

1. $\|A\|_2 \leq \|A\|_F \leq \sqrt{n}\|A\|_2$

2. $\frac{1}{\sqrt{n}}\|A\|_\infty \leq \|A\|_2 \leq \sqrt{n}\|A\|_\infty$

3. $\frac{1}{\sqrt{n}}\|A\|_1 \leq \|A\|_2 \leq \sqrt{n}\|A\|_1$

4.1.2 Solution Concepts

Remember: $A \times \vec{x} = \vec{b}$ where the sizes are $n \times n$, $n \times 1$ and $n \times 1$ respectively.

1. If $\vec{b} = \vec{0}$ then it is a <u>homogeneous</u> system

   - Trivial solution of $\vec{x} = \vec{0}$

   - A non-trivial solution exists if $\det(A) = 0$

2. If $\vec{b} \neq \vec{0}$, then it is a <u>non-homogeneous</u> system, denoted as *augmented* matrix

$$A' = \left[A / \vec{b} \right]$$

   - System has a solution $\iff \operatorname{rank}(A) = \operatorname{rank}(A')$

   - Solution is unique if $\operatorname{rank}(A) = n$; A is considered **full rank**

- If $\text{rank}(A) < n$, then it is denoted as **inconsistent**

Definition 51. *Linearly dependent rows and equations*

$$A = \begin{pmatrix} 1 & -1 & 1 \\ 2 & 1 & -1 \\ 8 & 1 & -1 \end{pmatrix} \rightsquigarrow \begin{cases} r_1 \\ r_2 \\ r_3 \end{cases}$$

And we have: $2r_1 + 3r_2 = r_3$. And r_1, r_2 and r_3 are linearly dependent.

4.2 Rank and Nullspace of a Matrix $(A{:}\, m \times n)$

We can have:

$$\begin{aligned} \text{range}(A) &= \left\{ \vec{y} \in \mathbb{R}^m \colon \vec{y} = A\vec{x}, \text{for some } \vec{x} \in \mathbb{R}^n \right\} \\ \text{rank}(A) &= \dim(\text{range}(A)) \\ \text{nullspace}(A) &= \left\{ \vec{x} \in \mathbb{R}^n \colon A\vec{x} = \vec{0} \right\} \end{aligned}$$

Theorem 52. $\dim(\text{nullspace}(A)) + \text{rank}(A) = n$

Where the $\text{rank}(A)$ is the maximum, linearly independent number of rows.

Definition 53. *A is a full rank if*

$$\text{rank}(A) = \min(m, n)$$

A is rank-defficient if

$$\text{rank}(A) < \min(m, n)$$

4.3 Cramer's Method

We have $A\vec{x} = \vec{b}$ where A is an $n \times n$ matrix. We define:

$$A_i = \begin{pmatrix} \vdots & \begin{pmatrix} b_1 \\ \vdots \\ b_n \end{pmatrix} & \vdots \end{pmatrix}$$

with $i = 1, ..., n$. Then, we can have $x_i = \frac{|A_i|}{|A|}$ with $i = 1, ..., n$.

Example 54. Given:

$$\begin{aligned} x_1 - x_2 + x_3 &= 3 \\ x_1 + x_2 - x_3 &= 0 \\ 3x_1 + 2x_2 + 2x_3 &= 15 \end{aligned}$$

That looks like:

$$|A| = \begin{pmatrix} 1 & -1 & 1 \\ 2 & 1 & -1 \\ 3 & 2 & 2 \end{pmatrix} = 1 \times \begin{pmatrix} 1 & -1 \\ 2 & 2 \end{pmatrix} - (-1) \times \begin{pmatrix} 2 & -1 \\ 3 & 2 \end{pmatrix} + 1 \times \begin{pmatrix} 2 & 1 \\ 3 & 2 \end{pmatrix}$$

We then have:

$$|A_1| = \begin{pmatrix} 3 & -1 & 1 \\ 0 & 1 & -1 \\ 15 & 2 & 2 \end{pmatrix} = 12, x_1 = \frac{|A_1|}{|A|} = \frac{12}{12} = 1$$

Next:

$$|A_2| = \begin{pmatrix} 1 & 3 & 1 \\ 2 & 0 & -1 \\ 3 & 15 & 2 \end{pmatrix} = 24, x_2 = \frac{24}{12} = 2$$

And:

$$|A_3| = \begin{pmatrix} 1 & -1 & 3 \\ 2 & 1 & 0 \\ 3 & 2 & 15 \end{pmatrix} = 48, x_3 = \frac{48}{12} = 4$$

4.4 Gauss Elimination

The **strategy** is reduce to [upper] triangular form, and then run back substitution. This reduction is carried out by *elementary row operations*:

- Multiply divide by any row or constant value

- Any row can be added/subtracted to/from any row

- Interchange rows

Example 55. Suppose we have the system:

$$\begin{aligned} 2x_1 - x_2 + x_3 &= 4 \\ 4x_1 + 3x_2 - x_3 &= 6 \\ 3x_1 + 2x_2 + 2x_3 &= 15 \end{aligned}$$

Use elementary row operations to obtain:

$$\begin{aligned} x_3 &= 4 \\ x_2 &= 2 \\ x_1 &= 1 \end{aligned}$$

4.4.1 Determinant Computation via GEM

If we have $A \times \vec{x} = \vec{b}$ and by GE we reduce it to $\widetilde{A} \times \vec{x} = \vec{b}$. We can then say:

$$\det(A) = \det\left(\widetilde{A}\right)$$

We can then define the property:

$$\det(B) = \prod_{i=1}^{n} b_{i_i}$$

where B is triangular. From the previous example, we have

$$\det(A) = 2 \times 5 \times \frac{13}{5} = 26$$

where those numbers come from the diagonal of the [upper] triangle matrix.

4.5 Gauss-Jordan

It is an extension of GEM. Use a *pivot* to reduce (to 0). Element below and above the main diagonal - apply back substitution as needed.

$$A \overset{\text{GJ}}{\rightsquigarrow} I_n$$

What happens is we end up finding the solution, in the augment, by transforming A in I_n.

4.5.1 Inverse Matrix Computation via GJE

$$(\ A|I_n \ ) \overset{\text{GJ}}{\rightsquigarrow} (\ I_n|A^{-1} \ )$$

The way this one works, is transforming $A \to I_n$ and the augment now has the inverse.

4.6 LU Decomposition

$$A = L \times U$$

Where L is a lower triangular matrix and U is an upper triangular matrix. We can start by saying A has n^2 elements, L has $\frac{n(n+1)}{2}$ and U has $\frac{n(n+1)}{2}$.

We have n extra variables in LU wrt A. There are 3 LU variations:

1. $u_{ii} = 1$ where $i = 1, ..., n \longrightarrow$ Crout

2. $l_{ii} = 1$ where $i = 1, ..., n \longrightarrow$ Doolittle

3. $l_{ii} = u_{ii}$ where $i = 1, ..., n \longrightarrow$ Choleski

This proposes 2 issues:

1. Find LU given A

2. Solve $A \times \vec{x} = \vec{b}$

The second:

$$\left(\text{LU} \times \vec{x} \right) = \vec{b}$$

and denote $U \times \vec{x} = \vec{z}$. We then have $l \times \vec{z} = \vec{b}$.

Example 56. Let's say we have $A = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}$. Find the LU decomposition, of A, using Crout's method.

$$A \ = \ L \times U \rightsquigarrow$$
$$\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} = \begin{pmatrix} l_{11} & 0 & 0 \\ l_{21} & l_{22} & 0 \\ l_{31} & l_{32} & l_{33} \end{pmatrix} \times \begin{pmatrix} 1 & u_{12} & u_{13} \\ 0 & 1 & u_{23} \\ 0 & 0 & 1 \end{pmatrix}$$
$$9 \, a_{ij} \text{ variables} \qquad 6 \, l_{ij} \text{ variables and } 3 \, u_{ij} \text{ variables}$$

Computation:

$$= \begin{pmatrix} l_{11} & l_{11}\,u_{12} & ... \\ l_{21} & l_{21}\,u_{12} + l_{22} & ... \\ l_{31} & l_{31}\,u_{12} + l_{32} & ... \end{pmatrix}$$

Our objective is to find l_{ij} and u_{ij} in terms of a_{ij}. Equate A and $LU \rightsquigarrow$

$$\begin{aligned} l_{11} &= a_{11} \\ l_{21} &= a_{21} \\ l_{31} &= a_{31} \\ u_{12} &= \frac{a_{12}}{a_{11}} \\ \vdots \quad & \vdots \quad \vdots \end{aligned}$$

We can find the rest of the matrix entries but solving the rest of the computation.

Example 57. Use LU decomposition of A to solve the linear system $A \times \vec{x} = \vec{b}$.

$$A = \begin{pmatrix} 2 & -1 & 1 \\ 4 & 3 & -1 \\ 3 & 2 & 2 \end{pmatrix}, \vec{b} = \begin{pmatrix} 4 \\ 6 \\ 15 \end{pmatrix}$$

$$A = L \times U = \begin{pmatrix} 2 & 0 & 0 \\ 4 & 5 & 0 \\ 3 & \frac{7}{2} & \frac{13}{5} \end{pmatrix} \times \begin{pmatrix} 1 & -\frac{1}{2} & \frac{1}{2} \\ 0 & 1 & -\frac{3}{5} \\ 0 & 0 & 1 \end{pmatrix}$$

We can then denote $\vec{z} = U \times \vec{x}$ (2), and then the original system becomes: $L \times \vec{z} = \vec{b}$ (1). We can then solve (1) to obtain:

$$\vec{z} = \begin{pmatrix} 2 \\ -\frac{2}{5} \\ 4 \end{pmatrix}$$

and solve (2) to obtain:

$$\vec{x} = \begin{pmatrix} 1 \\ 2 \\ 4 \end{pmatrix}$$

Note: LU is especially efficient when we need to solve several linear systems with the same A and different constant vectors, $\vec{b_i}$ because we need to find the LU decomposition of A, only once; and use it k times.

Theorem 58. *An $n \times n$ matrix, A, has an LU decomposition if $\det(A(1\!:\!k, 1\!:\!k)) \neq 0$ for $k = 1, ..., n-1$.*

Notation 59. *This $A(1\!:\!k, 1\!:\!k)$ is called a **leading principal minor** of A. If $k = 1$, we take the first element of the matrix being the leading principal minor of $k = 1$. If $k = 2$, then we take 4 elements, and that is the leading principal minor for $k = 2$. This increases by an exponential factor of 2. Then can continue until $n-1$.*

Example 60. $n = 3$, $A = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 4 & 7 \\ 3 & 5 & 3 \end{pmatrix}$.

This matrix does not have a LU decomposition, because, for the previous theorem, for $k = 2$, there is a determinant of $\begin{vmatrix} 1 & 2 \\ 2 & 4 \end{vmatrix} = 0$.

Example 61. We have $A = \begin{pmatrix} 4 & -1 & 1 \\ -1 & 6 & 4 \\ 1 & -4 & 5 \end{pmatrix}$. For $k = 1, 2$ the leading principal minors have $\det \neq 0$.

NOTE: If $a_{11} = 0$, we cannot compute the LU decomposition.

4.7 Iterative Methods to Solve Linear Systems

1. Jacobi Method, $A \times \vec{x} = \vec{b}$

$$
\begin{aligned}
a_{11}\, x_1 + a_{21}\, x_2 + \ldots + a_{1n}\, x_n &= b_1 \rightsquigarrow x_1 = \frac{1}{a_{11}}\left(b_1 - a_{12}\, x_2 - \ldots - a_{1n}\, x_n\right) \\
\vdots &= \vdots \\
a_{n1}\, x_1 + \ldots + a_{nn} x_n &= b_n \rightsquigarrow x_n = \frac{1}{a_{nn}}\left(b_n - a_{n1}\, x_1 - \ldots - a_{nn-1}\, x_{n-1}\right)
\end{aligned}
$$

In summary, $x_i = \frac{1}{a_{ii}}\left(b_i - \sum_{j=1}^{n} a_{ij}\, x_j\right)$, for $i = 1, \ldots, n$. We need to exclude $j = i$ from the sum, so we have $n - 1$ terms.

Our initial guess is: $x_1^{(1)}, x_2^{(1)}, \ldots, x_n^{(1)}$. For example, we could have $x_1^{(1)} = 0, x_2^{(1)} = 0, \ldots, x_n^{(1)} = 0$.

We then substitute our initial guess into the Jacobi iteration formula and obtain $x_1^{(2)}, x_2^{(2)}, \ldots, x_n^{(2)}$. This would be the next approximation to the solution.

In general:

Substitute $x_i^{(k)}$ for $i = 1, \ldots, n$ into the Jacobi iteration formula to obtain $x_i^{(k+1)}$, the next iteration.

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

excluding $j = i$ so we have $n - 1$ terms.

Convergence/stopping criterion:

$$
\left| x_i^{(k+1)} - x_i^{(k)} \right| \leq \epsilon, \forall i = 1, \ldots, n
$$

There is a condition for the convergence of the Jacobi matrix: if A, is *diagonally dominant*, then Jacobi will converge to the solution.

Definition 62. *Matrix A, is **diagonally dominant** if*

$$
|a_{ii}| > \sum_{j=1}^{n} |a_{ij}|
$$

excluding $j = i$ and $\forall i = 1, \ldots, n$.

So basically, if the diagonal element of that row is larger than the sum of the absolute value of all other elements in the same row, and this occurs for every row in the matrix, then the matrix is considered diagonally dominant. Sexy.

Example 63. We have:

$$
\begin{aligned}
-5x_1 - x_2 + 2x_3 &= 1 \\
2x_1 + 6x_2 - 3x_3 &= 2 \\
2x_1 + x_2 + 7x_3 &= 32
\end{aligned}
$$

Check if this is diagonally dominant. The first row:

$$|-5| > |-1| + |2|$$

This checks out.

$$|6| > |2| + |-3|$$

This also checks out.

$$|7| > |2| + |1|$$

Nice! It works. Let's call it a *domimatrix*. Sorry. It is diagonally dominant.

$$
\begin{aligned}
x_1 &= -\frac{1}{5}(1 + x_2 - 2x_3) \\
x_2 &= \frac{1}{6}(2 - 2x_1 - 3x_3) \\
x_3 &= \frac{1}{7}(32 - 2x_1 - x_2)
\end{aligned}
$$

Our initial approximation is $x_1^{(1)} = 0, x_2^{(1)} = 0, x_3^{(1)} = 0$. The next approximation is:

$$
\begin{aligned}
x_1^{(2)} &= -\frac{1}{5} \\
x_2^{(2)} &= \frac{1}{3} \\
x_3^{(2)} &= \frac{32}{7}
\end{aligned}
$$

The next approximation is:

$$
\begin{aligned}
x_1^{(3)} &= 1.56 \\
x_2^{(3)} &= 2.68 \\
x_3^{(3)} &= 4.58
\end{aligned}
$$

The Jacobi converges to the solution $x_1 = 1$, $x_2 = 2$ and $x_3 = 4$.

2. Gauss-Seidel

This is an improvement upon the Jacobi method: $x_i^{(k+1)}$ are generated for $x_i^{(k)}$.

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

If A is diagonally dominant, the $G - S$ method converges to the solution.

5 Ill-conditions and Condition Numbers

Definition 64. *A system of equations is said to be **ill-conditioned** if small changes in the coefficients lead to very large changes in the solution.*

Example 65.

$$x_1 - x_2 = 5$$
$$k\,x_1 - x_2 = 4$$

There are k parameters, $k \neq 1$ and $k = 1$ has no solutions.

$$\det(A) = \begin{vmatrix} 1 & -1 \\ k & -1 \end{vmatrix} = k - 1$$

The solution is:

$$x_1 = \frac{1}{1-k}, x_2 = \frac{5\,k - 4}{1 - k}$$

We then have (k approaching 1 from negative and positive side):

$$\text{if } k \to 1^- \quad \text{then} \quad x_1 \in [3000, 10000]$$
$$\text{if } k \to 1^+ \quad \text{then} \quad x_2 \in [-10000, -3000]$$

Thus we have an ill-condition around $k = 1$.

We can quantify ill-conditionness using the **condition number**.

Definition 66.

$$\text{cond}(A) = \|A\| \cdot \|A^{-1}\|$$

(using various norms). This is a mesasure of how ill-conditioned a problem is.

Properties:

$$\text{cond}(I_n) = 1$$
$$\text{cond}(A) \geq 1$$

If we have a large $\text{cond}(A)$*, example 10000, then we say the linear system is ill-conditioned.*

Example 65. (cont.)

$$A^{-1} = \frac{1}{\det(A)} \times \begin{pmatrix} -1 & 1 \\ -k & 1 \end{pmatrix}$$

We then have two cases: [we will use the ∞ norm - max. row sum]

1. $k > 1$

$$\|A\|_\infty = k + 1$$
$$\|A^{-1}\|_\infty = \frac{k+1}{k-1}$$

We then have $\text{cond}(A) = \frac{(k+1)^2}{k-1}$.

$$k = 1.0001 \rightsquigarrow \text{cond}(A) \approx 40000$$
$$k = 1.0002 \rightsquigarrow \text{cond}(A) \approx 20000$$

2. $k < 1$

$$\|A\|_\infty = 2$$
$$\|A^{-1}\|_\infty = \frac{2}{1-k}$$

We have $\text{cond}(A) = \frac{4}{1-k}$.

$$k = 0.998 \rightsquigarrow \text{cond}(A) \approx 20000$$
$$k = 0.999 \rightsquigarrow \text{cond}(A) \approx 40000$$

The condition number is $\approx 10^s$. Thus, we may end up losing s significant digits.

5.1 Positive Definite Matrices

Definition 67. *A $(n \times n)$ matrix is **positive-definite** if:*

define $\vec{x}$ as an $n \times 1$.

$$\vec{x} \cdot A \cdot \vec{x} > 0, \forall \vec{x} \neq \vec{0}$$

Example 68. Show that $A = \begin{pmatrix} 2 & 2 \\ 2 & 5 \end{pmatrix}$ is positive-definite. Let's use $n = 2$.

Take $\vec{x} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$ and prove that:

$$\begin{pmatrix} x_1 & x_2 \end{pmatrix} \times \begin{pmatrix} 2 & 2 \\ 2 & 5 \end{pmatrix} \times \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} > 0$$

for every x_1, x_2. Then $\rightsquigarrow 2(x_1 + x_2)^2 + 3 x^2 \geq 0$. This will be equal to 0 when

$$\begin{cases} x_1 + x_2 = 0 \longrightarrow x_1 = 0 \\ x_2 = 0 \longrightarrow x_2 = 0 \end{cases}$$

Example 69. Show that $A = \begin{pmatrix} 2 & 4 \\ 4 & 5 \end{pmatrix}$ is **not** positive-definite. Thus, exhibit $\vec{x}$ such that

$$\vec{x} \cdot A \cdot \vec{x} \leq 0$$

<u>Fact:</u>

Suppose A is symmetric and positive-definite, then A is non-singular.

<u>Fact:</u>

If A is symmetric and positive-definite then $\exists$ upper triangular matrix U s.t. $A = U^T \cdot U$.

6 Matrix Eigenvalue Problems

Standard eigenvalue problem:

$$A \cdot \vec{x} = \lambda \cdot \vec{x}$$

where:

$$
\begin{aligned}
\vec{x} &= n \times 1 \,\text{column vector} \longrightarrow \text{the eigenvector} \\
\lambda &= \text{scalar, the eigenvalue} \\
A &= n \times n \,\text{matrix}
\end{aligned}
$$

We have an equivalent formulation where:

$$
(A - \lambda \cdot I_n) \cdot \vec{x} = \vec{0}
$$

This is a homogenous system of linear equations.

Note: If we want a non-trivial solution to exist, then $\det(A) = 0$ and thus the system is homogenous.

Then: ** $|A - \lambda \cdot I_n| = 0$.

$$
\begin{vmatrix}
a_{11} - \lambda & a_{12} & ... & a_{1n} \\
a_{21} & a_{22} - \lambda & ... & a_{2n} \\
\vdots & \ddots & \ddots & \vdots \\
a_{1n} - \lambda & ... & ... & a_{nn} - \lambda
\end{vmatrix} = 0
$$

** is the characteristic polynomial of the standard equation eigen problem has degree n and its roots are the eigenvalues:

$$
\lambda_1, ..., \lambda_2
$$

We have then, for each eigenvalue λ_i, we can determine an eigenvector $\vec{x}_{(i)}$ such that $A \cdot \vec{x}_{(i)} = \lambda_i \cdot I_n$ and $\left(\lambda_i, \vec{x}_{(i)} \right)$ come in pairs. Thus, $\vec{x}_{(i)}$ is the eigenvector associated to the eigenvector associated to the eigenvalue λ_i.

Example 70. $A = \begin{pmatrix} 4 & 1 \\ 3 & 2 \end{pmatrix}$. Solve the standard eigen problem.

$$
\begin{aligned}
|A - \lambda \cdot I_2| &= 0 \\
\begin{pmatrix} 4 - \lambda & 1 \\ 3 & 2 - \lambda \end{pmatrix} &= 0 \\
\rightsquigarrow \lambda^2 - 6\lambda + 5 &= 0 \,(\text{char poly}) \\
\rightsquigarrow \lambda_1 = 1 \quad, \quad \lambda_2 &= 5
\end{aligned}
$$

Thus, we have two (eigenvalue, eigenvector) pairs.

$$
\begin{aligned}
A \cdot \vec{x}_{(1)} &= \lambda_1 \cdot \vec{x}_{(1)} \rightsquigarrow \vec{x}_{(1)} = \begin{pmatrix} -\frac{1}{3} \\ 1 \end{pmatrix} \\
A \cdot \vec{x}_{(2)} &= \lambda_2 \cdot \vec{x}_{(2)} \rightsquigarrow \vec{x}_{(2)} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}
\end{aligned}
$$

Thus:

$$
\begin{aligned}
\begin{pmatrix} -\frac{1}{3} \\ 1 \end{pmatrix} &= \begin{pmatrix} -\frac{1}{3} \\ 1 \end{pmatrix} \\
\begin{pmatrix} 1 \\ 1 \end{pmatrix} &= 5 \cdot \begin{pmatrix} 1 \\ 1 \end{pmatrix}
\end{aligned}
$$

6.1 Generalized Eigenvalue Problem

$$A \cdot \vec{x} = B \cdot \vec{x}$$

Where A, B are symmetric matrices, λ is the eigenvalue and $\vec{x}$.

1. B is diagonal, $B = C \cdot C$ with C diagonal, $c_{ii} = \sqrt{b_{ii}}$

$$C^{-1} \cdot A \cdot C^{-1} \cdot \vec{x} = \lambda \cdot \vec{x}$$

2. B is symmetric and positive-definite, $B = U^T \cdot U$

$$(U^T)^{-1} \cdot A \cdot U^{-1} \cdot \vec{x} = \lambda \cdot \vec{x}$$

Characteristics of Eigen Problems:

A	$\lambda_1, ..., \lambda_n$
singular	at least one $\lambda_i = 0$
non-singular	all $\lambda_i \neq 0$
symmetric	all λ_i are real
diagonal	$\lambda_i = a_{ii}$, $i = 1, ..., n$
A^{-1}	eigenvalues are $\frac{1}{\lambda_i}$
$P^T \cdot A \cdot P$ (orthogonal)	remain unchanged

6.2 Computational Methods

- Determinant method

- F-L method

- Power method

6.2.1 Determinant Method

$$
\begin{aligned}
A \cdot \vec{x} &= \lambda \cdot \vec{x} \rightsquigarrow \\
|A - \lambda \cdot n| &= 0 \rightsquigarrow \\
\text{characteristic poly.} &\rightarrow (-1)^n (\lambda^n - p_1 \cdot \lambda^{n-1} - ... - p_{n-1} \cdot \lambda - p_n) = 0 \\
p_1 &= a_{11} + a_{22} + ... + a_{nn} \\
&= \text{Trace}(A)
\end{aligned}
$$

Example 71. We have $A = \begin{pmatrix} 12 & 6 & -6 \\ 6 & 16 & 2 \\ -6 & 2 & 16 \end{pmatrix}$, with $n = 3$. A is symmetric, so the eigenvalues are real.

We need to determine p_1, p_2, p_3:

$$
|A - \lambda I_3| = 0 \qquad , \qquad \begin{pmatrix} 12 - \lambda & 6 & -6 \\ 6 & 16 - \lambda & 2 \\ -6 & 2 & 16 - \lambda \end{pmatrix} = 0
$$

$$\text{polynomial} \quad \rightsquigarrow \quad -\lambda^3 + 44\lambda^2 - 564\lambda + 1728 = 0$$

$$\lambda_1 = 18, \quad \lambda_2 = 13 + \sqrt{73}, \quad \lambda_3 = 13 - \sqrt{73}$$

Since all λ_i are positive, we conclude that A is positive-definite.

$$p_1 = \text{Trace}(A) = 12 + 16 + 16 = 44$$

The eigenvector associated to $\lambda_1 = 18$ comes after we solve: $A \cdot \vec{x} = 18 \cdot \vec{x} \rightsquigarrow \vec{x} = \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}$.

6.2.2 Faddeev-Leverrier Method

The idea behind this method is to generate the coefficients $p_1, ..., p_n$ of the characteristic polynomial by trace computations of the matrices $P_1, ..., P_n$.

$$\begin{aligned}
P_1 &= A &\rightsquigarrow\quad p_1 &= \text{Trace}(P_1) = \text{Trace}(A) \\
P_2 &= A\,(P_1 - p_1\,I_n) &\rightsquigarrow\quad p_2 &= \frac{1}{2}\,\text{Trace}(P_2) \\
&\quad\vdots\quad\vdots\quad\vdots \\
P_i &= A\,(P_{i-1} - p_{i-1}\,I_n) &\rightsquigarrow\quad p_i &= \frac{1}{i}\,\text{Trace}(P_i) \\
&\quad\vdots\quad\vdots\quad\vdots \\
P_n &= A\,(P_{n-1} - p_{n-1}\,I_n) &\rightsquigarrow\quad p_n &= \frac{1}{n}\,\text{Trace}(P_n)
\end{aligned}$$

Example 72. Use the power method to compute the dominant eigenvalue; $A = \begin{pmatrix} 12 & 6 & -6 \\ 6 & 16 & 2 \\ -6 & 2 & 16 \end{pmatrix}$. The initial trial vector, $\vec{X_1} = \begin{pmatrix} 1.0 \\ 0.5 \\ -0.5 \end{pmatrix}$.

We then have: $\vec{X_2} = A \cdot \vec{X_1} = \begin{pmatrix} 18.0 \\ 13.0 \\ -13.0 \end{pmatrix}$ with $c = 18.0 \rightsquigarrow \begin{pmatrix} 1 \\ 0.722 \\ -0.722 \end{pmatrix}$.

The next iteration will be: $\vec{X_3} = A \cdot \vec{X_2} = \begin{pmatrix} 20.66 \\ 16.11 \\ 16.11 \end{pmatrix}$ with $c = 20.66 \rightsquigarrow \begin{pmatrix} 1 \\ 0.779 \\ -0.779 \end{pmatrix}$.

This will go through 8 iterations to obtain $\lambda_1 = 21.5439$.

Example 73. Given $A = \begin{pmatrix} 12 & 6 & -6 \\ 6 & 16 & 2 \\ -6 & 2 & 16 \end{pmatrix}$.

$$P_1 = A \quad\rightsquigarrow\quad p_1 = \text{Trace}(A) = 44$$

$$P_2 = A \cdot (P_1 - p_1\,I_n) = \begin{pmatrix} -312 & -108 & 108 \\ -108 & -408 & -60 \\ 108 & -60 & -408 \end{pmatrix} \quad\rightsquigarrow\quad p_2 = \frac{1}{2} \cdot \text{Trace}(P_2) = 564$$

$$P_3 = A \cdot (P_2 - p_2\,I_n) = \begin{pmatrix} 1728 & 0 & 0 \\ 0 & 1728 & 0 \\ 0 & 0 & 1728 \end{pmatrix} \quad\rightsquigarrow\quad p_3 = \frac{1}{3} \cdot \text{Trace}(P_3) = 1728$$

The characteristic polynomial is $(-1)^3\,(\lambda^3 - p_1\,\lambda^2 - p_2\,\lambda - p_3) = 0$.

6.3 The Power Method (in Google's PageRank)

Given:

$$A^{(n \times n)} \rightsquigarrow |\lambda_1| \geq |\lambda_2| \geq ... \geq |\lambda_n|$$

Note: If $\lambda_i \in \mathbb{C}$, then $|\lambda_i| = \sqrt{\text{Re}(\lambda_i)^2 + \text{Im}(\lambda_i)^2}$. Where λ_1 is the *dominant* eigenvalue.

This is an iterative method to compute λ_1 and it's corresponding vector.

The idea is to choose an aribitrary trial vector, x_1, and refine it by premultiplication by A and generate a new trial vector.

Notation 74. $\vec{X}^{(1)}, ..., \vec{X}^{(2)}$: the eigenvectors of A

$$
\begin{aligned}
\vec{X}_1 &= & c_1 \cdot \vec{X}^{(1)} + ... + c_n \cdot \vec{X}^{(n)} \\
\vec{X}_2 = A \cdot \vec{X}^{(1)} &= & A\left(\sum_{i=1}^{n} c_i \vec{X}^{(i)}\right) = \sum_{i=1}^{n} c_i A \cdot \vec{X}^{(i)} = \sum_{i=1}^{n} c_i \lambda_i \cdot \vec{X}^{(i)} \\
\vec{X}_3 &= & A \cdot \vec{X}^{(2)} \longrightarrow \sum_{i=1}^{n} c_i \lambda_i \cdot \vec{X}^{(i)} \\
\vdots \quad \vdots \quad &\vdots& \\
\vec{X}_{r+1} &= & A \cdot \vec{X}_r = \sum_{i=1}^{n} c_i x_i^r \cdot \vec{X}^{(i)} \\
&= & \lambda_1^r \cdot \left(c_1 \vec{X}^{(1)} + \left(\frac{\lambda_2}{\lambda_1}\right)^r c_2 \cdot \vec{X}^{(2)} + ... \right)
\end{aligned}
$$

So, it works out such that: $\frac{\lambda_2}{\lambda_1}, ..., \frac{\lambda_n}{\lambda_1}$ *are* <1.

Letting $r \to \infty$, *we get* $\rightsquigarrow \vec{X}_{r+1} = \lambda_1^r \cdot c_1 \cdot \vec{X}^{(1)}$

Algorithm 6

- Input: $n \times n$ matrix, A
- Output: dominant eigenvalue λ_1

1. $\vec{X}_1$: Trial vector, with all items ≤ 1 in abs. value
2. $k = 1$
3. $\vec{X}_{k+1} = A \cdot \vec{X}_k$
4.
   ```
   if |(X_{k+1} - X_k^i)/X_k^i| < ε which converges, λ_1 = X_{k+1}^i / X_k^i
   else c_{k+1} = max_{i=1,...,n} |X_{k+1}^i|
   ```
   Normalize $\vec{X}_{k+1}$ by dividing c_{k+1} and $k = k + 1$.

6.4 Symmetric Tridiagonal Matrices

$A = \begin{pmatrix} a_1 & b_2 & 0 & 0 \\ b_2 & a_2 & \ddots & 0 \\ 0 & \ddots & \ddots & b_n \\ 0 & 0 & b_n & a_n \end{pmatrix}$, with $2n - 1$ elements and $O(n)$.

We will compute the characteristic polynomial of A by a recursive construction.

Note: The char. polynomial of $A = |A - \lambda \cdot I_n|$.

$$
\begin{aligned}
f_0(\lambda) &= & 1 \\
f_1(\lambda) &= & a_1 - \lambda \\
f_2(\lambda) &= & f_1(\lambda) \cdot (a_2 - \lambda) - b_2^2 \cdot f_0(\lambda) \\
\vdots \quad \vdots \quad &\vdots& \\
f_n(\lambda) &= & f_{n-1}(\lambda) \cdot (a_n - \lambda) - b_n^2 \cdot f_{n-2}(\lambda)
\end{aligned}
$$

We than have that $f_n(\lambda)$ is the characteristic polynomial of A.

Example 75. Given $A = \begin{pmatrix} 3 & -2 & 0 & 0 \\ -2 & 5 & -3 & 0 \\ 0 & -3 & 7 & -4 \\ 0 & 0 & -4 & 9 \end{pmatrix}$.

$$
\begin{aligned}
f_0(\lambda) &= 1 \\
f_1(\lambda) &= 3 - \lambda \\
f_2(\lambda) &= \lambda^2 - 8\lambda + 11 \\
&\vdots \quad \vdots \quad \vdots \\
f_4(\lambda) &= \lambda^4 - 24\lambda^3 - 177\lambda^2 - 444\lambda + 274
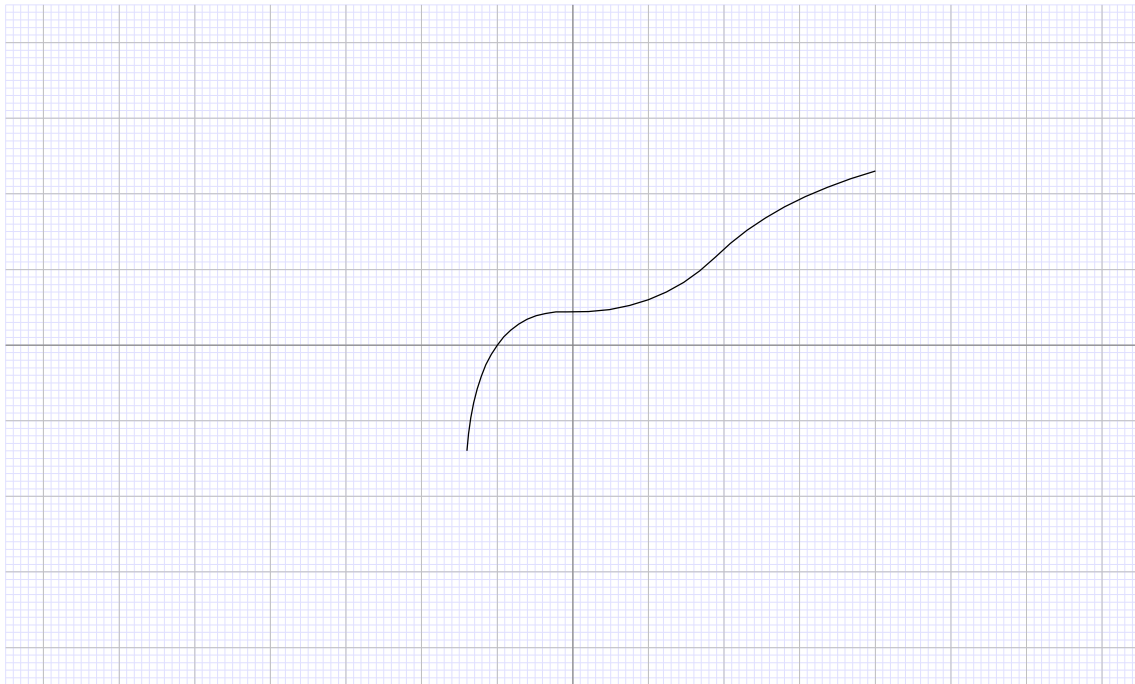\end{aligned}
$$

We know that it has 4 positive roots in $[0, 13]$. Thus, we know it is positive definite.

7 Interpolation (AKA Curve Fitting)

The **main idea** behind interpolation is that we have data available as discrete points, and we want to apply a smooth/continuous curve to this data.
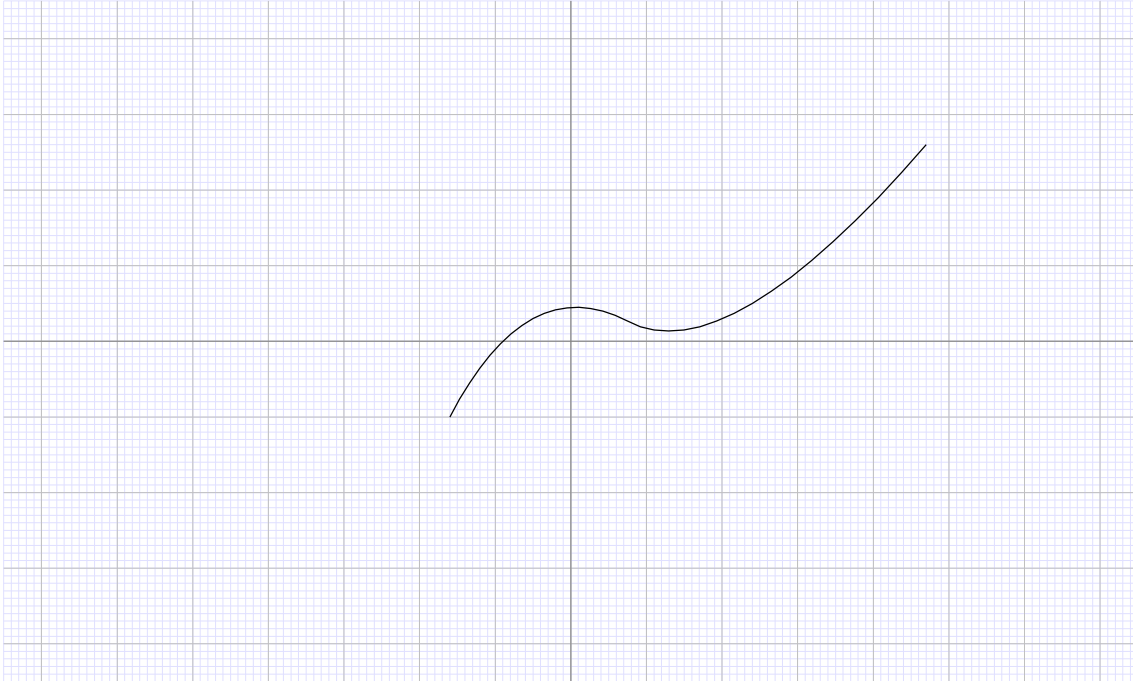
7.0.1 1$^{\text{st}}$ Approach: Collocation

The curve passes *exactly* through all the data points.

$$f(x) = a_n \cdot x^n + \ldots + a_x \cdot x + a_0$$

7.0.2 2$^{\text{nd}}$ Approach: Least Squares

The curve indicates a general <u>trend</u> of the data.

<u>Interpolation:</u> Find $f(x) = y$.

<u>Extrapolation:</u> Predict/deduce data values (y-values) outside of the given range. **Ex.** What is $(0, ??)$, or $(11, ??)$.

Method 1.

Example 76. Collocation, polynomial fit.

We have $n+1$ data points: $(x_0, y_0), ..., (x_n, y_n)$.

$$y = f(x) = a_n \cdot x^n + ... + a_1 \cdot x + a_0$$

With:

$$f(x_0) = y_0, ..., f(x_n) = y_n$$

Above, is a set of $n+1$ linear equations in $a_0, ...a_n$.

We will aim to get the form of $B \cdot \vec{a} = \vec{y}$, where $\vec{a} = \begin{pmatrix} a_0 \\ \vdots \\ a_n \end{pmatrix}$ and $\vec{y} = \begin{pmatrix} y_0 \\ \vdots \\ y_n \end{pmatrix}$. We can understand that B is a Vandermonde matrix.

$$B = \begin{pmatrix} 1 & x_0 & x_0^2 & ... & x_0^n \\ 1 & x_1 & x_1^2 & ... & x_1^n \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & x_n^2 & ... & x_n^n \end{pmatrix}$$

And thus:

$$|\det(B)| = \prod_{\substack{i > j \\ i = 0, ..., n \\ j = 0, ..., n}} (x_i - x_j)$$

Note: There is a **unique** polynomial of degree n, that passes through $n+1$ data points.

7.1 Lagrange Interpolation

The **idea** is to avoid solving a linear system by using a *semi-factored* form of the interpolation polynomial.

Example 77. Fit a quadratic through 3 $(=2+1)$ data points:

$$f(x) = a_0 + a_1 \cdot x + a_2 \cdot x^2$$

With

$$y = f(x) = a_0(x - x_1)(x - x_0) + a_1(x - x_0)(x - x_2) + a_2(x - x_0)(x - x_1)$$

And the three data points are:

$$(x_0, y_0)$$
$$(x_1, y_1)$$
$$(x_2, y_2)$$

We have

$$f(x_0) = y_0 \quad , \quad a_0(x_0 - x_1)(x_0 - x_2) = y_0 \rightsquigarrow a_0 = \frac{y_0}{(x_0 - x_1)(x_0 - x_2)}$$
$$f(x_1) = y_1 \quad , \quad a_1(x_1 - x_0)(x_1 - x_2) = y_1 \rightsquigarrow a_1 = \frac{y_1}{(x_1 - x_0)(x_1 - x_2)}$$
$$f(x_2) = y_2 \quad , \quad \ldots = y2 \rightsquigarrow a_2 = \frac{y_2}{(x_2 - x_0)(x_2 - x_1)}$$

Example 78. We have :

$$\begin{aligned}(x_0, y_0) &= (0, 0)\\(x_1, y_1) &= (1, 1)\\(x_2, y_2) &= (2, 3)\end{aligned}$$

We have $n + 1 = 3 \rightsquigarrow n = 2$. Further, writing this in the Lagrange form:

$$y = f(x) = \sum_{i=0}^{2} a_i \cdot \left(\prod_{\substack{j=0 \\ j \neq i}}^{2} (x - x_j) \right)$$

We then have:

$$\begin{aligned}a_0 &= \frac{y_0}{(x_0 - x_1)(x_0 - x_2)} &= \frac{0}{\ldots} = 0\\a_1 &= \frac{y_1}{(x_1 - x_0)(x_1 - x_2)} &= \frac{1}{(1 - 0)(1 - 2)} = -1\\a_2 &= \frac{y_2}{(x_2 - x_0)(x_2 - x_1)} &= \frac{3}{(2 - 0)(2 - 1)} = \frac{3}{2}\end{aligned}$$

Thus, we have the Lagrange interpolation polynomial is

$$\begin{aligned}y = f(x) &= -1(x - 0)(x - 2) + \frac{3}{2}(x - 0)(x - 1)\\&= \frac{x(x + 1)}{2}\end{aligned}$$

Using the Vandermonde method, we have $B \cdot \vec{a} = \vec{y}$ with

$$\begin{pmatrix} 1 & 0 & 0 \\ 1 & 1 & 1 \\ 1 & 2 & 4 \end{pmatrix} \cdot \begin{pmatrix} a_0 \\ a_1 \\ a_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 3 \end{pmatrix}$$

We need to solve this.

7.1.1 Lagrange Interpolation for $n+1$ Data Points (with a polynomial of degree n)

$$y = f(x) = \sum_{i=0}^{n} y_i \cdot \left(\prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{(x - x_j)}{(x_i - x_j)} \right)$$