Numerical Analysis ?

← subject of writing numerical approx to problems
Idea: Numerics is the heart of studying something which is closing to/close but not the same as the desired quantity

- Algorithms
- Analysis
- Implementation

(approximation)

Idea: get as close as possible to the original problem, construct a good approx

And we want to make sure this approx works within certain errors

(errors)

(python)

We can only approximate Def well posed problems . i.e.

1) there exist a unique solution
2) it depends continuously on the data

Idea behind numerics and numerical approx is that we simplify in a controlled manner

This means that we make the following replacements

infinite	finite
differential	algebraic
non-linear	linear problems

Difficult → "easy"

Example:

Given a function "f", a point x_0, compute "$f'(x_0)$" (derivative of f in x_0)

$f \in C^1[a,b]$ continuous in $[a,b]$ and first derivative continuous in $[a,b]$ $x_0 \in (a,b)$

Is it well posed? yes, because exist a UNIQUE derivative of f at x_0
If f is not derivable ⇒ problem is not well posed ⇒ WE MUST CHECK DOMAIN!

→ use finite difference

$$f'(x_0) \approx \frac{f(x_0+h) - f(x_0)}{h}$$

with small h ⇕ (s.t. $x_0+h \in (a,b)$)

(!! I'm not assuming to know anything about f except the evaluation of its body)

anything you choose here will have an effect of what you can do and what you can't

Error: Typical ways to estimate errors is → Taylor expansion around x_0:

$$f(x_0+h) = f(x_0) + h f'(x_0) + \frac{h^2}{2} f''(x_0) + \dots$$

When you compute powers of 2 (2**i , i ...),
The accuracy of computer is perfect up to
$\sim 10^{-4}$, and in reality is still perfect unto
$15^{14} \cdot 10^{-15}$

In theory, as $h \to 0$, the finite approx should get close to the exact result (exact derivative)

In practice much else happens

$$f(x_0+h) \approx \sum_{i=0}^{n} \frac{f^{(i)}(x_0)\, h^i}{i!}$$

For $n \to \infty$, $\approx \to =$ provided that function is analytical, so that I can do it for n functions at each step

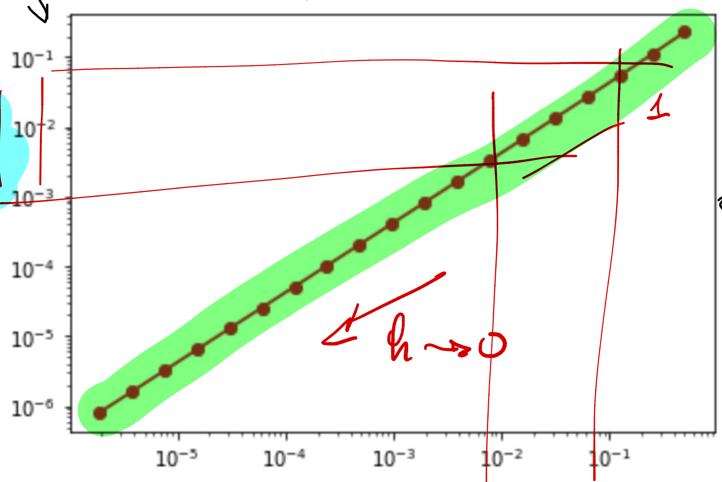
$$FD := \frac{f(x_0+h) - f(x_0)}{h} \approx f'(x_0) + \frac{1}{2} f''(x_0)\, h + O(h^2)$$

exact derivative + something small that when $h \to 0$ means that it's way smaller compared to h

The error is computable as

Error: $|FD(f) - f'| \approx \frac{f''(x_0)\, h}{2} + O(h^2)$

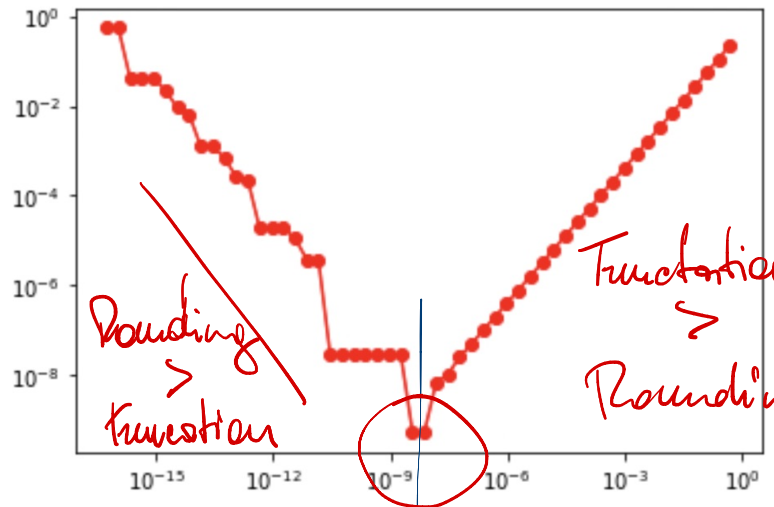
for h down to 2^{-20} ($\sim 10^{-6}$)



linearity in h (slope is = 1)

interesting things happens when h keeps getting smaller, but the algorithm above doesn't tell us that: it tells us that the error, being $\sim h$, will go to zero in a linear fashion as h goes down

h goes at lower values (10^{-15})



$\sqrt{\varepsilon}$ ~ optimal h

ε: precision of machine (Rounding precision)

$\sim 10^{-15}$

10^{-8}

Types of error are

- Data error → always present (Data) — If you have error in measurements of data, i.e. the x_0 above, and the function
- Computational Error (Algorithm) — depends on used algorithms — (gathering of the following)
  - Truncation error (Algorithm error in Exact Arithmetics) — not the one of PCs — ← error you make on the algorithm level by assuming that happens by putting exact at in the act
  - Rounding Error (Finite Arithmetic) — the one of PC — Due to ≠ arithmetics of computers and numbers we deal with every day

diff between what you expect from algorithm by putting in exact, and what you get when using your algorithm (the approximation)

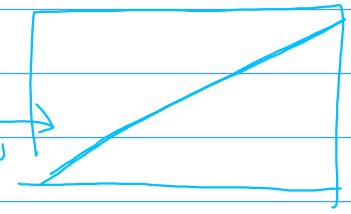
It doesn't take account of the fact that machines operate in a different arithmetics

arithmetics in pc is of power of 2

FINITE DIFF:

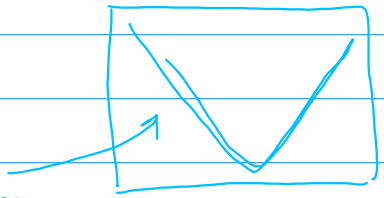
Infinite series - Truncated series

linear the graph above is TRUNCATION ERROR ONLY



because trunc. error dominates over rounding error

but, as h drops, rounding error starts becoming more relevant



here it dominates over the trunc error

The problem to solve is

Pb: Compute value of a function "F"

$$F : \mathbb{R} \longrightarrow \mathbb{R}$$

at a argument x

So we have

- x : true value of input
- $F(x)$: desired value of output ← what to compute
- $\hat{x}$: approximate input (may be "off" for rounding) — affected by rounding, data error, … — Error on input data
- $\hat{F}(\hat{x})$: computed output (may be "off" for both rounding and truncation) — Error on outcome due to algorithm; due to approximation

$$\hat{F}(\hat{x}) - F(x) =$$

effect of rounding in input data on the algorithm → ROUNDING ERROR or COMPUTATIONAL OUTPUT DUE TO ROUNDING ERROR IN INPUT (ROUNDING ERROR IN APPROXIMATED PROBLEM)

Truncation error in exact arithmetic

$$= \underbrace{\hat{F}(\hat{x}) - \hat{F}(x)}_{1} + \underbrace{\hat{F}(x) - F(x)}_{2}$$

or

(consistency evaluated at ≠ points)

sensitivity of algorithm with respect to the original problem; sensitivity of original problem with respect to perturbation in the data → ROUNDING ERROR IN EXACT PROBLEM

$$= \underbrace{\hat{F}(\hat{x}) - F(\hat{x})}_{3} + \underbrace{F(\hat{x}) - F(x)}_{4}$$

/!\ You only control the algorithm, and only know that rounding is there, but you can't remove it → (don't choose $h < 10^{-8}$!)

COMPUTATIONAL ERROR (diff between algorithm and expected output)

② in exact arithmetic
③ in rounding arithmetics

Rounding Precision (machine precision) : ε the largest number s.t.

$$fl(1+\varepsilon) = fl(1)$$

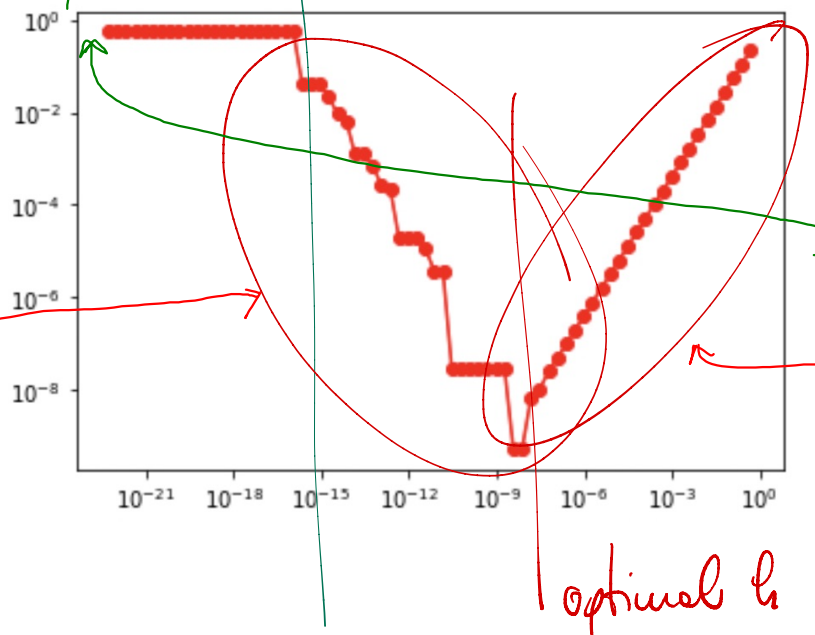
fl = floating point representation of a number

gives optimal $h \sim \sqrt{\varepsilon}$

$h < \sqrt{\varepsilon}$ rounding err dominates

$fl(f(x+h)) = fl(f(x))$ in a computer $\rightarrow$ $f(x+h) - f(x) = 0$

false in exact arithmetic



in the example, the error here is exactly the value of the function at the point!

error here is order of 1!

Rounding error dominates

Truncation error dominates

optimal $h \simeq \sqrt{\varepsilon}$

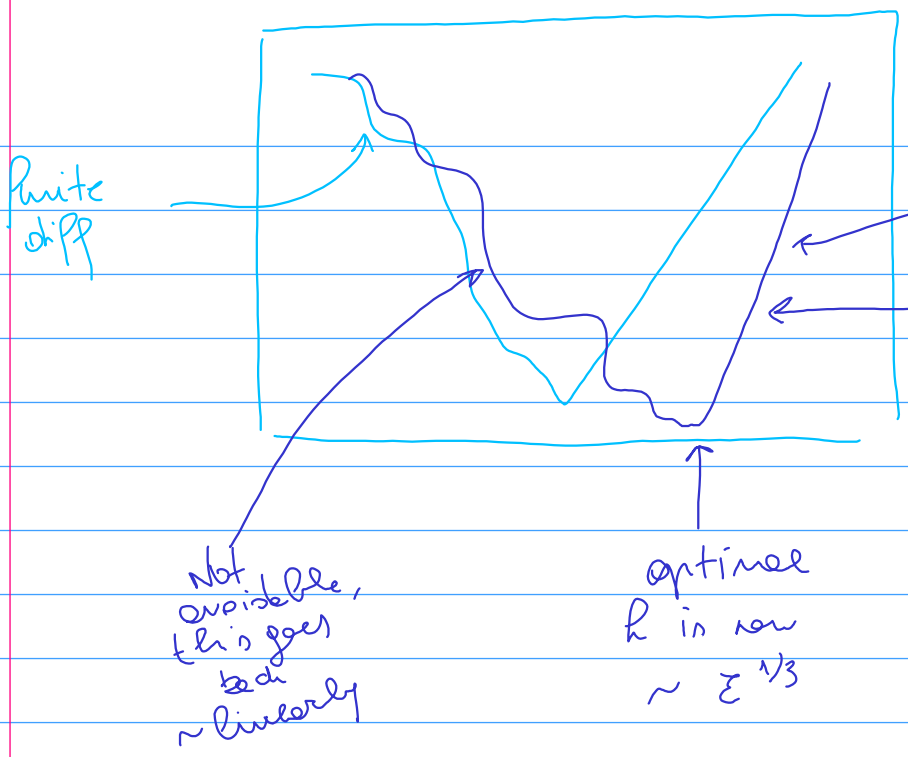
for 64 bits doubles (python) $\varepsilon \sim 10^{-15}$

$\sin(1) = 0.8414709848078965$

$$\frac{f(x+h) - f(x)}{h}$$ ← this h must be chosen according to property on f' and $\sqrt{\varepsilon}$, otherwise you'll get good results for some f' and bad for others.

All of this also depends on where we evaluate $f'(x_0)$ and truncation error at the same time

⚠ Don't use abs error as a measure of error, but use the RELATIVE ERROR


finite diff
central finite difference. BETTER, because here we have another power of h, which is power of 2 (slope two in 2!)
Not available, this goes to 0 linearly
optimal h is now ~ ε^{1/3}

Numerical Analysis - lec. 2

8.10.2020

problems can be written in a functional approach

$y = F(x)$ where $F: \mathcal{X} \longrightarrow \mathcal{Y}$

data $\rightarrow x \longrightarrow y = F(x)$ ← output/result

Functional Evaluation → F is a given function

EXAMPLES

1) $\mathcal{X}: \mathbb{R}$, $\mathcal{Y}: \mathbb{R}$ F: continuous func.

$$y = F(x)$$

2) **Sum of two numbers:**

$\mathcal{X}: \mathbb{R}^2$ ← pair of numbers, $\mathcal{Y}: \mathbb{R}$: F: sum of numbers.

$x = (a, b)$ $\quad F(x) = F((a,b)) = a+b$

3) **Computation of derivative**

$\mathcal{X}: C^1([a,b])$ $\quad \mathcal{Y}: \mathbb{R}$

F: evaluation of first derivative in $x_0 \in [a,b]$

$$y = F(x) := x'(x_0)$$

← function

Only well posed problems are characterized by 2 properties

1) $\forall x \in \mathcal{X}$, $\exists!\ y \in \mathcal{Y}$ s.t. $F(x) = y$

2) $\exists\ k$ (condition number) s.t. $\forall x, \hat{x} \in \mathcal{X}$

$$\| F(x) - F(\hat{x}) \|_{\mathcal{Y}} \leq k \| x - \hat{x} \|_{\mathcal{X}}$$

← basically F is continuous (bounded for every pair)

each of these are norms

We assume that $\mathbb{K}$, $\mathbb{V}$

Real Vector Spaces (Normed)

Def (Real vector spaces)

RVS: collection of objects for which it makes sense "V" to "sum" and "scale"

$$+ : V \times V \longrightarrow V$$

$$(u, v) \longrightarrow w = u + v$$

$$\cdot : V \times \mathbb{R} \longrightarrow V$$

such that

$$\forall\, u, v \in V, \quad \forall\, \alpha, \beta \in \mathbb{R}$$

$$\alpha u + \beta v = w \in V$$

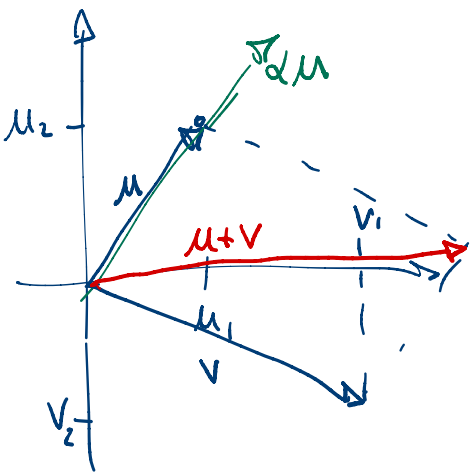
$\mathbb{R}^2$

$u = (u_1, u_2)$

$v = (v_1, v_2)$

$u + v = (u_1 + v_1, u_2 + v_2)$

$\alpha u = (\alpha u_1, \alpha u_2)$



$C^0([a,b])$

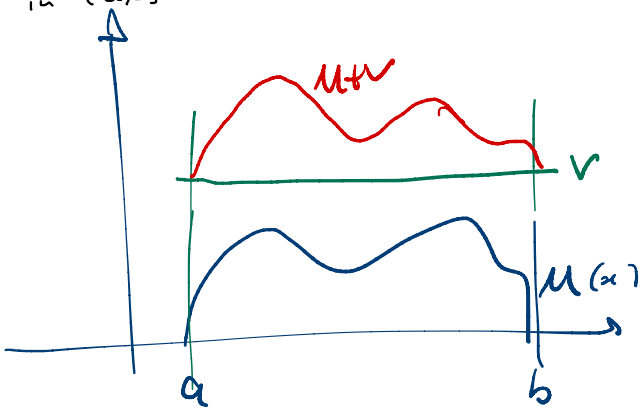
$u : [a,b] \longrightarrow \mathbb{R}$

$v : [a,b] \longrightarrow \mathbb{R}$

$w = u + v : [a,b] \longrightarrow \mathbb{R}$

because u, v are domained in $[a,b]$

$x \longrightarrow u(x) + v(x)$



Way to measure things

↓

introduce NORMS

Norms on Real Vector Spaces

a function $\|\cdot\| : V \longrightarrow \mathbb{R}_0^+$ ← positive or zero

1) $\|u\| \geq 0 \quad \forall u \in V$

2) $\|u+v\| \leq \|u\| + \|v\|$ Triangle inequality

3) $\|\alpha u\| = |\alpha| \|u\|$

optional 4) $\|u\| = 0 \Rightarrow u = 0$

without ④ it is a semi-norm

We will use

ℓ_p norms on $\mathbb{R}^n$

L_p norms on $\Omega \subset \mathbb{R}^d$

$\|\cdot\|_*$ operatorial norms induced by $\|\cdot\|_V$

Def:

$\mathbb{R}^n$: ℓ_p norm $\|u\|_p := \left(\sum_{i=1}^n |u_i|^p \right)^{\frac{1}{p}}$ ↘ $p \to \infty$

$\|u\|_\infty := \max_i |u_i|$ ℓ_∞ norm

↓ generalization to continuous domains

$\Omega \in \mathbb{R}^d$ L_p norms $\|u\|_p := \left(\int_\Omega |u|^p \right)^{\frac{1}{p}}$ ↘ $p \to \infty$

↙ L_∞ norm

$\|u\|_\infty := (\text{ess}) \sup_{x \in \Omega} |u(x)|$

$\|\cdot\|_*$ induced by vector space norm $\|\cdot\|_V$ on V and $\|\cdot\|_W$ on W

$A : V \longrightarrow W$ $\|A\|_* := \sup_{0 \neq x \in V} \frac{\|A(x)\|_W}{\|x\|_V}$

↑ used to measure how functionals / functions work / or what is their measure in a space

You def the norms of domain and codomain of A, and then you can def the operator norm

L_p norm of Matrices in $\mathbb{R}^{n\times m}$

(which is an obj of this kind)

$$A : \mathbb{R}^m \longrightarrow \mathbb{R}^n$$

$$A^{n\times m} \cdot x \qquad x \in \mathbb{R}^m$$

$$A \cdot x = y \in \mathbb{R}^n$$

$\|A\|_p$: L_p norm of the matrix → functional norm because I measure the norm of a function

$$\|A\|_p := \sup_{0 \neq x \in \mathbb{R}^n} \frac{\|Ax\|_p}{\|x\|_p} = \|A\|_*$$

$*$ operator id norm because A is a linear operator

induced by $\|\cdot\|_p$ on $\mathbb{R}^n$

$$A \in \mathbb{R}^{n\times m} \qquad A(x) = y \qquad \sum_{j=1}^{m} A_{ij} x_j = y_i$$

$$A \in \mathcal{L}(\mathbb{R}^m, \mathbb{R}^n)$$

$\|\cdot\|_*$ norm on $\mathcal{L}(\mathbb{R}^m, \mathbb{R}^n) \equiv \mathbb{R}^{n\times m}$

Why we need them? Every quantity related to a well posed problem can be put in a way between two spaces and their norms.

well posed problems

1) $\forall x \in \underline{\underline{X}}$, $\exists!\ y \in \underline{\underline{Y}}$ s.t. $F(x) = y$

$\underline{\underline{X}}$: Normed Vector Space; $\underline{\underline{Y}}$: Normed Vector Space

2) $\exists\ K$ (condition number) s.t. $\forall x, \hat{x} \in \underline{\underline{X}}$

$$\|F(x) - F(\hat{x})\|_{\underline{\underline{Y}}} \leq (K_{Abs}) \|x - \hat{x}\|_{\underline{\underline{X}}}$$

← Here we use norms

3) Relative cond. number (only if $x \neq 0$ and $F(x) \neq 0$!)

K_{rel} s.t. $\forall x, \hat{x}$

↑ INDEPENDENT ON x

$$\frac{\|F(x)-F(\hat{x})\|_{\mathcal{Y}}}{\|F(x)\|_{\mathcal{Y}}} \leq \boxed{K_{rel}} \frac{\|x-\hat{x}\|_{\mathcal{X}}}{\|x\|_{\mathcal{X}}}$$

No denominator

Prop

A problem is well posed if $K_{rel/abs}$ is "small" ⟷ Relation must be CONTROLLABLE

↳ with respect to what? → relative: depends on problem handled

Example: sum of two numbers: (ℓ_1 norm)

$\mathcal{X}: \mathbb{R}^2 \qquad \mathcal{Y}: \mathbb{R}$

$x \in \mathbb{R}^2 \to \|x\|_1 := |x_1| + |x_2| \qquad \|y\|_1 = |y|$

We have that

$$\frac{\|F(x)-F(\hat{x})\|_1}{\|F(x)\|_1} = \frac{|x_1-\hat{x}_1+x_2-\hat{x}_2|}{|x_1+x_2|} \leftarrow \|\cdot\|_{\mathcal{Y}=\mathbb{R}}$$

$$\frac{\|x-\hat{x}\|_1}{\|x\|_1} = \frac{|x_1-\hat{x}_1|+|x_2-\hat{x}_2|}{|x_1|+|x_2|}$$

$\Delta y, \quad \Delta x \qquad \Delta x = x-\hat{x} \qquad \Delta y = F(x)-F(\hat{x})$

Now Find K_{abs}: $\exists K_{abs} \mid \forall x_1, x_2, \quad |\Delta y| \leq K \|\Delta x\|$?

$$|\Delta y| \leq K\|\Delta x\| \leq K\left(|\Delta x_1|+|\Delta x_2|\right)$$

Assume that $\Delta x \neq 0$

$$\frac{|\Delta y|}{|\Delta x|} \leq K$$

$$\frac{|\Delta x_1 + \Delta x_2|}{|\Delta x_1| + |\Delta x_2|} \leq \frac{|\Delta x_1| + |\Delta x_2|}{|\Delta x_1| + |\Delta x_2|} \leq 1$$

From pts of absolute K: this is perfect: you perturb data, and the perturbation of the result reduces proportionally the ptb of the inputs ($K_{abs} = 1$)

$K_{abs} = 1$ but ~~$\exists K < 1$ s.t.~~ Indeed:

$$\frac{|\Delta y|}{|\Delta x|} \cdot \frac{|x|}{|y|} \leq \frac{|x|}{|y|} \leq K_{rel}$$

$K_{abs} \leq 1$

because

$$\frac{|x|}{|y|} = \frac{|x_1| + |x_2|}{|x_1 + x_2|}$$

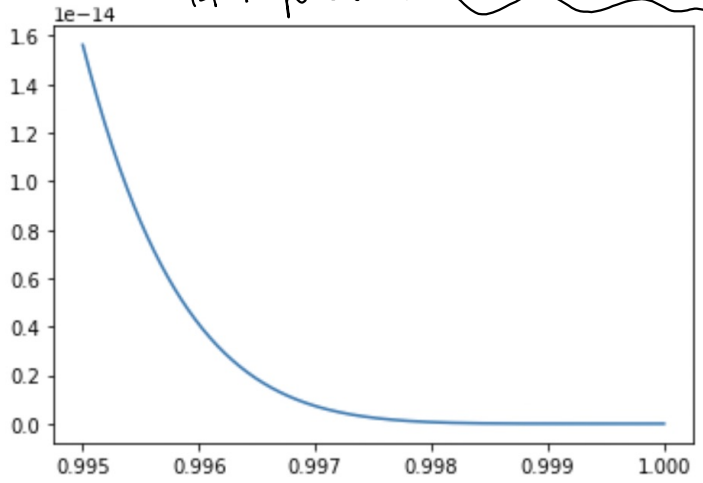
we cannot control this number!

can be as large as we want

=> If you try to sum 2 numbers with closing values and opposite signs, you're dealing with an ill posed problem, but the sum of 2 numbers is not ill posed by 6

Example: $(1-x)$ in $[1-\epsilon, 1]$ ϵ is small

If I plot




```
x = linspace(.995, 1,1029)
```

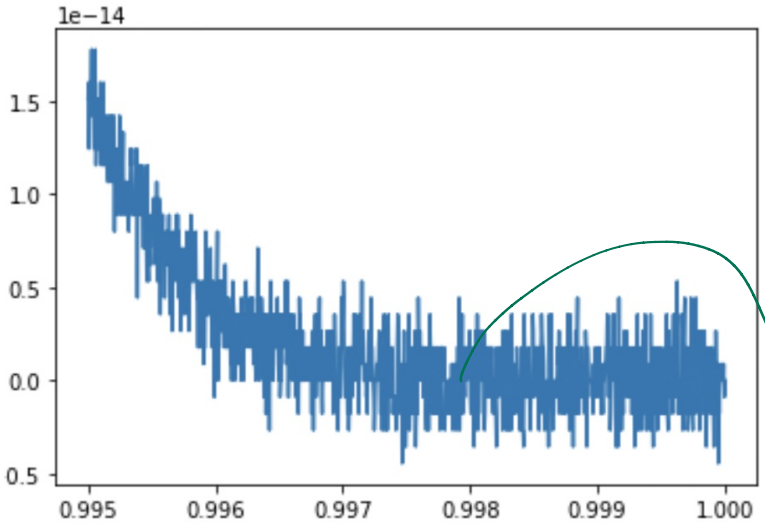
```
y = (x-1)**6
```

but if I expand the power I get a bad result

```
y = x**6 - 6*x**5 + 15*x**4 - 20*x**3 + 15*x**2 - 6*x + 1
```

↖ due to addition of very close numbers (in value) but with ≠ signs → we really that this is an ill posed problem

$x - \hat{x}$ = floating point errors (rounding errors)



Δy

Consider:

If $x_1 = -(x_2 + \varepsilon)$ with ε "small"

So what we obtain from procedure above

$$\frac{|x|}{|y|} = \frac{|x_2+\varepsilon| + |x_2|}{|-x_2 - \varepsilon + x_2|} \leq \frac{2|x_2|+|\varepsilon|}{|\varepsilon|}$$

($|x| \leq |x_2+\varepsilon| + |x_2|$; $x_1 = -x_2 - \varepsilon$)

if x_2 not close to zero then

$$\frac{|x|}{|y|} \leq \frac{2|x_2|}{|\varepsilon|} + 1$$

↖ if $|\varepsilon|$ is too small we get a problem

So, relating this to the true quantity

$$\frac{|\Delta y|}{|y|} \cdot \frac{|x|}{|\Delta x|} \leq K_{rel} \Rightarrow$$

which makes $K_{rel} = \infty$ to agree with its def (it has to be greater for every chosen ε)

$$\frac{|\Delta y|}{|\Delta x|} \frac{|x|}{|y|} \leq K_{rel}$$

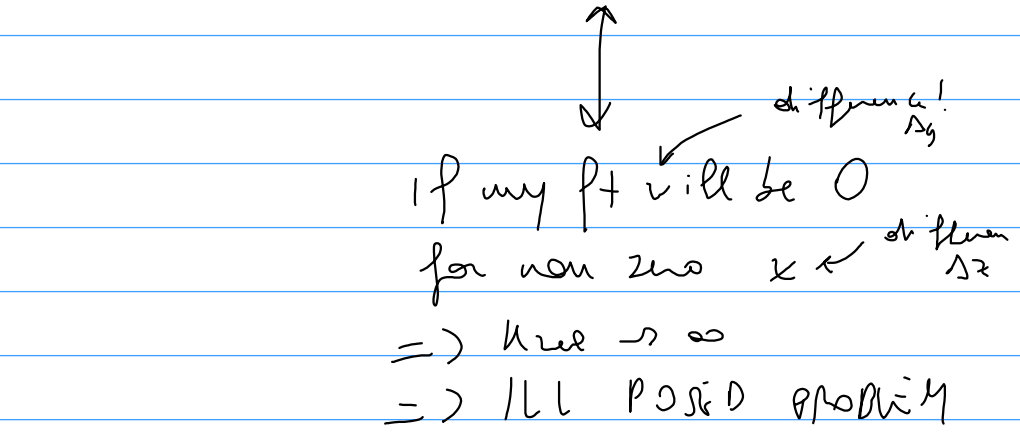
↖ in this case, it may also depend on x

Sum of 2 number is not a "RELATIVELY" well posed problem ($\leftrightarrow$ in relative terms $\leftrightarrow$ k rel)

But it is an "ABSOLUTELY" well posed problem

relative change in results caused by relative change in input, what you get is NOT controllable

THIS DEPENDS ON THE EVALUATION POINT



! Rounding errors are MAGNIFIED by big cancellation numbers

Numerical Analysis — Lec. 3 — LH — 13.10.2020

1) ∃! solution
2) pb. is stable ⟺ well posed ⟺ finite cond. Num.

X, Y Normed Vector spaces

$F: X \longrightarrow Y$ ← ∃! solution ⇒ F is an INVERTIBLE FUNCTION

We had

1) $K_{abs} \in \mathbb{R}^+ \cup \{+\infty\}$ ← positive and possibly infinite

s.t. $x, \hat{x} \in X$ LIPSCHITZ PROPERTY, $\|F(x) - F(\hat{x})\|_Y \leq K_{abs} \|x - \hat{x}\|_X$

used whenever is required to study stability of a problem and implies that there is a continuous dependency on data (how much you perturb the input ⟺ when you perturb the input data)

which is ⟺ to $K_{abs} \geq \dfrac{\|F(x) - F(\hat{x})\|_Y}{\|x - \hat{x}\|_X}$

You choose the smallest number greater than that fraction ⇒ $K_{abs} = \sup_{x, \hat{x} \in X,\ x - \hat{x} \neq 0} \dfrac{\|F(x) - F(\hat{x})\|_Y}{\|x - \hat{x}\|_X}$

If $K_{abs} \neq \infty$ ⇒ problem is stable (well conditioned)

1) $K_{rel} \in \mathbb{R}^+ \cup \{+\infty\}$

s.t. $x, \hat{x} \in X$

$$\frac{\|F(x) - F(\hat{x})\|_Y}{\|F(x)\|_Y} \leq K_{rel} \frac{\|x - \hat{x}\|_X}{\|x\|_X}$$

denominators make the relativity

Similarly as before, the smallest number greater than is

$$K_{rel} = \sup_{x, \hat{x} \in X,\ x - \hat{x} \neq 0,\ F(x) \neq 0} \frac{\|F(x) - F(\hat{x})\|_Y}{\|x - \hat{x}\|_X} \frac{\|x\|_X}{\|F(x)\|_Y}$$

I split the sup because I have INEQUALITIES and then I can bound the OVERALL definition and put K_{rel} equal to this

$= K_{abs} \sup_{x, \hat{x} \in X,\ x - \hat{x} \neq 0,\ F(x) = 0} \dfrac{\|F^{-1}(F(x)) - F^{-1}(F(\hat{x}))\|_X}{\|F(x)\|_Y}$ (remember F is invertible)

$= K_{abs} \|F^{-1}\|_*$

If F is not linear ⇒ K_{abs} is basically the Lipschitz constant of F^{-1}

use def of operatorial norm applied to F^{-1}: cond to be sure that F is invertible

$\delta x = x - \hat{x}$, $\delta y = y - \hat{y}$ (⟺ F is affine)

if operator is linear

Example: $Ax = y$ ($\Leftrightarrow y = F(x)$) $\quad y = F(x)$

Absolute stability: $A\hat{x} = \hat{y}$ ($\Leftrightarrow \hat{y} = F(\hat{x})$) → $A\,\delta x = \delta y$

$$\|Ax - A\hat{x}\| = \|A(x - \hat{x})\| = \|\delta y\|$$

I can collect the A thanks to the linearity of the problem

Expl. it property of operatorial norm of a matrix (follows from its definition)

$$\|\delta y\| \leq \|A\|_* \|\delta x\|$$

and we get Kabs

Finding Krel gives (by applying the def of Krel above)

$$\frac{\|\delta y\|}{\|y\|} \leq \|A\|_* \|A^{-1}\|_* \frac{\|\delta x\|}{\|x\|}$$

Condition number of A (this is a def: CONDITION NUMBER OF A MATRIX IS $\|matrix\| \|matrix^{-1}\|$)

it will depend on the norm you use

Prop

A problem is (Absolutely) Relatively well posed if

(Kabs) Krel is $< +\infty$.

What is an approximation?

Sequence of problems F_n $(n \in \mathbb{N})$ applied to a sequence of "approximated data" x_n (implied approximated sequence of domains $\mathbb{X}_n$)

s.t.

$$\lim_{n\to\infty} |F_n(x_n) - F(x)| = 0$$

← CONVERGENCE OF THE PROBLEM: this is really what we want to check

Note 1: "$\mathbb{X}_n \to \mathbb{X}$"

simple case: $\mathbb{X}_n \subset \mathbb{X}$

consistency ↦ Approximated problem converges to the exact problem that we have

2) Note 2: "$F_n \to F$"

this is the algorithm

Assume that $\mathbb{X}_n \equiv \mathbb{X}$ $\forall n$ → I can apply the algorithm to all pt of the "complicated space"

2) can be rewritten → $\lim_{n\to\infty} |F_n(x) - F(x)| \to 0$

I'm asking that the algo applied to exact input minus the exact problem (in modulus) goes to zero for increasing n

LAX-RICHTMEYR THEOREM:

For consistent pb $\left(\lim_{n\to\infty} |F_n(x) - F(x)| = 0\right)$

CONVERGENCE $\Longleftrightarrow$ STABILITY

err

input $\rightarrow x$ $\xrightarrow{F}$ y $\leftarrow$ output

Proof

if F is well posed $\Rightarrow$ sure exist $F^{-1}(y_n) = \hat{x}$ $\xrightarrow{F}$ y_n

can be an approx of x (a ntl or x itself) $\rightarrow x_n$ $\xrightarrow{F_n}$ y_n

evaluate it with algorithm

if you want to prove convergence you must show that

Convergence $\lim_{n\to\infty} |F_n(x_n) - F(x)| \rightarrow 0$

We have:

adding and subtracting

$$|F_n(x_n) - F(x_n) + F(x_n) - F(\hat{x}) + F(\hat{x}) - F(x)| = \dots \rightarrow 0$$

consistency $\rightarrow 0$

stability $\Leftarrow \leq K|x_n - \hat{x}_n|$

stability $\Downarrow$ $K|\hat{x} - x|$

All the errors falls into 3 categories

- **stability errors** (of continuous pb)
- " " (of discrete pb)
- **consistency error**

If we control this, convergence is implied by stability of the problem

If continuous prob is stable, and the discrete problem is stable and consistent $\Rightarrow$ we have convergence

Example: Interpolation (Polynomial interpolation)

for simplicity but it is gen topic

We consider the case of One dimension. $\mathcal{X} := C^0([a,b])$ ← continuous functions

and we study the following problem

Pb: Find a polynomial of order n (at most) that coincides with the input function at (given) $n+1$ interpolation points

! They are not inputs! They are part of the problem itself

CONSIDERATIONS

1. in $\mathcal{X}$ we use the L^∞ norm:

We want to understand what F is and what's the condition number of the problem

$$\|u\|_\infty := \max_{x\in[a,b]} |u(x)|$$

2. the space $\mathcal{Y}$ is $\mathbb{P}^n([a,b])$ (because the outcome is a polynomial of degree n): we use again $\|\cdot\|_\infty$ as a norm (same norm as norm chosen for $\mathcal{X}$, because polys are also continuous fcts)

$\mathcal{X}$ is FINITE DIM, while $\mathcal{Y}$ IS NOT!

Note 1: $\mathcal{Y}$ is finite dimensional (with dimension $n+1$), and we can write it as

$$\mathcal{Y} = \mathbb{P}^n([a,b]) = \text{span}\{v_i\}_{i=0}^{n}$$ (linear combination; same basis functions)

$$\Updownarrow$$

$$\forall p \in \mathcal{Y} = \mathbb{P}^n([a,b]) \quad \exists! \ \{p^i\}_{i=0}^{n} \in \mathbb{R}^{n+1} \text{ s.t.}$$ (p^i: coefficients)

$$p(x) = \sum_{i=0}^{n} p^i v_i(x)$$

linear independence of v_i, i.e. $\iff$ $p^i = 0 \quad i = 0, \dots, n \iff p(x) = 0 \ \forall x \in [a,b]$

Polynomial interpolation: (Given $n+1$ points $\{x_i\}_{i=0}^{n}$)

The algorithm takes a function (continuous) and returns a polynomial

$$F: \mathcal{X} = C^0([a,b]) \longrightarrow \mathcal{Y} = \mathbb{P}^n([a,b])$$

where u function $\longrightarrow$ p polynomial

$$p(x_i) = u(x_i) \quad i = 0, \dots, n$$

($n+1$ conditions; the given points)

$$\sum_{j=0}^{n} p^j v_j(x_i) = u(x_i)$$

(p^j: contravariant coefs)

(Can do this because I know that the space $\mathbb{P}^n$ is finite dimensional, meaning that I can uniquely identify every element of that space with a vector of coefficients with respect to a given basis)

$$\Downarrow$$

$$\sum_{j=0}^{n} V_{ij} p^j = u_i \iff V p = u$$

(u_i: covariant coefs)

must invent index summing to einstein notation

$$V_{ij} = v_j(x_i)$$

Vandermond Matrix (when $v_i(x) = \text{pow}(x, i)$)

what we doing: going from a vector of values of a pt in $C^0([a,b])$ to a vector of coefficient of a basis in $\mathbb{P}^n([a,b])$

Einstein notation: $V_{iJ}\, p^J \equiv \sum_{J=0}^{n} V_{iJ}\, p^J$

we set $\left(V_{iJ}\right)^{-1} = V^{iJ}$ so that $\boxed{V^{iJ} V_{Jk} = \delta^i_k = \begin{cases} 1 & \text{if } i=k \\ 0 & \text{if } i\neq k \end{cases}}$

So if needed

$$V_{iJ}\, p^J = u_i \quad \Updownarrow \quad p^J = V^{Ji}\, u_i \iff \underline{p} = \mathbb{V}^{-1}\, \underline{u}$$

If you want to solve the prob of interpolation $\Rightarrow$ solve a linear system $\Rightarrow$ condition number of problem is related to condition number of $\mathbb{V}$

we define the "Reduced problem": $\mathcal{X} \equiv \mathbb{R}^n \longrightarrow \mathcal{Y} \equiv \mathbb{R}^n$ ← LINEAR PROBLEM NOW!

where

$\mathcal{X}$:= set of values of u in x_i $\mathcal{Y}$:= coefficients of the polynomial

with norm $\|\underline{u}\|_2 := \left(\sum_{i=0}^{n} u_i^2\right)^{\frac{1}{2}}$ and same for $\mathcal{Y}$

The original problem can be thought in this problem with 2 additional functions

We want to find Condition number of F: $\underline{u} \longrightarrow \mathbb{V}\,\underline{u} = \underline{p}$ ← by similarity

that is input $\{u_i\}_{i=0}^n \longrightarrow$ output $\{p^J\}_{J=0}^n$

If I was suppose to perturb the input, starting from $\hat{p} = \mathbb{V}^{-1}\hat{u}$

$$\|p - \hat{p}\|_2 \leq K_{abs}\, \|u - \hat{u}\|_2$$

We KNOW ALREADY THAT THE K_{abs} is given by the norm of the matrix (find out starting from $\|p-\hat{p}\|$ and using)

$$\|p - \hat{p}\|_2 \leq \|\mathbb{V}^{-1}\|\, \|u - \hat{u}\|_2$$

∠' As long as $\mathbb{V}$ is invertible, problem is always well posed, and $\|\mathbb{V}^{-1}\|_*$ is not infinite

The op norm is defined here as: $\|\mathbb{V}^{-1}\|_* := \left|\rho\left(\mathbb{V}^{-1}\right)\right| = \max_i \left|\lambda_i\left(\mathbb{V}^{-1}\right)\right| = \|\mathbb{V}^{-1}\|_2$

eigenvalues of $\mathbb{V}^{-1}$

op norm induced by the 2-norm

To make the problem better conditioned, we need to minimize $K_{abs} = \|\mathbb{V}^{-1}\|_2$ that is $\mathbb{V} \equiv \mathbb{I}$

then we have

$$V = I \Rightarrow V_j(x_i) = \delta_{ji}$$

which means we have a

Polynomial that is zero on every point x_i except on x_j where it is 1. We call this polynomial

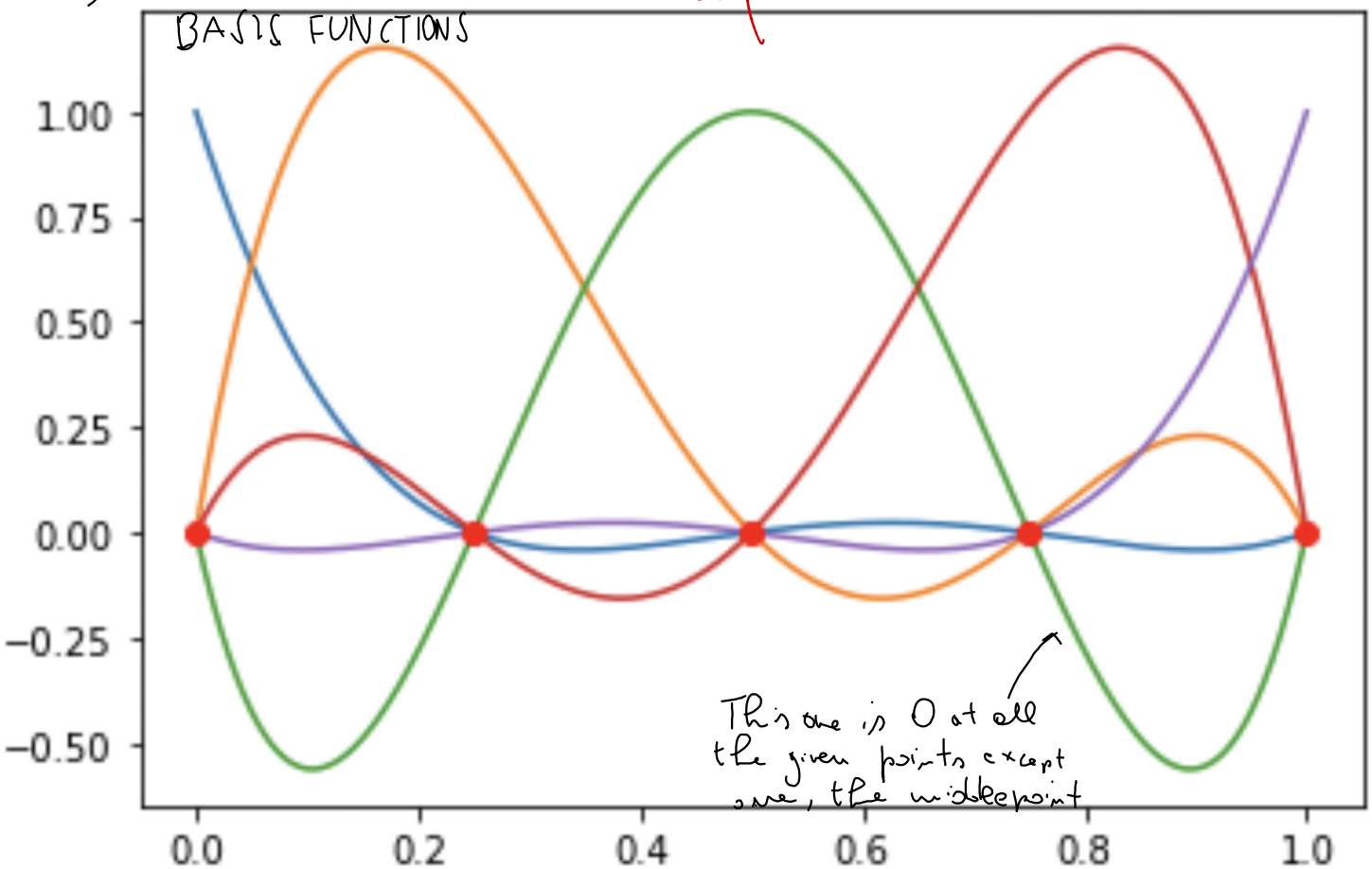
$$l_i := \prod_{\substack{j=0 \\ i \neq j}}^{n} \frac{(x - x_j)}{(x_i - x_j)}$$

Lagrange Basis

poly of order n

$\Rightarrow l_i(x_j \neq x_i) = 0, l_i(x_i) = 1$

example with $n = 5$



This example shows you how to choose the basis function such that

$$V = I$$

And you can use directly these basis functions to construct the polynomial interpolation

$$p(x) = \sum_{j=0}^{n} u(x_j) V_j(x)$$

where the coefficient are exactly

$$p^j = u(x_j)$$

because $V^{-1} = I$

! If you have columns of V that are very similar to one another (i.e. because basis fct get close and close to one another) V will still be invertible but the condition number will be very bad!

The condition number of Vandermont matrix will deteriorate as we increase the number of points (simply because, the more points we have the similar all the basis functions will get!)

Numerical Analysis — lec 4 L+H — 15.10.2020

is a linear problem

General interpolation problem from $\mathcal{X} := C^0([a,b])$ (continuous fcts)
to the space $\mathcal{Y} := V := \text{span}\{v_i\}_{i=0}^n$ finite dimensional with dimension $(n+1)$
with fixed support points $\{x_i\}_{i=0}^n$

$$\Pi : C^0([a,b]) \longrightarrow V$$
$$u(x) \longrightarrow p(x) := \sum_{i=0}^{n} p^i v_i(x)$$

the choice of this (#of nmber pts) is important in principle you could have an higher # of points but then it would'nt be possible to satisfy exactly the relationship in which the points coincide at those higher # of points

such that p and u coincides in $\{x_i\}_{i=0}^n$ (higher than the # of basis fcts)

Indeed
$$\sum_{j=0}^{n} p^j v_j(x_i) = u(x_i)$$
this is a linear system
$$\equiv$$
$$\mathbb{V}_{ij} := v_j(x_i) \qquad \mathbb{V}\,\underline{p} = \underline{u}$$
$$\{\underline{p}\}^j = p^j$$
$$\{\underline{u}\}_i = u(x_i)$$

POWER BASIS IN $[0,1]$

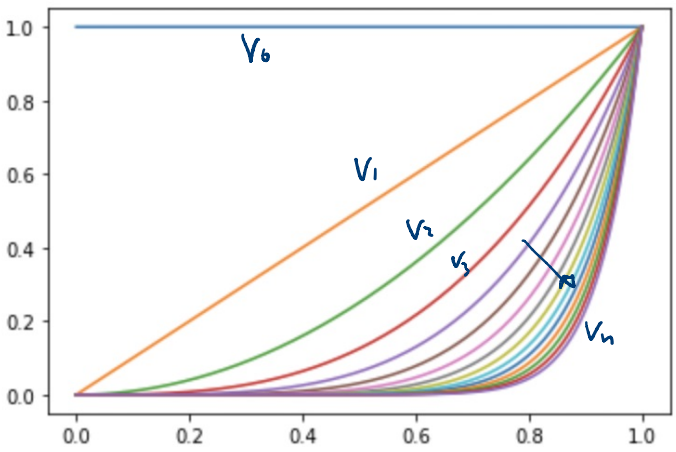
The basis functions $v_i \in C^0([a,b])$
basis fcts can be chosen among
(polynomials, cos/sin, sigmoids)

Example: $[a,b] = [0,1]$

$$v_i = \text{pow}(x,i) = x^i$$

if we fix $n+1 = 5$ $\quad \underline{p} := [1,0,0,2,3]$

$$p(x) = 1 + 2x^3 + 3x^4$$
$$= p^i v_i(x)$$



$$\underline{u} + \underline{v} = (u+v)$$
$$(\underline{u}+\underline{v})_i = u(x_i) + v(x_i)$$

then here we use

Linearity implies
$$\Pi(u+v) = \Pi(u) + \Pi(v)$$
because
$$\Pi(u) = \left(\mathbb{V}^{-1}\underline{u}\right)^i v_i(x) \qquad \Pi(v) = \left(\mathbb{V}^{-1}\underline{v}\right)^i v_i(x)$$
$$\Pi(u+v) = \left(\mathbb{V}^{-1}(\underline{u}+\underline{v})\right)^i v_i(x)$$

Condition number for interpolation problem

We use as norms in $C^0([a,b])$ $\|\cdot\|_\infty$, the same in V:

exploit the fact that the interpol. problem as we defined it is a linear problem

$$\|\mathbb{I}(u) - \mathbb{I}(\hat{u})\|_\infty = \|\mathbb{I}(u-\hat{u})\|_\infty \leq \|\mathbb{I}\|_* \, \|u-\hat{u}\|_\infty$$

by def. — $\|\mathbb{I}\|_*$ can be seen as $\sim K_{abs}$

What is $\|\mathbb{I}\|_*$?

Let's apply the definition of a norm

$$\|\mathbb{I}\|_* := \sup_{0 \neq u \in C^0([a,b])} \frac{\|\mathbb{I}(u)\|_\infty}{\|u\|_\infty} = \sup_{0\neq u \in V} \frac{\left\| V^{ij} u(x_j)\, v_i(x) \right\|_\infty}{\|u\|_\infty}$$

domain of the function "symbolized" by the problem $\mathbb{I}$

norm of V; inverse of matrix V; p^i; $p = \mathbb{I}u$

$$\leq \sup_{0\neq u \in V} \frac{\|V^{-1}\|_\infty \|u\|_\infty \max_i \|v_i\|_\infty}{\|u\|_\infty} \leq \|V^{-1}\|_\infty \max_i \|v_i\|_\infty$$

because for sure the maximum of the absolute value of u is greater than all the values of u at x_j, since x_j is a smaller number in the interval than all points in the interval!

u disappears $\Rightarrow$ can get rid of the sup

in finite dimensions all norms are equivalent

$$\text{cond}(V^{-1}) \max_i \|v_i\|_\infty \Rightarrow$$

cond number of the problem deteriorates if matrix deteriorates and deteriorates when basis function become too large

To minimize cond number of the problem you can play with 2 things: $\{x_i\}_{i=1}$, v_i

Two things: $\{x_i\}_{i=1}$, v_i

$\Rightarrow$ min $\text{cond}(V^{-1}) \equiv \{v_i\}_{i=0}^n$ are the Lagrange basis functions:

For power basis:

n = 1 : 1.0
n = 2 : 2.6180339887498953
n = 3 : 15.099657722502098
n = 4 : 98.86773850722759
n = 5 : 686.4349418185955
n = 6 : 4924.371056611224
n = 7 : 36061.16088021232
n = 8 : 267816.7009075794
n = 9 : 2009396.3800421846
n = 10 : 15193229.677753646
n = 11 : 115575244.54431371
n = 12 : 883478687.0721825
n = 13 : 6780588492.454725
n = 14 : 52214926084.1525
n = 15 : 403234616528.72504

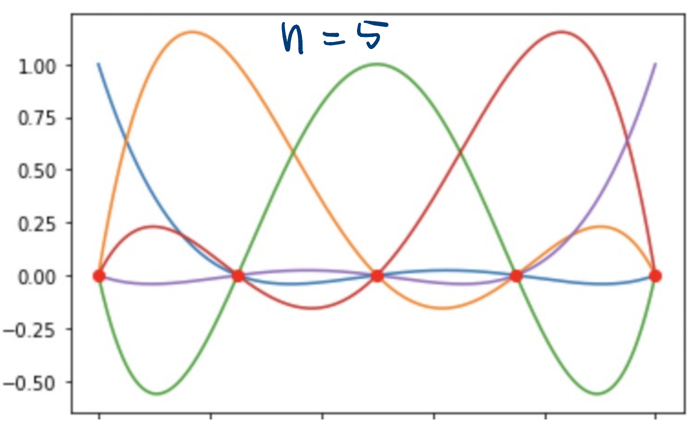
cond(V) for power basis

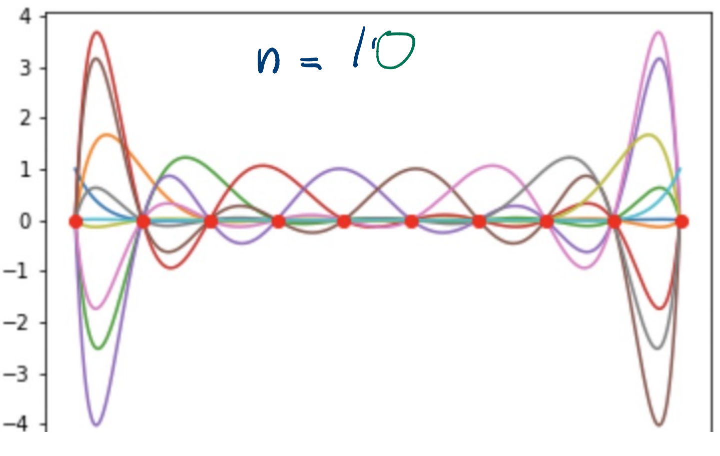
$$l_i := \prod_{\substack{j\neq i \\ j=0}}^{n} \frac{(x - x_j)}{(x_i - x_j)}$$

$\hookrightarrow V = \mathbb{I}d$ by construction

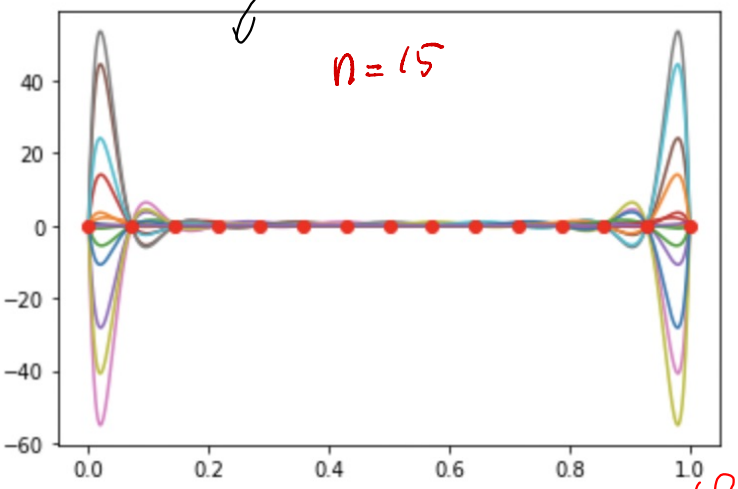
$$\rightsquigarrow V_{ij} := l_j(x_i) = \delta_{ij} = \begin{cases} 1 & \text{if } i=j \\ 0 & \text{if } i\neq j \end{cases}$$

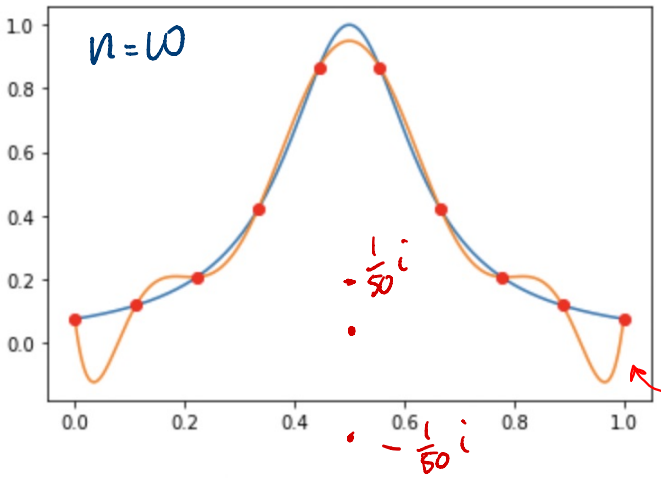
We should choose x_i s.t. $\max_i \|l_i\|_\infty$ is small

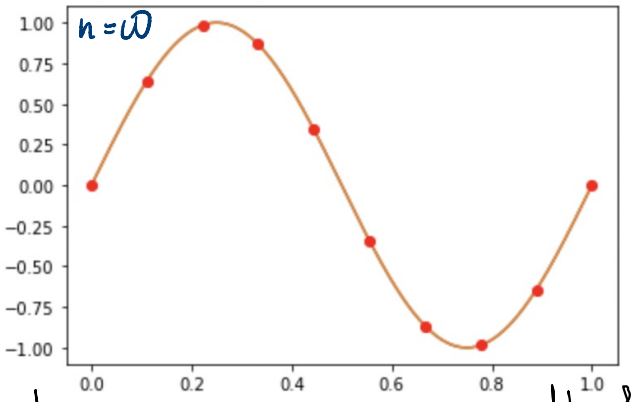




then you start getting bad oscillations







Is interpolation a good strategy for approximating a function?

the orange line represents, using LAGRANGE interpolation $\sum_{i=0}^{n} u(x_i)\, l_i(x) = p(x)$ with lagrange basis

blue line is the interpolated function $f(x) = \frac{1}{1+50(x-\frac{1}{2})^2}$

BAD BEHAVIOR HERE (away from the center) while at the center things are good

but this is FUNCTION DEPENDENT $f(x) = \sin(2\pi x)$

for sine results are perfect

Can we do better?

What can we say for smooth fcts about interpolation pities of pol interpol

Thm $f \in C^{(n+1)}([a,b])$ if $x_i \in (a,b)$, $\forall x \in (a,b)\ \exists \xi \in (a,b)$

(we here n+1 pb derivatives => needs for n+1 derivatives)

$$\left(f - \Pi^n f\right)(x) = \frac{1}{(n+1)!} f^{(n+1)}(\xi)\, \omega(x)$$

Interpolation of f using n points

This is our error treasurement

where $\omega(x)$ is the characteristic polynomial of $\{x_i\}_{i=1}^{n}$

$$\omega(x) = \prod_{i=0}^{n} (x - x_i)$$

can we make these two numbers small?

First consequence: $\|\Pi f - f\|_\infty \leq \frac{\|\omega\|_\infty}{(n+1)!} \|f^{(n+1)}\|_\infty$

If can control the n+1 derivative of the function ANYWHERE :) you have a bound on the error at every point, simply bound by the norm of the n+1 derivative and the norm of the w function

proof: $\forall x$ define $G(t)$ s.t. it is equal to 0 in all points in which the polynomials and the function coincide (support points) plus the point x

$$G(t) = \big(f(t) - p(t)\big)\,\omega(x) - \big(f(x) - p(x)\big)\,\omega(t)$$

where $p(t) = \sum_{i=0}^{n} f(x_i)\,\ell_i(t) = (\mathbb{I}f)(t)$ ↝ interpolation function of f

$G(t)$ has $n+2$ ($n+1$ support points + x) zeros: $\{x_i\}_{i=0}^{n} \cup \{x\}$

According to Rolle's theorem (applied iteratively): $\exists\, \xi \in (a,b)$ s.t. $\dfrac{d^{n+1} G(\xi)}{dt^{n+1}} = 0$

f with two zeros $\Rightarrow$ $\exists\, \xi$ s.t. $f'(\xi) = 0$

writing explicitly the derivative

$$\frac{d^{n+1}}{dt^{n+1}}\,G(\xi) = f^{(n+1)}(\xi)\cdot\omega(x) - \big(f(x) - p(x)\big)\,(n+1)! = 0$$

$\frac{d^{n+1}}{dt^{n+1}}(\omega(t))$ — just removed

$$\Rightarrow\quad f(x) - (\mathbb{I}f)(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!}\,\omega(x) \qquad \blacksquare \quad \text{QED}$$

How to apply this?

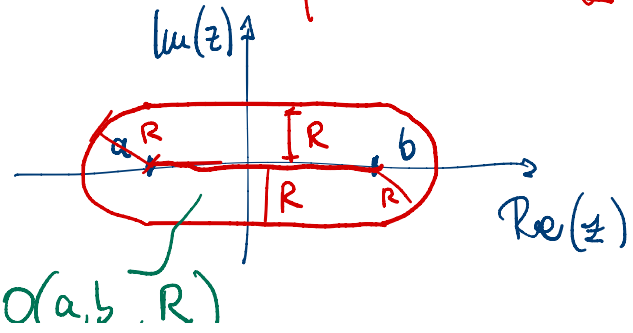
Thm 2: If f is analytically extendible in an ovoid $O(a,b,R)$ with $R > 0$

Then $\|f^{(n+1)}\|_\infty \le \dfrac{(n+1)!}{R^{n+1}}\,\|\tilde{f}\|_{L^\infty(O(a,b,R))}$

Analytically extendible means: it

Take x, and replace with $z \in \mathbb{C}$

we are asking that $f \in C^\infty$ in $O(a,b,R)$

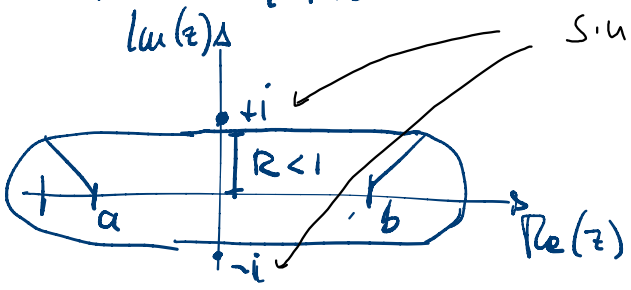


EXAMPLE

Runge function: $f = \frac{1}{1+x^2}$

extension to $\mathbb{C}$

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



f is analytical in $\mathcal{O}(-\infty, +\infty, 1-\varepsilon) \quad \forall \varepsilon > 0$

What are the consequences?

$$\| f^{(n+1)} \| \leq \frac{(n+1)!}{R^{n+1}} \| f \|_\infty$$

$R < 1$ otherwise i get singularities

So, by the previous theorem:

$$\| p - f \|_\infty \leq \| f^{(n+1)} \|_\infty \frac{\| w \|_\infty}{(n+1)!} \leq \frac{(n+1)!}{(n+1)!} \frac{\| w \|_\infty}{R^{n+1}} \| f \|_\infty$$

where

$$\| w \|_\infty = \left\| \prod_{i=0}^{n} (x - x_i) \right\| \leq |b-a|^{(n+1)} \quad x \in (a,b)$$

since $x \in (a,b) \Rightarrow |x - x_i| \leq |b-a|$

$$\| p - f \|_\infty \leq \left(\frac{|b-a|}{R} \right)^{n+1} \| f \|_\infty$$

↳ good only when $|b-a| < R$, otherwise $\| p - f \|_\infty$ IS NOT BOUNDED

$\Rightarrow$ Runge: $\frac{1}{1+x^2}$ in $(-1, 1)$ everything ok

Can we do better?

Best Approximation. Definition:

Restrict ourselves

$\mathcal{X}$ Banach, reflexive, strictly convex

V subspace of $\mathcal{X}$

We call p the best approximation in V of f in $\mathcal{X}$ when:

$$\|f-p\| \leq \|f-q\| \quad \forall q \in V$$

in other words

$$\|f-p\| = E(f) = \inf_{q \in V} \|f-q\|$$

Thm: $\exists! p$ only in these cases (mandatory conditions)

How does polynomial interpolation compare to best approximation?

We can say that

$$\|f - \Pi^n f\|_\infty = \|f - p + p - \Pi^n f\|_\infty =$$

add and subtract best approx

p is a polyn of deg n $\Rightarrow$ its polyn interpolation is itself

$$= \|f - p + \Pi^n(p - f)\|_\infty$$

$$\text{triangular inequality} \leq \|f-p\|_\infty + \|\Pi^n\|_* \|p-f\|_\infty$$

$$\text{property of norms} \leq \left(1 + \|\Pi^n\|_*\right) \|p-f\|_\infty$$

how away we are from best interpolation

For Lagrange interpolation:

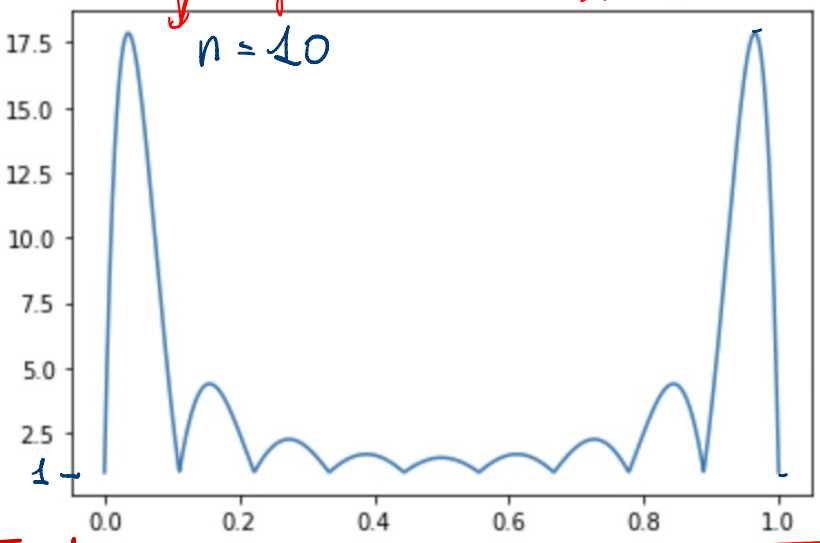
$$\|\Pi^n\|_* := \sup_{u \in C^0([a,b])} \frac{\|\sum_{i=0}^n u(x_i)\, l_i(x)\|_\infty}{\|u\|_\infty} \leq$$

$$= \|\sum_{i=0}^n |l_i(x)|\|_\infty$$

def: $\Lambda(x) := \sum_{i=1}^n |l_i(x)|$ LEBESGUE FUNCTION

$\Rightarrow \| \Pi^n_* \| = \| \Lambda \|_\infty$

Lebesgue functions are such that => bad results. Indeed $\| \Lambda \|_\infty$ for equispaced points grows quickly



$$\| \Lambda \|_\infty \leq \frac{2^{n+1}}{e n \log n}$$

A collection of points: $\{x_i\}_{i=0}^n$ is a list of lists of points with increasing size

Erdos

$\forall$ collection of points $\{x_i\}_{i=0}^n$ $\exists\, c > 0$ s.t.

$$\| \Lambda \|_\infty \geq \frac{2}{\pi} \log(n+1) - c$$

independently of how you choose the points, at best you get logarithmic with the number of the points

Faber

$\forall$ collection of points $\{x_i\}_{i=0}^n$ $\exists f$ s.t.

$\lim_{n \to \infty} \| \Pi^n f - f \|_\infty \to \infty$

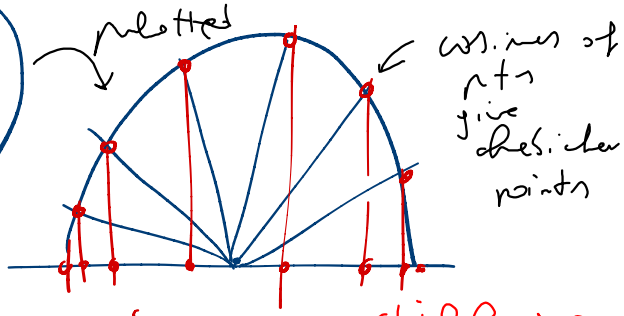
$\Leftrightarrow$ you can always find a f that destroys all

The best is $\alpha := \{x_i\}_{i=0}^n$ s.t. $\| \Lambda^\alpha \|_\infty \leq \| \Lambda^\beta \|_\infty$

$\forall\, \beta = \{\tilde{x}_i\}_{i=0}^n$

such $\alpha := \{x_i\}_{i=0}^n$ are called Chebyshev points: between $[-1, 1]$

defined as $x_i = \cos\left(\frac{(2i+1)\pi}{2n+2}\right)$



There's an estimate that says

$$\| \Lambda^\alpha \|_\infty \leq \frac{2}{\pi} \log(n+1) + 1$$

Best case scenario

still grows logarithmically

$$\frac{2}{\pi} \log(n+1) - c \leq \| \Lambda^\alpha \|_\infty \leq \frac{2}{\pi} \log(n+1) + 1$$

=) π INTERPOLATION IS GOOD BUT NOT π SO GOOD

Nonlinear equations

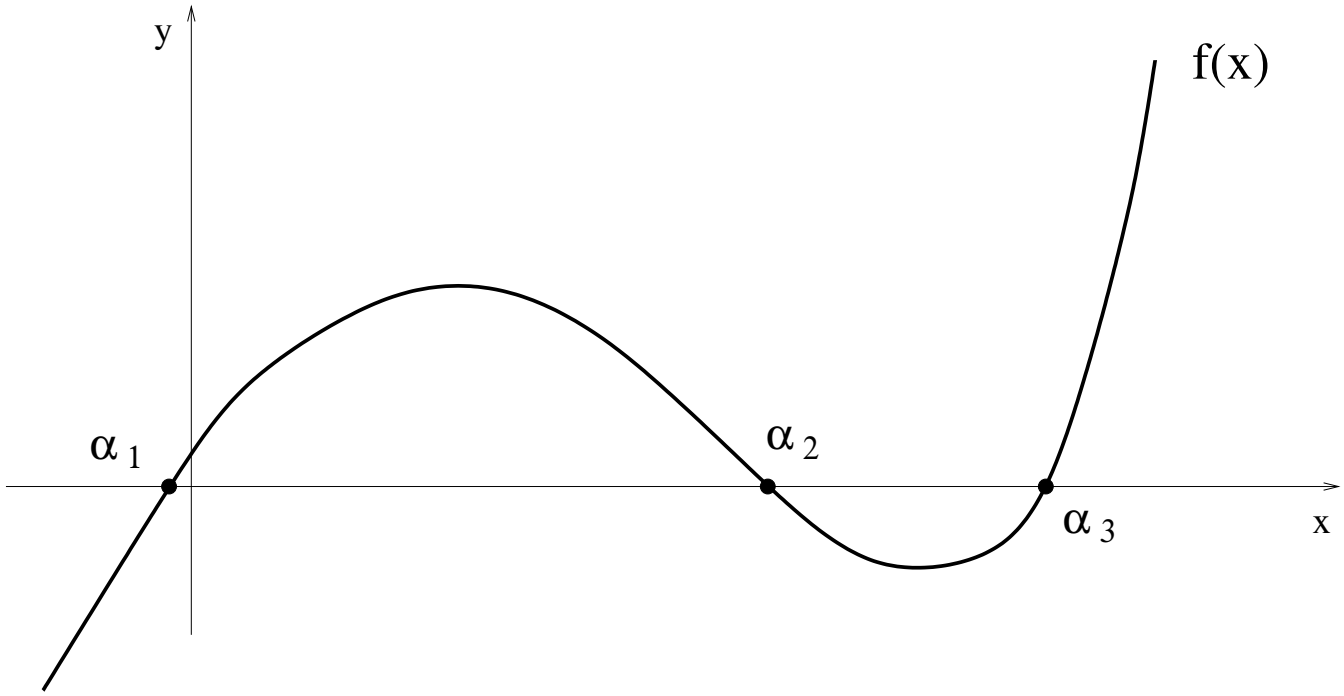
Numerical Analysis

Profs. Gianluigi Rozza - Luca Heltai

2019-SISSA mathLab Trieste

Nonlinear equations

Objective: Find the root of scalar (or vector) non-linear functions, i.e., find $\alpha \in \mathbb{R}$ such that $f(\alpha) = 0$.



Examples and motivation

Example 1 (Interest rates)**.** We want to compute the mean interest rate I of a portfolio over several years. We invest $v = 1000$ Euro every year. After 5 years we end up with $M = 6000$ Euro.
The relation between M, v, I and the number of years n is

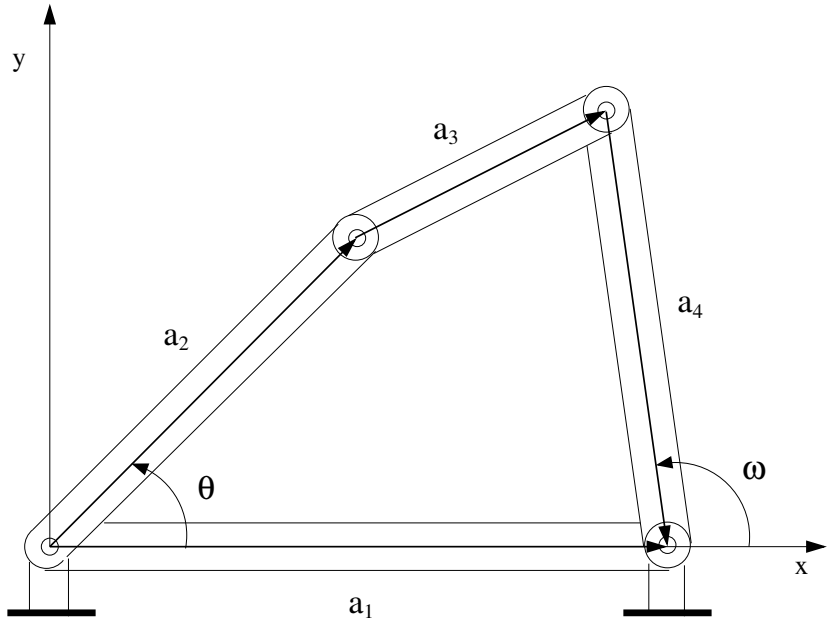
$$M = v \sum_{k=1}^{n} (1+I)^k = v \frac{1+I}{I} \left[(1+I)^n - 1 \right]$$

This can be rewritten as: *find I such that*

$$f(I) = M - v \frac{1+I}{I} \left[(1+I)^n - 1 \right] = 0 \tag{1}$$

Therefore we have to solve a nonlinear equation in I, for which we can't find an analytical solution.

Example 2 (Rods system)**.** Let us consider the mechanical system represented by four rigid rods



For any admissible angle ω, we want to compute the angle θ between $\mathbf{a}_1$ and $\mathbf{a}_2$.
Thanks to the vector identity

$$\mathbf{a}_1 - \mathbf{a}_2 - \mathbf{a}_3 - \mathbf{a}_4 = 0$$

and keeping $\mathbf{a}_1$ on the x-axis, we can derive the following equation: involving ω and θ:

$$\frac{a_1}{a_2}cos(\omega) - \frac{a_1}{a_4}cos(\theta) - cos(\omega - \theta) = -\frac{a_1^2 + a_2^2 - a_3^2 + a_4^2}{2a_2a_4} \qquad (2)$$

where a_i is the length of the ith rod. Equation (2) is nonlinear and can be solved only for particular values of ω. For a general ω it is not possible to find an analytic solution.

Example 3 (State equation of a gas)**.** We want to determine the volume V occupied by a gas at temperature T and pressure p. The state equation (i.e. the equation that relates p, V et T) is

$$\left[p + a\left(\frac{N}{V}\right)^2\right](V - Nb) = kNT\ ,$$

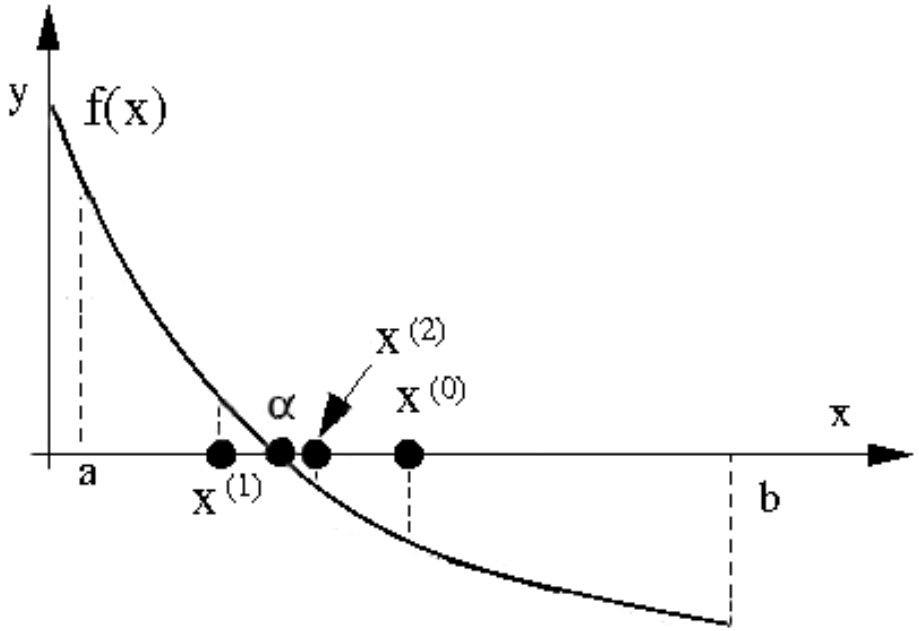
where a and b are two coefficients that depend on the specific gas, N is the number of molecules which are contained in the volume V and k is the Boltzmann constant. We need therefore to solve a nonlinear equation whose root is V.

Bisection method

(Book Sec. 2.2)

This method is used to compute the root of a continuous function f, i.e., the point α such that $f(\alpha) = 0$. We can build a *sequence* $x^{(0)}, x^{(1)}, \ldots, x^{(k)}$, ($x^{(0)}$ such that $\lim_{k\to\infty} x^{(k)} = \alpha$.

We assume that $f : (a, b) \to \mathbb{R}$ and $a < b$. If $f(a)f(b) < 0$, since f is continuous, we know that there exists (at least) one root α of f in the interval (a, b).



Then

1. We set $a^{(0)} = a$, $b^{(0)} = b$ and $x^{(0)} = \frac{a^{(0)}+b^{(0)}}{2}$,
2. if $f(x^{(0)}) = 0$, then $x^{(0)}$ is the zero.
3. if $f(x^{(0)}) \neq 0$, then:

   (a) if $f(x^{(0)})f(a^{(0)}) > 0 \Rightarrow$ the zero $\alpha \in (x^{(0)}, b^0)$ and we define $a^{(1)} = x^{(0)}$, $b^{(1)} = b^{(0)}$ and $x^{(1)} = (a^{(1)} + b^{(1)})/2$

   (b) if $f(x^{(0)})f(a^{(0)}) < 0 \Rightarrow$ the zero $\alpha \in (a^{(0)}, x^{(0)})$ and we define $b^{(1)} = x^{(0)}$, $a^{(1)} = a^{(0)}$ et $x^{(1)} = (a^{(1)} + b^{(1)})/2$

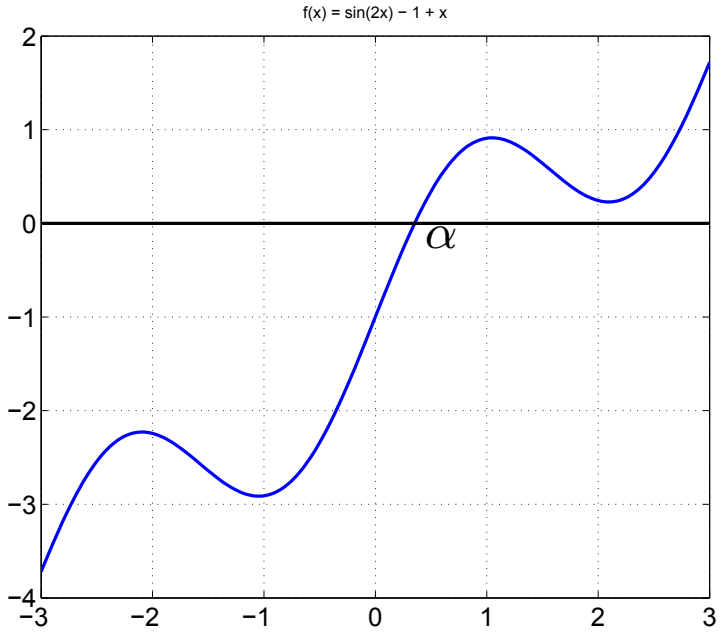
By the divisions of this type, we construct the sequence $x^{(0)}, x^{(1)}, \ldots, x^{(k)}$ that satisfies for all k,

$$|e^{(k)}| = |x^{(k)} - \alpha| \leq \frac{b-a}{2^{k+1}},$$

because we divide the interval by 2 at every step, starting from step 0

Example 4. We want to find the zero of the function $f(x) = \sin(2x) - 1 + x$. We draw the graph of the function f using the following commands in Matlab/Octave:

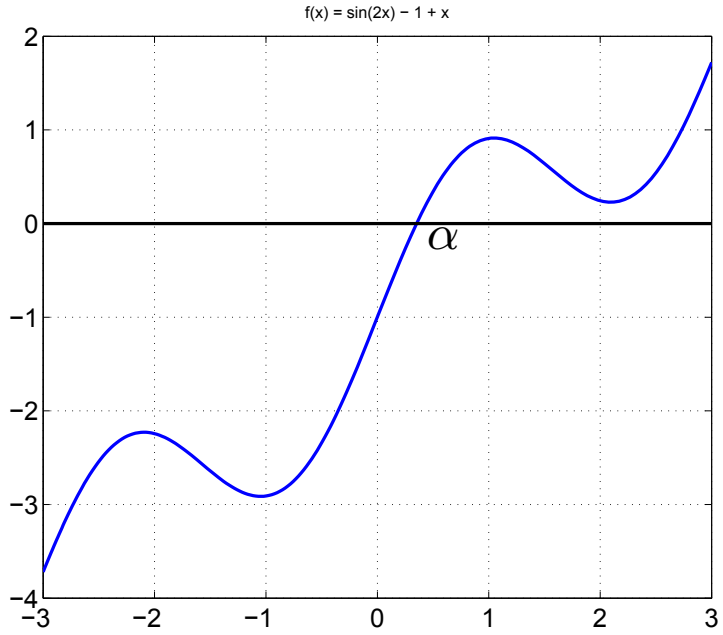
```
>> f = @(x) sin(2*x) -1 + x;
>> x=-3:0.1:3;
>> plot(x,f(x)); grid on;
```



If we appply the bisection method in the interval $[-1, 1]$ with a tolerance 10^{-8} and maximum number of iterations $k_{max} = 1000$

```
>> [zero,res,niter]=bisection(f,-1,1,1e-8,1000);
```

We find the value $\alpha = 0.352288462$ after 27 iterations.



APRIORI KNOWLEDGE OF # OF MAX ITERATION

Assume stopping criterion is based on size of interval.

At it k:

$$\frac{b-a}{2^k} < \varepsilon \quad \text{(} \varepsilon \text{: set tolerance)} \quad \rightarrow \text{solve for } k: \quad k \geq \log_2 \frac{b-a}{\varepsilon} = \frac{\ln(b-a) - \ln(\varepsilon)}{\ln 2}$$

Newton's method

(Chapt. 2.3 of the book)

Let $f : \mathbb{R} \to \mathbb{R}$ be a differentiable function.
Let $x^{(0)}$ be an initial guess. Let us consider the equation $y(x)$ which passes through the point $(x^{(k)}, f(x^{(k)}))$ and which has the slope $f'(x^{(k)})$:

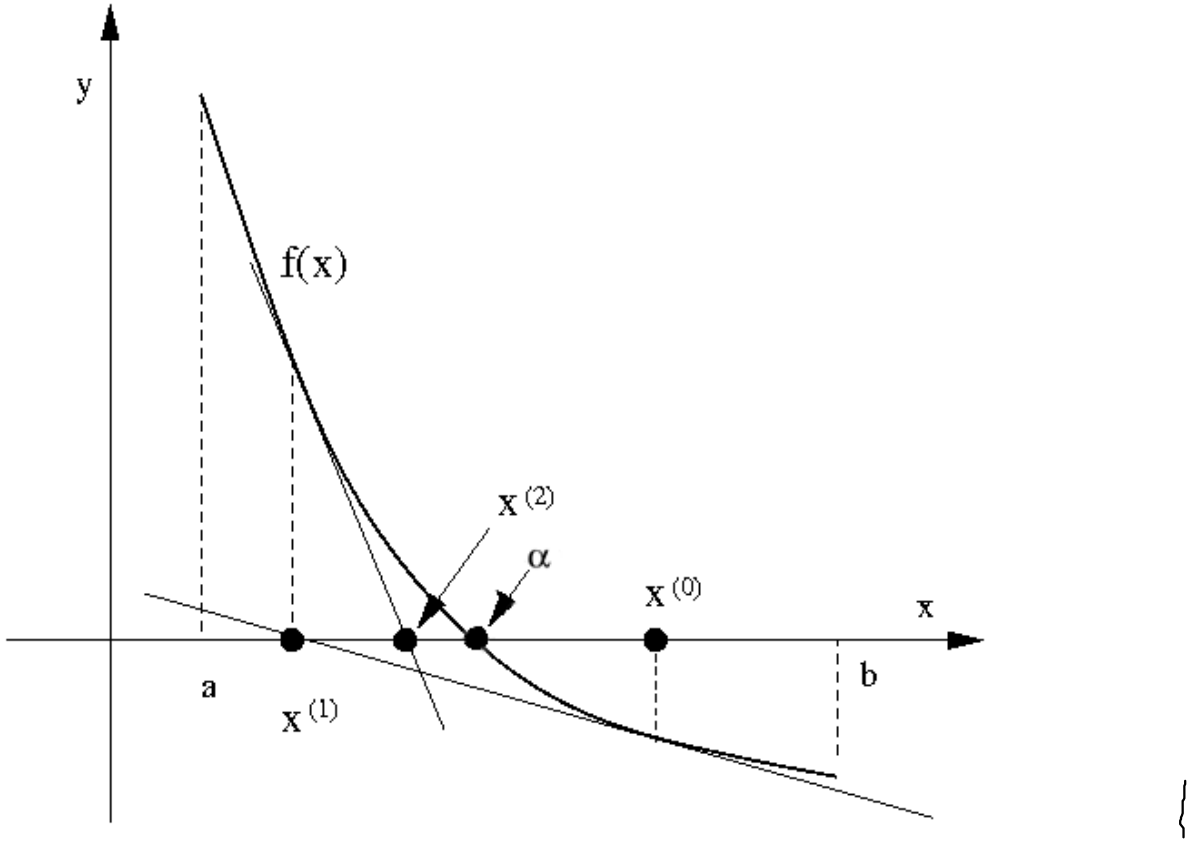
$$y(x) = f'(x^{(k)})(x - x^{(k)}) + f(x^{(k)}).$$

We define $x^{(k+1)}$ by the point where this line intersects the axis x, i.e. $y(x^{(k+1)}) = 0$. We deduce that:

$$x^{(k+1)} = x^{(k)} - \frac{f(x^{(k)})}{f'(x^{(k)})}, \quad k = 0, 1, 2 \ldots . \tag{3}$$

Newton's method

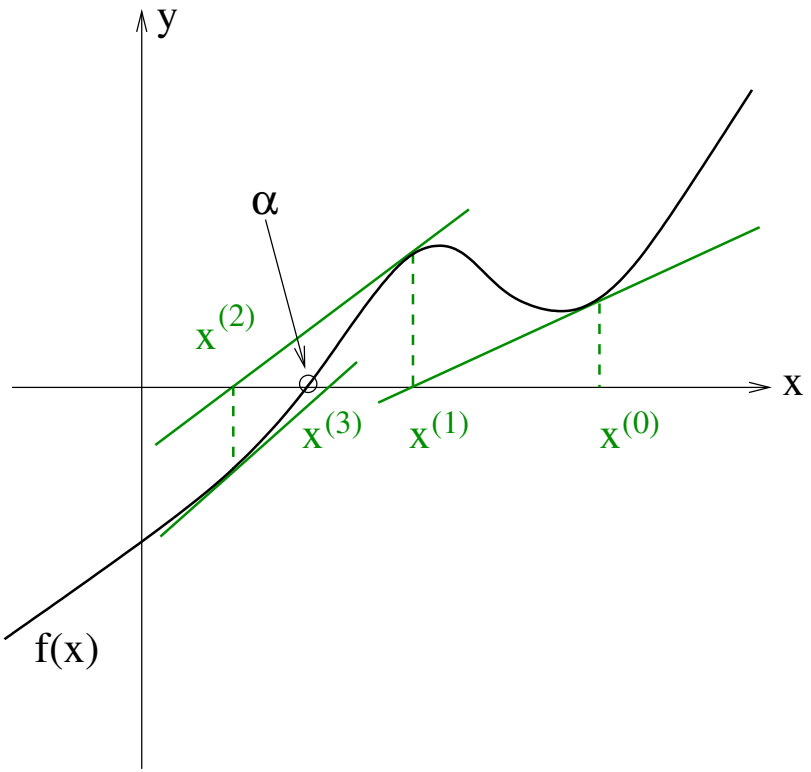
Starting from the point $x^{(0)}$, the sequence $\{x^{(k)}\}$ converges to the root of f

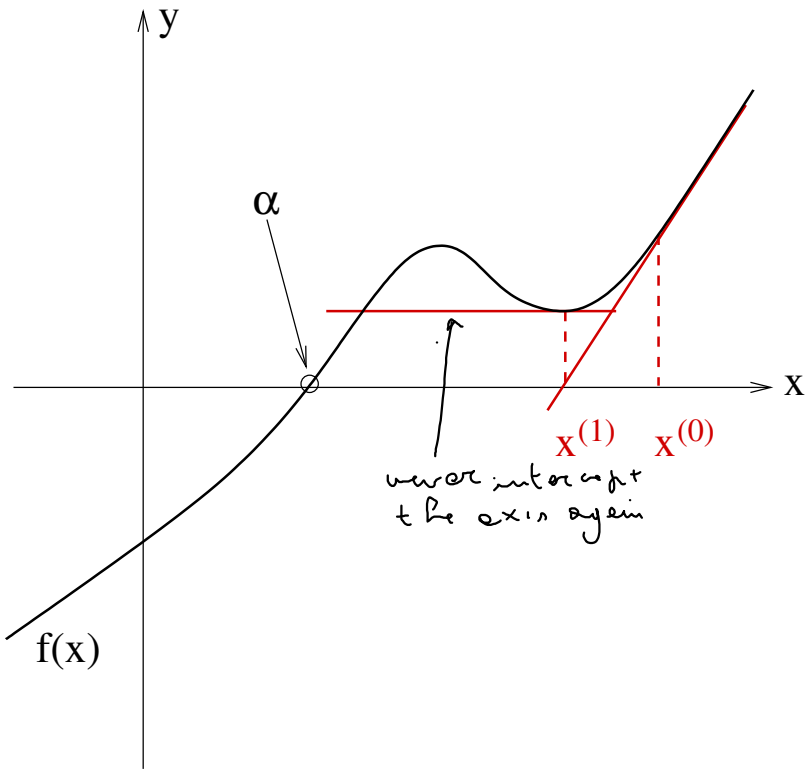


Convergence?

Does this method always converge?

- it depends on the property of the function;
- and on the initial guess.





Fixed point iterations.

(Chapt. 2.4 in the book)

A general method for finding the roots of a nonlinear equation $f(x) = 0$ is the transformation of the problem in an equivalent problem $x - \phi(x) = 0$, where the auxiliary function $\phi : [a, b] \to \mathbb{R}$ must have the following property :

$$\phi(\alpha) = \alpha \qquad \text{if and only if} \qquad f(\alpha) = 0.$$

and ϕ is called CONTRACTION

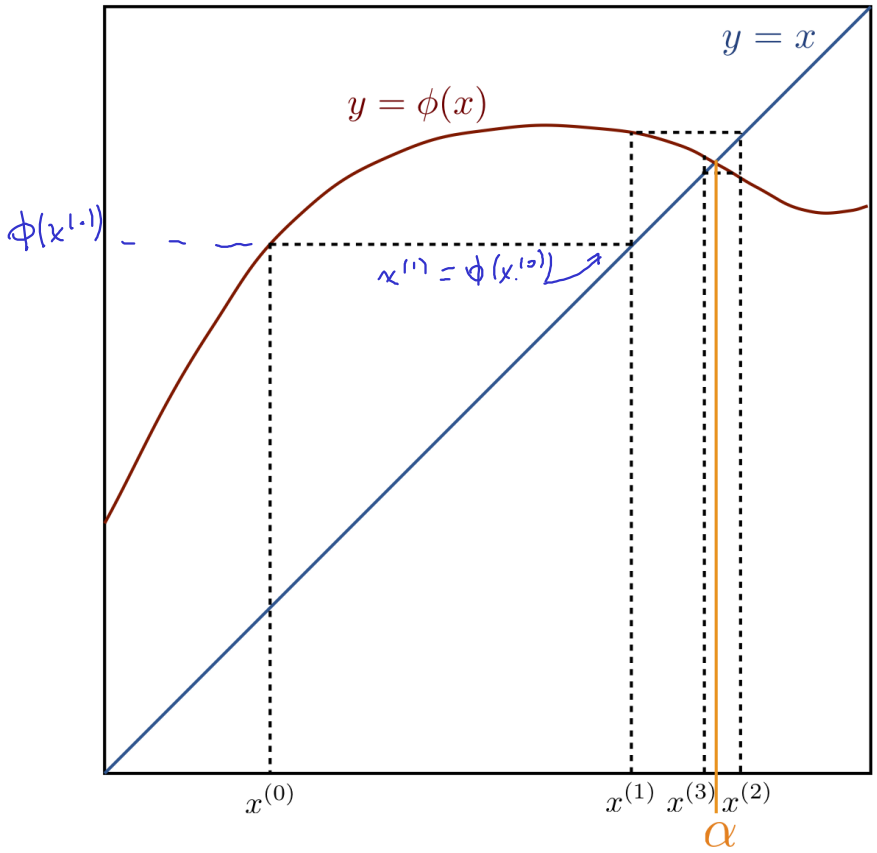
The point α is called *a fixed point* of ϕ. Searching the zeros of f is reduced to the problem of determining the fixed points of ϕ.

Idea : It could be computed by the following algorithm: $x^{(k+1)} = \phi(x^{(k)})$, $k \geq 0$. Indeed, if $x^{(k)} \to \alpha$ and if ϕ is continuous on $[a, b]$, then the limit α satisfies $\phi(\alpha) = \alpha$.

$x^{(k+1)} = \phi(x^{(k)}) \longrightarrow \phi(\alpha) = \alpha$ (follows from the definition of fct ϕ)

$x^{(k)} \to \alpha$

Starting from the point $x^{(0)}$, the sequence $\{x^{(k)}\}$ converges to the fixed point α

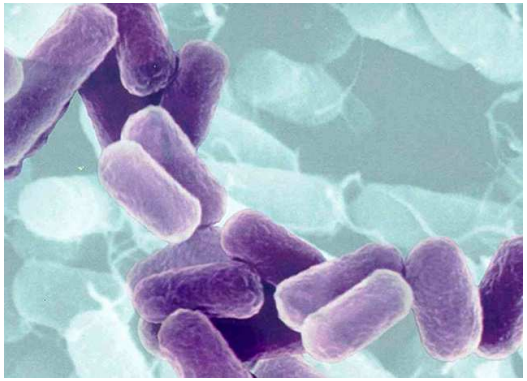


Example 5 (Population dynamics)**.**

In the survey population (e.g. bacteria), we want to establish a link between the number of individuals in the generation x and the number of individuals in the next generation x^+:

$$x^+ = \phi(x) = xR(x), \tag{4}$$

where $R(x)$ represents the rate of growth (or decay) of the considered population.



Several models are available for $R(x)$:

- The Malthusian growth model (Thomas Malthus 1766-1834),

$$x^+ = \phi_1(x) = xR_1(x) \text{ with } R_1(x) = r, \quad r \text{ is a positive constant}$$

- the model of growth with limited resources (Pierre François Verhulst, 1804-1849),

$$x^+ = \phi_2(x) = xR_2(x) \text{ with } R_2(x) = r/(1 + x/K), \quad r > 0, K > 0$$

K may be some kind of measurement for available resources → x/K is the number of members of population per resource

that improve the Malthausian growth model by taking into account the growth of a population is limited by the resources.

- the predator/prey model

$$x^+ = \phi_3(x) = xR_3(x) \text{ with } R_3(x) = rx/(1 + (x/K)^2)$$

that represents the change of the Verhulst model by presence of an antagonist population.

The dynamics of a population is defined by a iterative process, starting from a given initial guess ($x^{(0)}$),

$$x^{(k+1)} = \phi(x^{(k)}), \quad k \geq 0,$$

where $x^{(k)}$ represents the number of individuals in k-th generation.
In addition, the steady states (equilibriums) x^* of a considered population are identified by the following problem,

$$x^* = \phi(x^*), \tag{5}$$

or equivalently,

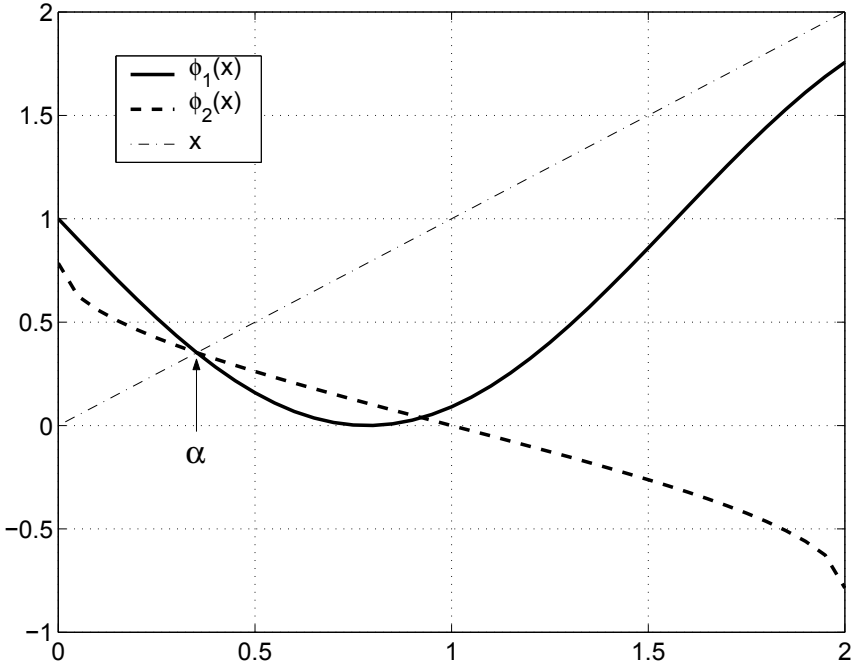
$$x^* = x^* R(x^*), \quad \text{i.e.} \quad R(x^*) = 1. \tag{6}$$

In both cases, we ask to solve a non-linear problem. In particular the problem is called the fixed point problem.

Example 6. We consider the equation $f(x) = \sin(2x) - 1 + x = 0$. We can rewrite it in two different fashions:

$$x = \phi_1(x) = 1 - \sin(2x)$$

$$x = \phi_2(x) = \frac{1}{2}\arcsin(1-x), \qquad 0 \le x \le 1$$



that is: the pair $(x, \phi(x))$ belongs to a square

Proposition 1. *(Global convergence)*

1. Assume that $\phi(x)$ is continuous on $[a, b]$ and such that $\phi(x) \in [a, b]$ for all $x \in [a, b]$; then there exists at least one fixed point $\alpha \in [a, b]$ of ϕ.

2. If $\exists L < 1$ such that $|\phi(x_1) - \phi(x_2)| \leq L|x_1 - x_2|$ $\forall x_1, x_2 \in [a, b]$,

then there exists a unique fixed point $\alpha \in [a, b]$ and the sequence $x^{(k+1)} = \phi(x^{(k)})$, $k \geq 0$ converges to α, for any initial guess $x^{(0)} \in [a, b]$.

Proof.

1. The function $g(x) = \phi(x) - x$ is continuous in $[a, b]$ and, thanks to assumption made on the range of ϕ, it holds $g(a) = \phi(a) - a \geq 0$ and $g(b) = \phi(b) - b \leq 0$. By applying the theorem of zeros of continuous functions, we can conclude that g has at least one zero in $[a, b]$, i.e. ϕ has at least one fixed point in $[a, b]$.

2. Indeed, should two different fixed points α_1 and α_2 exist, then

$$|\alpha_1 - \alpha_2| = |\phi(\alpha_1) - \phi(\alpha_2)| \leq L|\alpha_1 - \alpha_2| < |\alpha_1 - \alpha_2|,$$

which cannot be. There exists a unique fixed point $\alpha \in [a, b]$ of ϕ. □

Let $x^{(0)} \in [a,b]$ and $x^{(k+1)} = \phi(x^{(k)})$. We have

$$0 \leq |x^{(k+1)} - \alpha| = |\phi(x^{(k)}) - \phi(\alpha)| \leq L|x^{(k)} - \alpha| \leq \ldots \leq L^{k+1}|x^{(0)} - \alpha|,$$

fixed point; (1); (2); by applying 1 and 2 iteratively

i.e.

$$\frac{|x^{(k)} - \alpha|}{|x^{(0)} - \alpha|} \leq L^k.$$

Because $L < 1$, for $k \to \infty$, we obtain

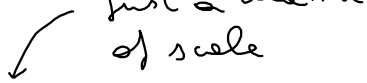
$$\lim_{k\to\infty} |x^{(k)} - \alpha| \leq \lim_{k\to\infty} L^k = 0.$$

ok, because $|x^{(0)} - \alpha|$ is constant

So, $\forall x^{(0)} \in [a,b]$, the sequence $\{x^{(k)}\}$ defined by $x^{(k+1)} = \phi(x^{(k)})$, $k \geq 0$ converges to α when $k \to \infty$.

Remark 1.
If $\phi(x)$ is differentiable in $[a, b]$ and

$\exists K < 1$ *such that* $|\phi'(x)| \leq K \ \forall x \in [a, b]$,



then the condion 2 of the proposal (1) is satisfied. This assumption is stronger, but is more often used in practice because it is easier to check.

Definition 1. *For a sequence of real numbers* $\{x^{(k)}\}$ *that converges,* $x^{(k)} \to \alpha$, *we say that the convergence to* α *is linear if exists a constant* $C < 1$ *such that, for* k *that is large enough*

$$| x^{(k+1)} - \alpha | \leq C | x^{(k)} - \alpha | .$$

If exists a constant $C > 0$ *such that the inequality*

$$| x^{(k+1)} - \alpha | \leq C | x^{(k)} - \alpha |^2$$

is satisfied, we say that convergence is quadratic.
In general, the convergence is with order p, $p \geq 1$, *if exists a constant* $C > 0$ *(with* $C < 1$ *when* $p = 1$*) such that the following inequality is satisfied*

$$| x^{(k+1)} - \alpha | \leq C | x^{(k)} - \alpha |^p .$$

$C > 1$ => doesn't converge

Proposition 2. *(Local convergence - Theorem 2.1 in the book)*
Let ϕ be a continuous and differentiable function on $[a,b]$ and α be a fixed point of ϕ. If $|\ \phi'(\alpha)\ | < 1$, then there exists $\delta > 0$ such that, for all $x^{(0)}$, $|\ x^{(0)} - \alpha\ | \leq \delta$, the sequence $\{x^{(k)}\}$ defined by $x^{(k+1)} = \phi(x^{(k)})$ converges to α when $k \to \infty$.
Moreover, it holds

$$\lim_{k\to\infty} \frac{x^{(k+1)} - \alpha}{x^{(k)} - \alpha} = \phi'(\alpha).$$

Proof: exp $\phi(x^{(k)})$ around α, proceed as in proof of next prop

Note that, if $0 <|\ \phi'(\alpha)\ | < 1$, then for any constant C such that $|\phi'(\alpha)| < C < 1$, if k is large enough, we have:

$$|\ x^{(k+1)} - \alpha\ | \leq C\ |\ x^{(k)} - \alpha\ |\ .$$

$\frac{x^{(k+1)} - \alpha}{x^{(k)} - \alpha}$ will reach $\phi'(\alpha)$ from above or below $\Rightarrow$ in any case, it will be $< C$

Proposition 3. *(Proposition 2.2 in the book) Let ϕ be a twice differentiable on $[a, b]$ and α be a fixed point of ϕ. Let us consider that $x^{(0)}$ converges locally. If $\phi'(\alpha) = 0$ and $\phi''(\alpha) \neq 0$, then the fixed point interations converges with order 2 and*

$$\lim_{k\to\infty} \frac{x^{(k+1)} - \alpha}{(x^{(k)} - \alpha)^2} = \frac{\phi''(\alpha)}{2}.$$

Proof. Using the Taylor series for ϕ with $x = \alpha$, we have

$$x^{(k+1)} - \alpha = \phi(x^{(k)}) - \phi(\alpha) = \underbrace{\phi'(\alpha)}_{0}(x^{(k)} - \alpha) + \frac{\phi''(\eta)}{2}(x^{(k)} - \alpha)^2$$

where η is between $x^{(k)}$ and α. So, we have

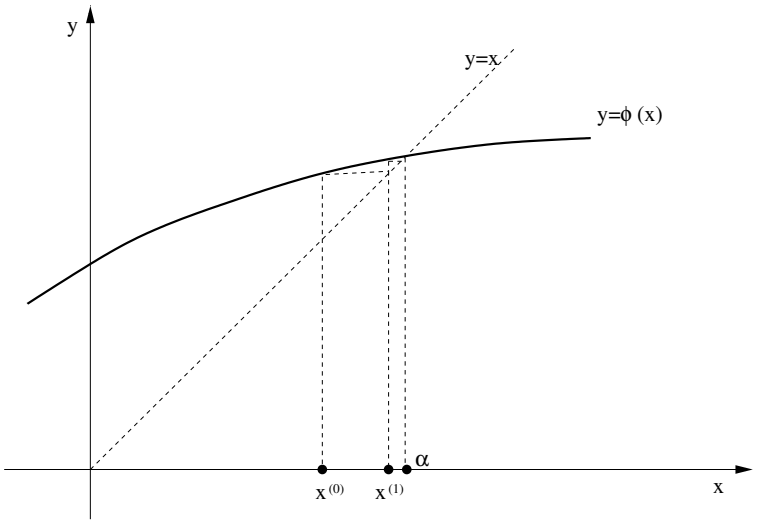
$$\lim_{k\to\infty} \frac{x^{(k+1)} - \alpha}{(x^{(k)} - \alpha)^2} = \lim_{k\to\infty} \frac{\phi''(\eta)}{2} = \frac{\phi''(\alpha)}{2}.$$

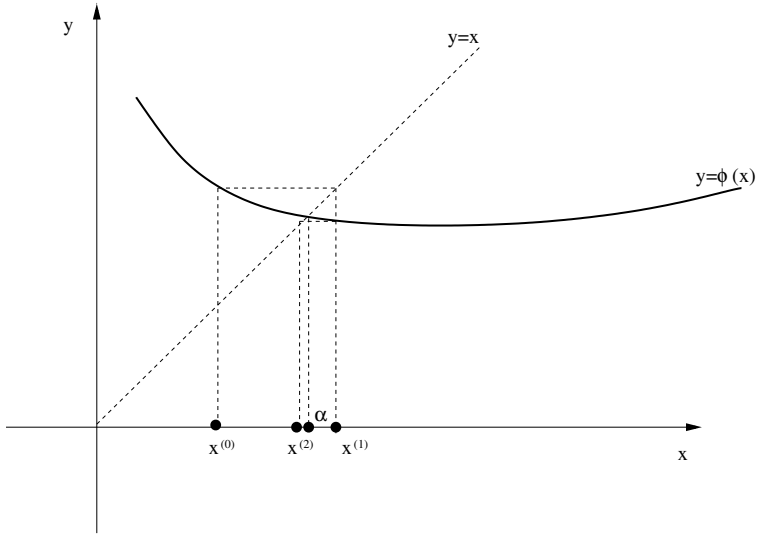
$\square$

Some examples on how the value $|\ \phi'(\alpha)\ |$ influences the convergence

Convergent cases:

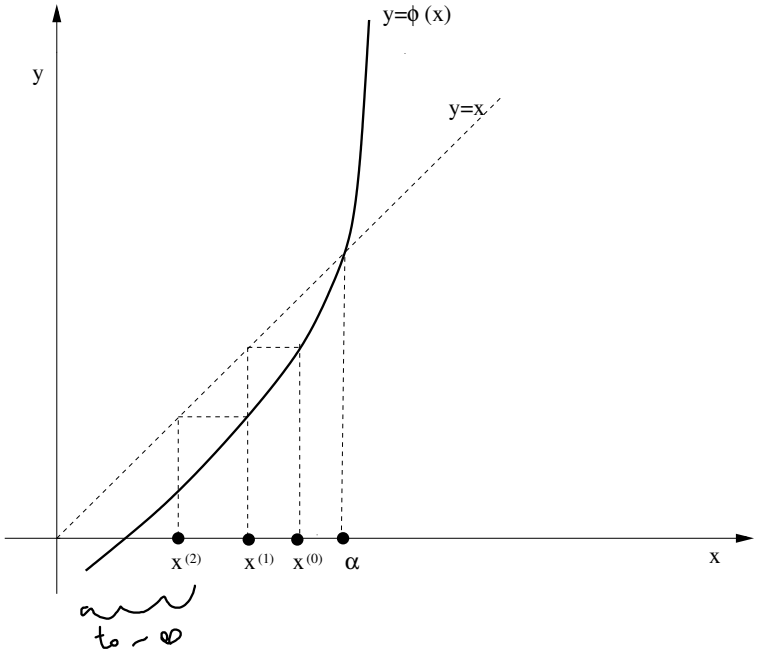
$$0 < \phi'(\alpha) < 1, \qquad -1 < \phi'(\alpha) < 0.$$

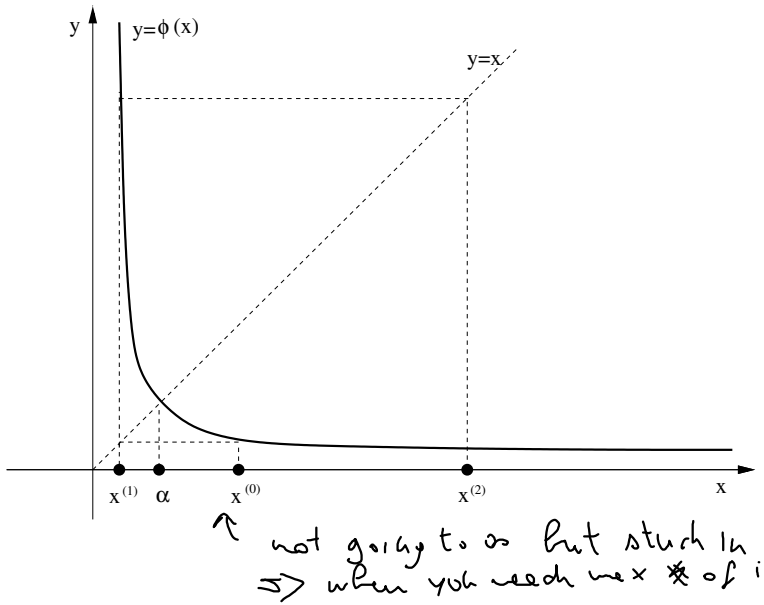




Divergent cases:

$$\phi'(\alpha) > 1, \qquad \phi'(\alpha) < -1.$$



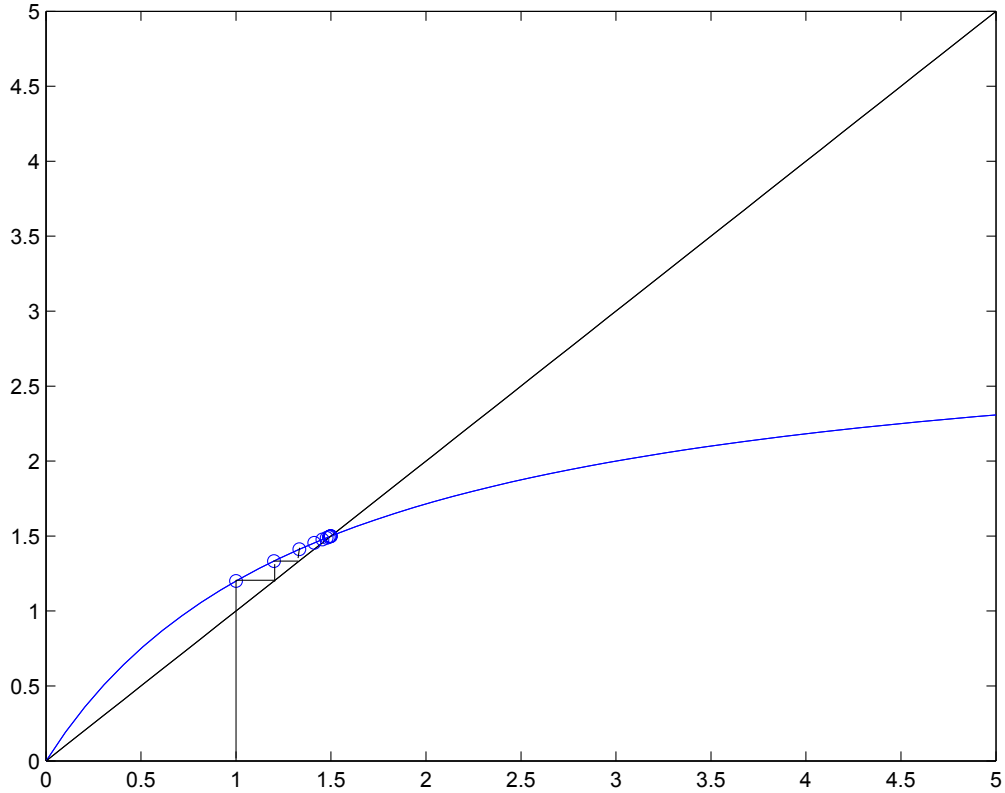


Example. 5 (suite) We apply the fixed point iterations on functions $\phi_2(x) = rx/(1 + x/K)$ and $\phi_3(x) = rx^2/(1 + (x/K)^2)$ that represent the Verhulst model and predator/prey model respectively, with $K = 1.5$ and $r = 2$. We consider the starting point $x^{(0)} = 1.0$.

```
>> phi2=@(x) x.*(2./(1+(x./1.5)));
>> phi3=@(x) x.*(2*x./(1+(x./1.5).^2));
>> x=linspace(0,5,50);
>> figure
>> plot(x,phi2(x),'b',x,x,'k');
>> [p2,res2,niter2]=fixpoint(phi2,1,1e-6,1000);
>> figure
>> plot(x,phi3(x),'b',x,x,'k');
>> [p3,res3,niter3]=fixpoint(phi3,1,1e-6,1000);
```

We find the stationary points $\alpha_2 = 1.5$ and $\alpha_3 = 3.9271$.

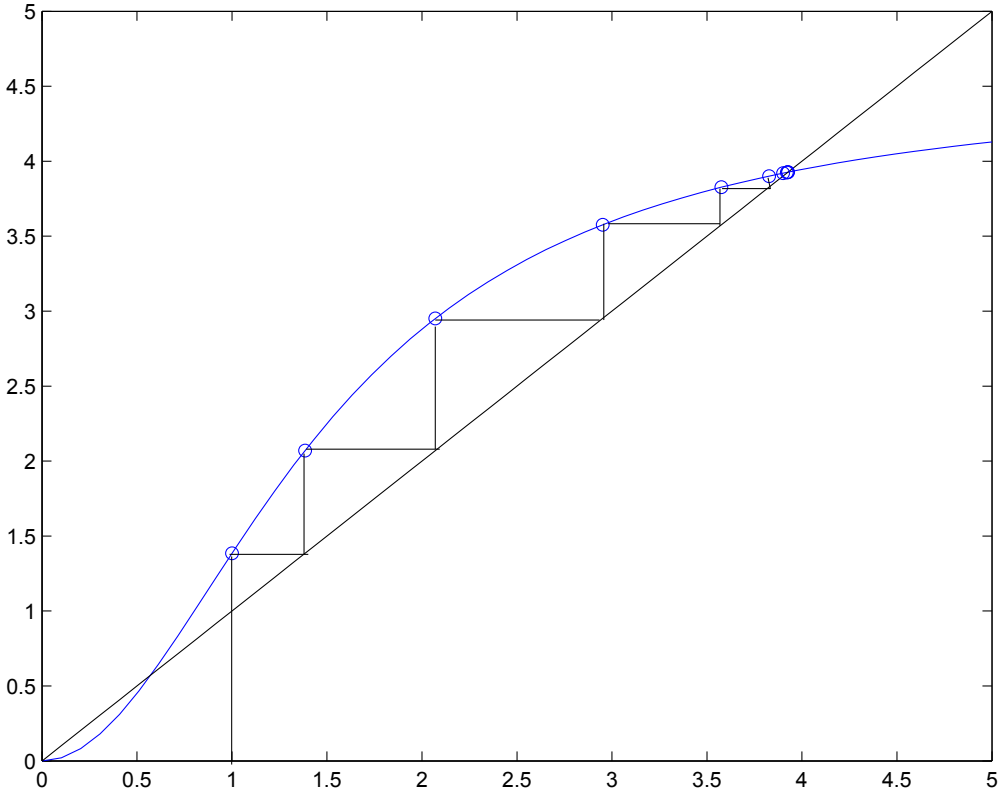
Function $\phi_2(x)$:



Careful to what first index is (0 or 1!)

$$
\begin{aligned}
x^{(0)} &= 1.0000, & |x^{(0)} - \alpha_2| &= 0.5000 \\
x^{(1)} &= 1.2000, & |x^{(1)} - \alpha_2| &= 0.3000 \\
x^{(2)} &= 1.3333, & |x^{(2)} - \alpha_2| &= 0.1667 \\
x^{(3)} &= 1.4118, & |x^{(3)} - \alpha_2| &= 0.0882
\end{aligned}
$$

Function $\phi_3(x)$:



$$
\begin{aligned}
x^{(0)} &= 1.0000, & |x^{(0)} - \alpha_3| &= 2.9271 \\
x^{(1)} &= 1.3846, & |x^{(1)} - \alpha_3| &= 2.5424 \\
x^{(2)} &= 2.0703, & |x^{(2)} - \alpha_3| &= 1.8568 \\
x^{(3)} &= 2.9509, & |x^{(3)} - \alpha_3| &= 0.9761
\end{aligned}
$$

Example. 6 (cont) We have used the fixed point algorithms using the two fonctions ϕ_1 and ϕ_2 with initial value $x^{(0)} = 0.7$. Remember that both have the same fixed point α.

easier, but not working!

$$x = \phi_1(x) = 1 - \sin(2x)$$

because $|\phi_1'(\alpha)| > 1$

! FIRST THING TO CHECK is I deriv!

more difficult but works

$$x = \phi_2(x) = \frac{1}{2}\arcsin(1-x), \qquad 0 \le x \le 1$$

```
>> [p1,res1,niter1]=fixpoint(phi1,0.7,1e-8,1000);
>> [p2,res2,niter2]=fixpoint(phi2,0.7,1e-8,1000);
```

The fixed point algorithm with the first function does not converge, while with the second one it converges to $\alpha = 0.352288459558650$ in 44 iterations. Indeed, $\phi_1'(\alpha) = -1.5237713$ and $\phi_2'(\alpha) = -0.65626645$.

More about the Newton method.

Very good convergence property (QUADRATIC)

Take the rest of Newton method and embed it in the whole fixed point framework

The Newton method is a fixed point method: $x^{(k+1)} = \phi(x^{(k)})$ for the function

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

Let α be a zero of f, i.e. such that $f(\alpha) = 0$. Note that $\phi'(\alpha) = 0$, when $f'(\alpha) \neq 0$. Indeed,

So good because we obtain fixed point with II procedure (less manipulation) and it is consistent with Newton method (II order)

use it one algorithm

image fixed point taking the property of Newton method

QUADRATIC CONVERGENCE to the fixed point which is "testified" by obtaining $\phi'(\alpha) = 0$

$$\phi'(x) = 1 - \frac{[f'(x)]^2 - f(x)f''(x)}{[f'(x)]^2}.$$

if $f'(\alpha) = 0$ UNLUCKY CASE

$\phi'(\alpha) = 1 - \dfrac{[f'(\alpha)]^2 - \overbrace{f(\alpha)}^{=0}\, f''(\alpha)}{[f'(\alpha)]^2}$ (α is root of f)

$= 1 - \dfrac{[f'(\alpha)]^2}{[f'(\alpha)]^2} = 0$

! Important that $\phi''(\alpha) \neq 0$

If this fails to happen failure is of Newton method (it is going to be linear)

↓

Solve by change a little bit the ϕ ft

(DEFLATION METHOD)

↓

modify Newton scheme by making sure that the II derivative $\neq 0$

Theorem 1. *If f is twice differentiable, $f(\alpha) = 0$ and $f'(\alpha) \neq 0$, then there exists $\delta > 0$ such that, if $| x^{(0)} - \alpha | \leq \delta$, the sequence defined by the Newton method converges to α.*
Moreover, the convergence is quadratic; more precisely

$$\lim_{k \to \infty} \frac{x^{(k+1)} - \alpha}{(x^{(k)} - \alpha)^2} = \frac{f''(\alpha)}{2f'(\alpha)}.$$

this represents $\phi''(\alpha)$

Proof. The property of convergence comes from the Proposition 2, while the quadratic convergence is a consequence of the Proposition 3, because

$\phi'(\alpha) = 0$ and $\frac{\phi''(\alpha)}{2} = \frac{f''(\alpha)}{2f'(\alpha)}$.

do second derivative of $\phi(x) = x - \frac{f(x)}{f'(x)}$

⇒ We recover quadratic convergence thanks to info coming from the function without the need to compute $\phi, \phi' \ldots$ but only f', f''

Definition 2. *Let α be a zero of f. α is said to have multiplicity m, $m \in \mathbb{N}$, if $f(\alpha) = \ldots = f^{(m-1)}(\alpha) = 0 \quad$ and $f^{(m)}(\alpha) \neq 0$.*
A zero that has multiplicity $m = 1$ is called simple zero.

$\frac{x^{(k+1)} - \alpha}{x^{(k)} - \alpha}$ IS UNCOMPUTABLE, because every ft empty related to α is UNCOMPUTABLE, since α IS NOT KNOWN

Remark 2. *If $f'(\alpha) = 0$, the convergence of the Newton method is linear, not quadratic. We can use the modified Newton method:*

$$x^{(k+1)} = x^{(k)} - m\frac{f(x^{(k)})}{f'(x^{(k)})}, \quad k = 0, 1, 2 \ldots. \tag{7}$$

at least = 2 since $f'(\alpha) = 0$

where m is the multiplicity of α.

If the multiplicity m of α is unknown, there are other methods, *the adaptive methods*, which can recover the quadratic order of convergence.

Multiplying f by m or reduce f' by m
=> IMPO: you can try to avoid updating f' at each iteration and delay the update of the most expensive computational ptics
↳ ADAPTIVITIES ↗ not free! you pay in ACCURACY

A stopping criterion for Newton

When to stop the Newton method? A good stopping criterion is the **control of the increment** : the iterations is completed when

$$|x^{(k+1)} - x^{(k)}| < \epsilon \tag{8}$$

where ϵ is a fixed tolerance.

Indeed, if we denote $e^{(k)} = \alpha - x^{(k)}$ is the error of the iteration k, we have

$$e^{(k+1)} = \alpha - x^{(k+1)} = \phi(\alpha) - \phi(x^{(k)}) = \phi'(\xi^{(k)})e^{(k)},$$

where $\xi^{(k)}$ is between $x^{(k)}$ and α, and

$$x^{(k+1)} - x^{(k)} \stackrel{\pm\alpha}{=} \alpha - x^{(k)} - \alpha + x^{(k+1)} = e^{(k)} - e^{(k+1)} = \left(1 - \phi'(\xi^{(k)})\right) e^{(k)}. \quad (9)$$

Assuming that if k is large enough, we have $\phi'(\xi^{(k)}) \approx \phi'(\alpha)$ and knowing that the Newton method for $\phi'(\alpha) = 0$, if α is a simple zero, we find the estimation

$$|e^{(k)}| \approx |x^{(k+1)} - x^{(k)}|.$$

The error that we commit when we adopt the criterion (8) is smaller than the fixed tolerance.

Stopping criteria: the general case

In general, for all discussed methods, we can use two different stopping criteria: the iterations is completed when

$$|x^{(k+1)} - x^{(k)}| < \epsilon \qquad \text{(control of the increment)},$$

or

$$|f(x^{(k)})| < \epsilon \qquad \text{(control of the residual)},$$

where ϵ is a fixed tolerance.

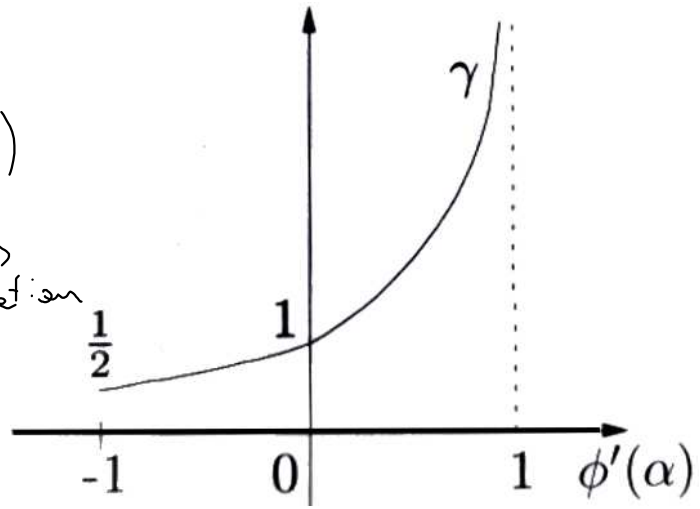
$f(x^{(k)})$ is the RESIDUAL, because $f(\alpha) = 0$, so there we should guarantee the consistency of the methodology

Using fixed point iterations we obtain the following estimation:

$$e^{(k)} \approx \frac{1}{(1-\phi'(\alpha))}(x^{(k+1)} - x^{(k)}).$$

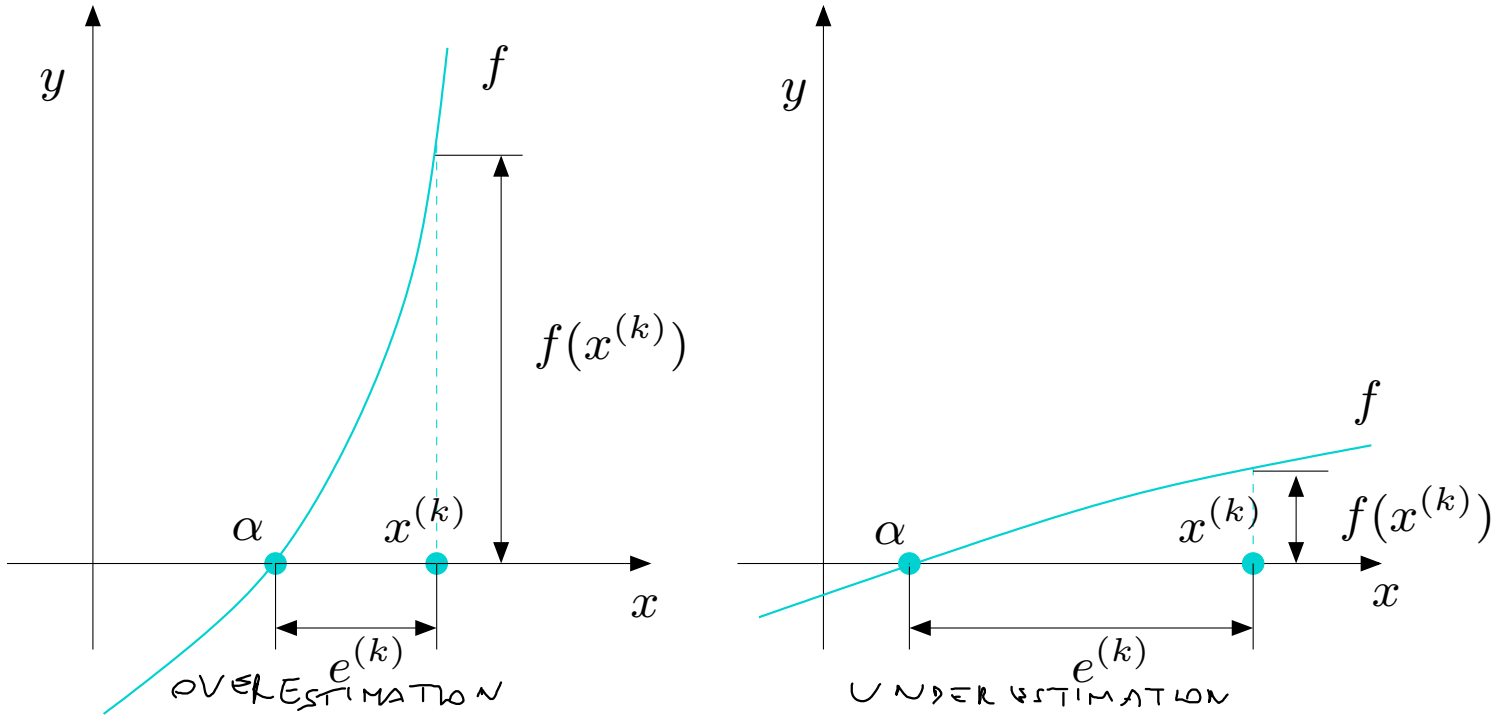
We can plot the graph of $\frac{1}{(1-\phi'(\alpha))}$ and comment on the relevance of the stopping criterium based on the increment:

- if $\phi\prime(\alpha)$ is near to 1 the test is not satisfactory
- for methods of order 2 ($\phi\prime(\alpha) = 0$), the criterium is optimal,
- if $-1 < \phi\prime(\alpha) < 0$ the criterium is still all right.



Stopping Criteria

The stopping criterium based on the control on the residual $|f(x^{(k)})| < \epsilon$ is satisfactory only if $|f'| \simeq 1$ near the root α. Otherwise it is too strong (if $|f'| \gg 1$) or too weak (if $|f'| \ll 1$):



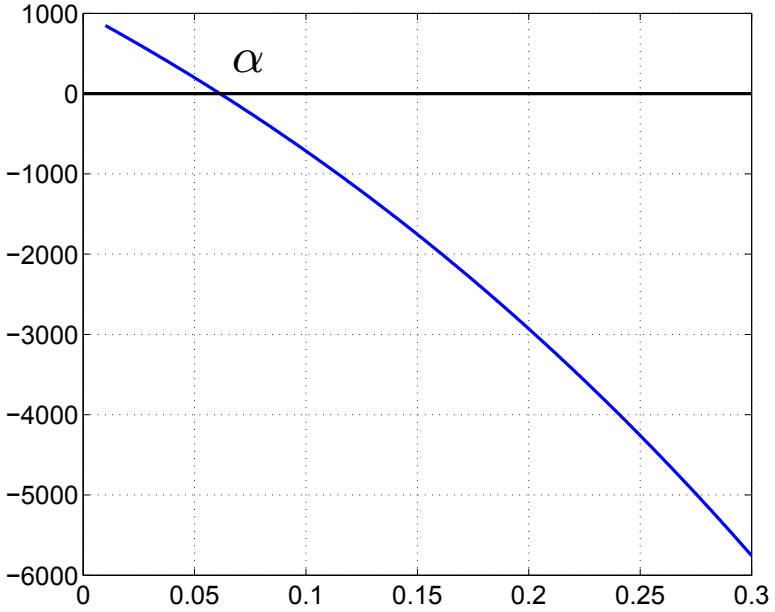
Two cases where the residual is a bad estimator of the error: $|f'(x)| \gg 1$ (left), $|f'(x)| \ll 1$ (right)) with x near to α

MYDEA: if divide $f(x^{(k)})$ by $f'(x^{(k)})$ (normalization)

Applications

Example. 1 (suite) We draw the graph of $f(I) = M - v\frac{1+I}{I}\left[(1+I)^n - 1\right]$ on the interval $[0.010.3]$ with $M = 6000$, $v = 1000$ and $n = 5$:

```
>> f=@(x) 6000-1000*(1+x).*((1+x).^5 - 1)./x;
>> I = [0.01:0.001:0.3];
>> grid on;plot(I,feval(f,x));
```



The root of f is between 0.05 and 0.1.

We can apply the bisection method on the interval $[0.05, 0.1]$ with a tolerance 10^{-5}

```
>> [zero,res,niter]=bisection(f,0.05,0.1,1e-5,1000);
```

The approximate solution after 12 iterations is $\bar{x} = 0.061407470703125$.

We can apply the Newton method with initial guess $x^{(0)} = 0.05$

```
>> df=@(x) 1000*((1+x).^5.*(1-5*x) - 1)./(x.^2);
>> [zero,res,niter]=newton(f,df,.05,1e-5,1000);
```

The result is approximately the same, but we need only 3 iterations

The interest rate is 6.14%.

! If you use Newton Method : you have to give also the I derivative of the nonlinear equation

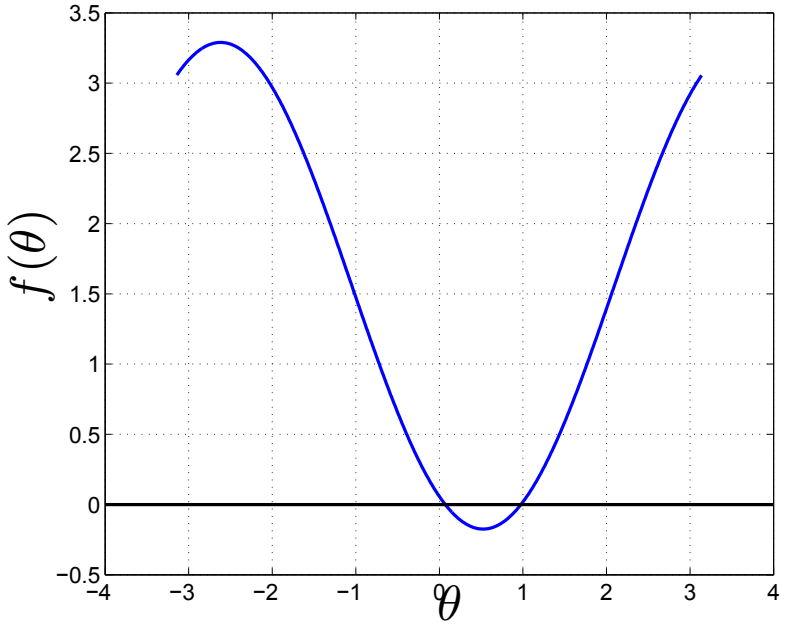
Example. 2 (cont) We would like to plot the angle θ as function of ω for $0 \leq \omega \leq \pi$ with $a_1 = 10\,cm$, $a_2 = 13\,cm$, $a_3 = 8\,cm$, $a_4 = 10\,cm$.
For each ω, we have to solve the nonlinear poblem

$$f(\theta) = \frac{a_1}{a_2} cos(\omega) - \frac{a_1}{a_4} cos(\theta) - cos(\omega - \theta) + \frac{a_1^2 + a_2^2 - a_3^2 + a_4^2}{2a_2a_4} = 0. \qquad (10)$$

To start with, we plot the graph of $f(\theta)$ for $\omega = \pi/3$:

```
>> F = @(x, a1, a2, a3, a4, omega) ...
       (a1/a2)*cos(omega) - (a1/a4)*cos(x) - cos(omega-x) ...
     + ( (a1.^2 + a2.^2 - a3.^2 + a4.^2) / (2*a2*a4) );
>> a1=10; a2=13; a3=8; a4=10; omega=pi/3;
>> f = @(x) F(x,a1,a2,a3,a4,omega);
>> x = [-pi:0.01:pi];
>> plot( x, f(x) ); grid on;
```

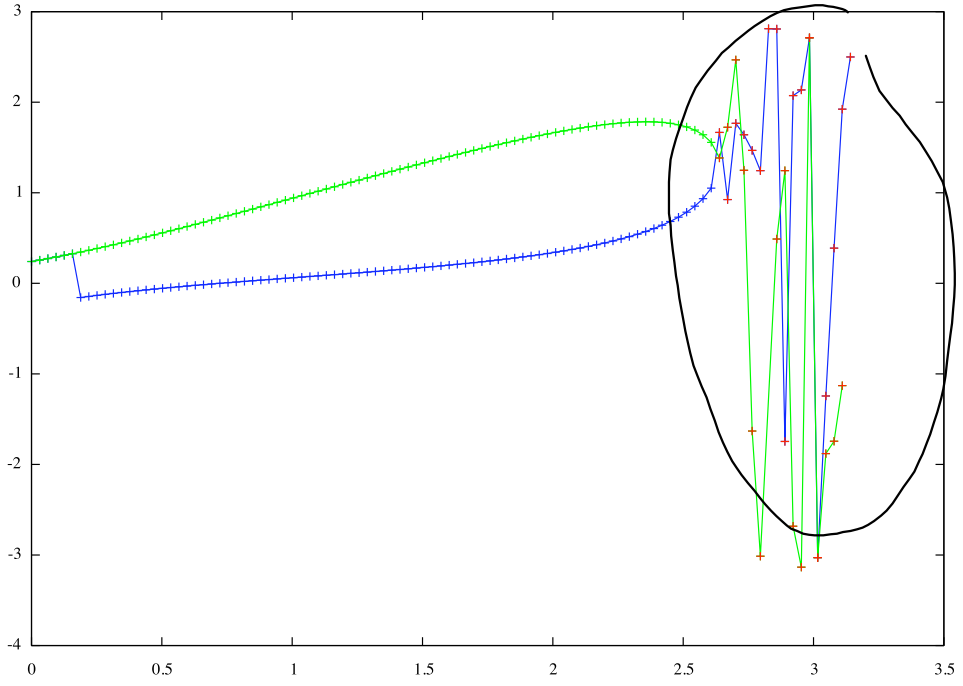
Function f with $\omega = \pi/3$.



We have two roots, which means that we have two possible configurations.

Now we chose 101 different values for ω, $\omega_k = k\frac{\pi}{100}$, $k = 0, \ldots, 100$ and for each of them solve the nonlinear problem (10) with the Newton method. Since we know that we may have two distinct solutions, we give two different initial guesses to our Newton method. For example $\theta_{01} = -0.1$ and $\theta_{02} = 2/3\pi$

The following figure shows the solutions as function of ω.
For $\omega > 2.6358$, the Newton algorithm does not converge anymore. In fact, with these values there is no configuration possible



no solution, but INCONSISTENT BEHAVIOR of MECHANICAL SYSTEM oscillation due to numerical wire : NOT PHYSICAL

Here are the Matlab/Octave commands that we have used:

```
>> n=101; x01=-0.1; x02=2*pi/3; nmax=100;
>> dF = @(x,a1,a2,a3,a4,w) a1/a4*sin(x)-sin(w-x);
>> for k=1:1:n
    omega(k) = (k-1)*pi/100;
    f  = @(x)  F(x,a1,a2,a3,a4,omega(k));
    df = @(x) dF(x,a1,a2,a3,a4,omega(k));
    [theta1(k),res,niter] = newton(f,df,x01,1e-5,nmax);
    [theta2(k),res,niter] = newton(f,df,x02,1e-5,nmax);
   end
>> plot(omega,theta1,'b:',omega,theta2,'g-')
```

Example. 3 (suite) We consider the carbon dioxide (CO_2), for which $a = 0.401\ Pa\,m^6$ and $b = 42.7 \cdot 10^{-6}\ m^3$.
We search the volume occupied by $N = 1000$ molecules of CO_2 in temperature $T = 300\ K$ and pressure $p = 3.5 \cdot 10^7\ Pa$. We know that the Boltzmann constant is $k = 1.3806503 \cdot 10^{-23}\ Joule\,K^{-1}$.

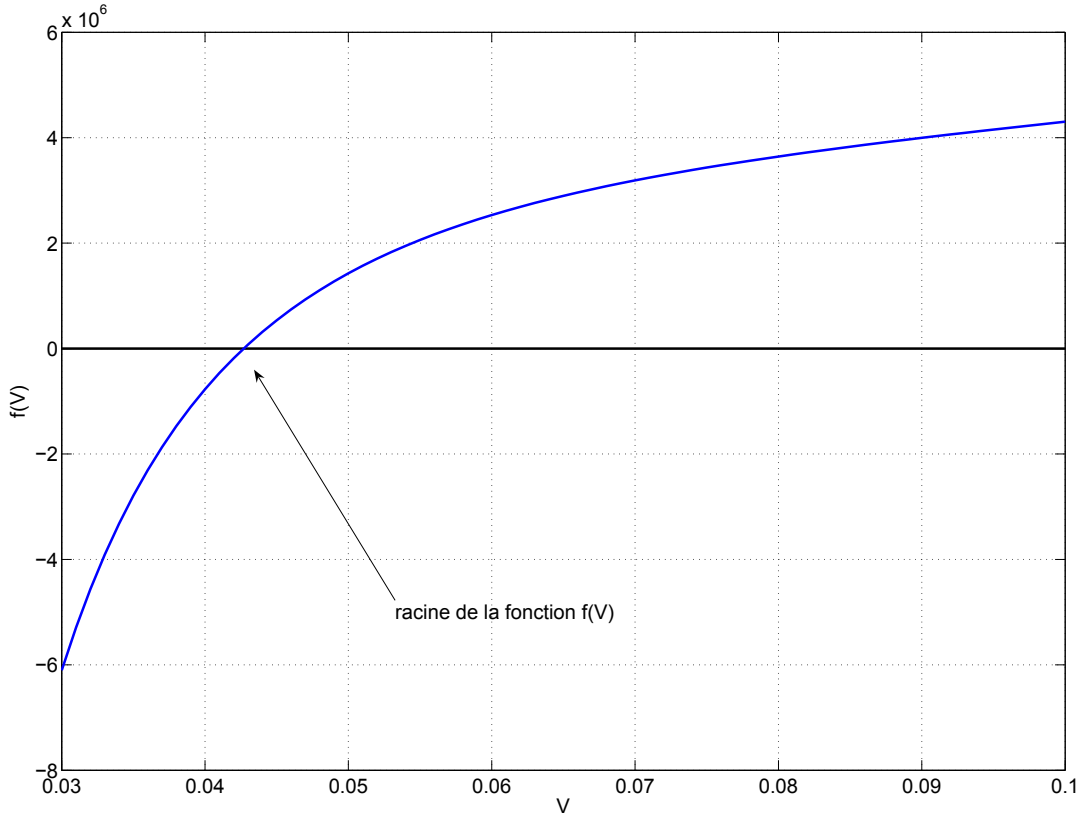
We draw the graph of the function

$$f(V) = \left[p + a\left(\frac{N}{V}\right)^2\right](V - Nb) - kNT$$

for $V > 0$. We do not consider $V < 0$ (it does not have physical meaning), because V is the volume of gas.
We use the commands in Matlab/Octave:

```
>> a=0.401; b=42.7e-6; p=3.5e7; T=300; N=1000; k=1.3806503e-23;
>> f = @(x,p,T,a,b,N,k)(p+a*((N./x).^2)).*(x-N*b)-k*N*T;
>> x=[0.03:0.001:0.1];
>> plot(x,f(x,p,T,a,b,N,k))
>> grid on
```

We obtain the graph of the function $f(V)$:



We see that there is a zero for $0.03 < V < 0.1$. If we apply the bisection method on the interval $[0.03, 0.1]$ with a tolerance 10^{-12}:

```
[zero,res,niter]=bisection(f,0.03,0.1,1e-12,1000,p,T,a,b,N,k);
```

then we find, after 36 iterations, the value $V = 0.0427$.
If we use the Newton method with the same tolerance, starting form the initial point $x^{(0)} = 0.03$,

```
>> df = @(x,p,T,a,b,N,k) -2*a*N^2/(x^3)*(x-N*b)+(p+a*((N./x).^2));
>> [zero,res,niter]=newton(f,df,0.03,1e-12,1000,p,T,a,b,N,k);
```

then we find the same solution after 6 iterations.
The conclusion is that the volume V occupied by the gas is $0.0427\ m^3$.

The rope method

This method is obtained by replacing $f'(x^{(k)})$ by a fixed q in the Newton method:

$$x^{(k+1)} = x^{(k)} - \frac{1}{q} f(x^{(k)}), \quad k = 0, 1, 2 \ldots . \tag{11}$$

We can take, for example, $q = f'(x^{(0)})$ or $q = \dfrac{f(b) - f(a)}{b - a}$, in the case when we search a zero in the interval $[a, b]$.

Example. 6 (suite) We apply the rope method and the Newton method to find the zero of f.

The rope method in the interval $[-1, 1]$, with $x^{(0)} = 0.7$:

```
>>  [zero,res,niter]=chord(f,-1,1,0.7,1e-8,1000)
```

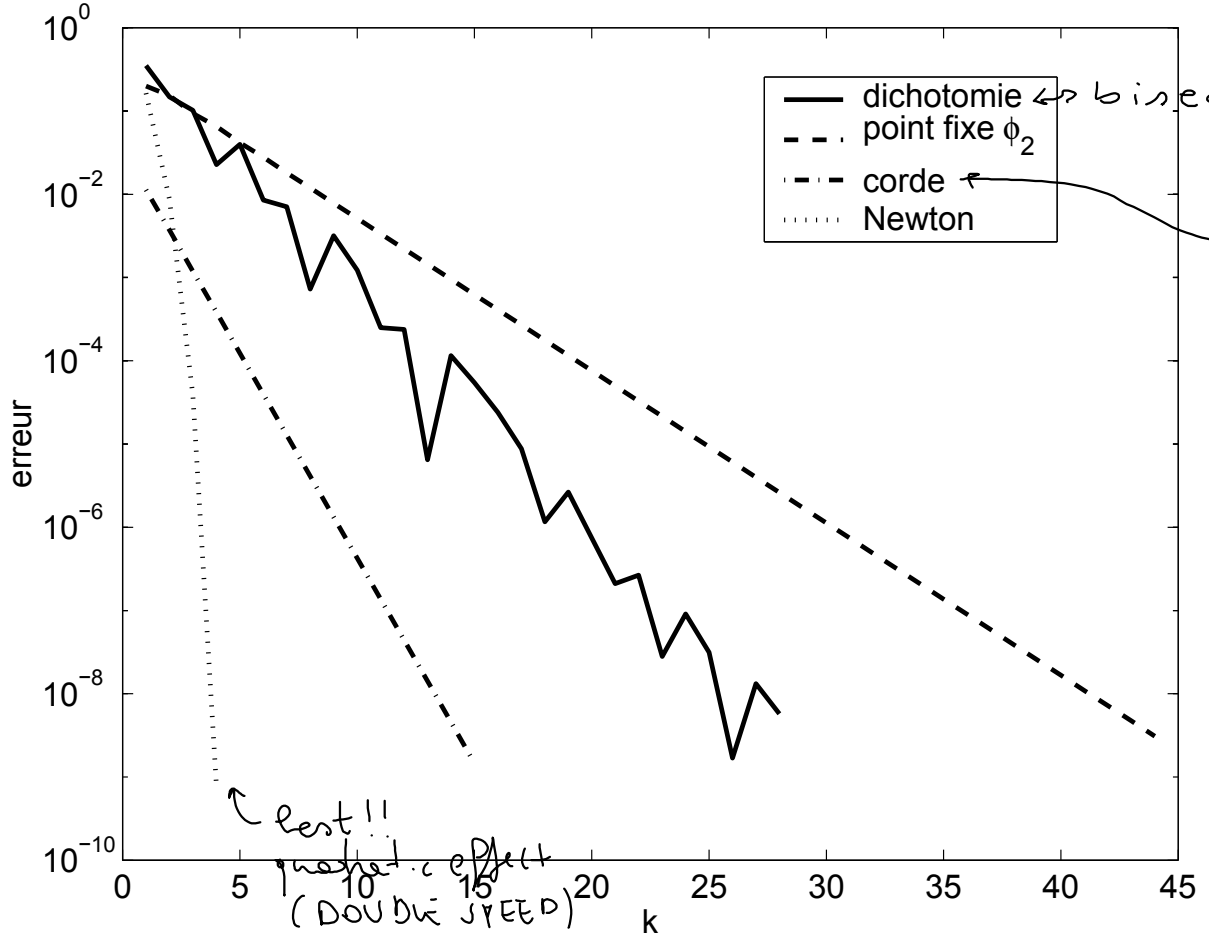
We find the result after 15 iterations.

The Newton method with the same $x^{(0)}$:

```
>>  df = @(x) 2*cos(2*x) + 1;
>>  [zero,res,niter]=newton(f,df,0.7,1e-8,1000);
```

We find the result after 5 iterations. Much faster.

Values of the errors plotted versus the number of iterations for 4 methods: bisection, fixed point ϕ_2, rope and Newton. There is logarithmic scale on the axis y.



Remark 3. *The rope method is also a fixed point method for*

$$\phi(x) = x - \frac{1}{q} f(x).$$

So, we have $\phi'(x) = 1 - \frac{1}{q} f'(x)$ *and thanks to the Proposition 2, we obtain that the method converges if the following condition is satisfied:*

$$| \, 1 - \frac{1}{q} f'(\alpha) \, | < 1 \, .$$

Lecture 11 - LH

5 Nov 2020

we want n to be ~~one~~ of interpolation => # of pts = # of basis fcts

Recap on interpolation: 1) a set of interpolation points $\{x_i\}_{i=0}^n$

2) a set of basis functions $\{v_i\}_{i=0}^n$

Interpolation of $f \in C^0([a,b])$ $x_i \in [a,b]$ $\forall i$

on the space $V = \text{span}\{v_i\}_{i=0}^n$ is defined as the solution to:

find p in V s.t. $p(x_i) = f(x_i)$ $\forall i$

Given $\{x_i\}_{i=0}^n$ best choice for $\{v_i\}_{i=0}^n$ is Lagrange basis

$$\Rightarrow \quad v_i(x) = \prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{(x - x_j)}{(x_i - x_j)}$$

So the interpolation poly becomes

$$p = \sum_{i=0}^{n} v_i(x) f(x_i) := \mathcal{L}^n f$$

Next step was:

Try to find the "best" set of $\{x_i\}_{i=0}^n$

Remember that L^2 [illegible] monic poly

best approx

$$\|\mathcal{L}^n f - f\|_\infty = \|\mathcal{L}^n(f - p) + p - f\|_\infty \leq \left(\|\mathcal{L}^n\|_* + 1\right) \|p - f\|_\infty$$

when Lagrange basis function is used

$$\|\mathcal{L}^n\|_* \leq \|\Lambda(\{x_i\}_{i=0}^n)\|_\infty$$

We try to min the sum of the absolute values of the basis fct (as before)

$$\Lambda := \sum_{i=0}^{n} |v_i|$$

← Lebesgue function

For Chebyshev points:

$$\frac{2}{\pi} \log(n+1) - c \leq \|\Lambda\|_\infty \leq \frac{2}{\pi} \log(n+1) + 1$$

Erdos — Phelyphen

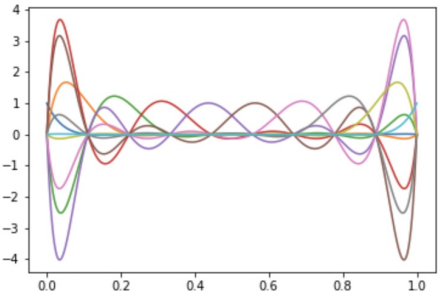
⚠ True only if the function is continuous

If you add more regularity, you get better things (Result for analytically extendable fct, with continuous derivatives up to the n-th derivative)

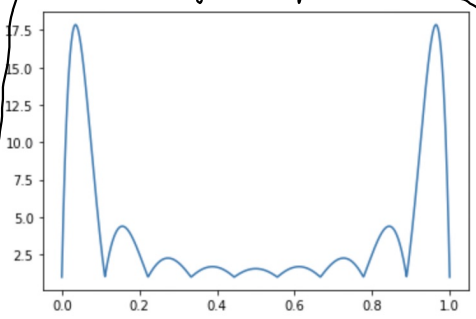
⚠ INTERPOL IS EXACT AT POINT OF INTERPOL

⇒ try to get exact approx every where in not exact way

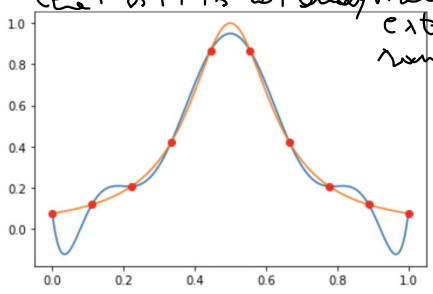
USING EQUISPACED PTS



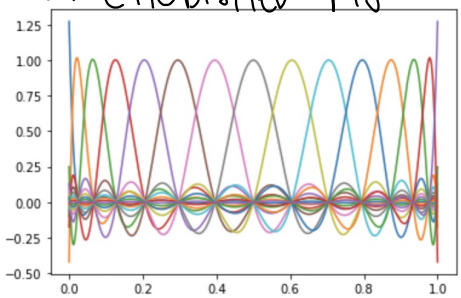
Lebesgue function

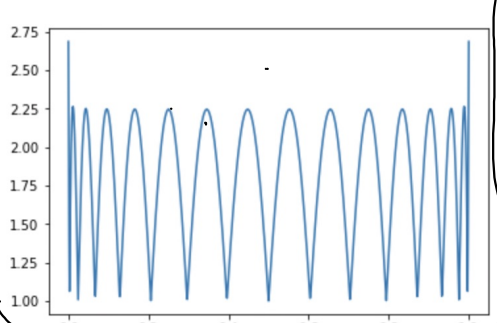


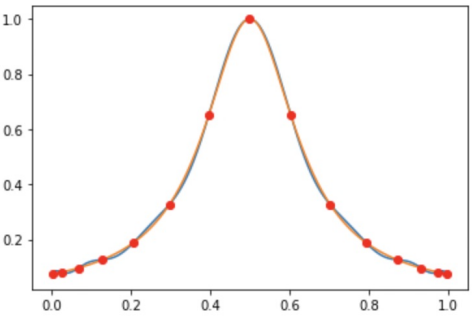
tells us if the pt is wrong that is it is not only totally extendible somehow



USING CHEBISHEV PTS







If interpolation is not good, what can we do in $C^0([a,b])$?

Yes: **Weierstrass Approximation Theorem**

$\forall f \in C^0([a,b])$, $\forall \varepsilon > 0$, $\exists n$, $p \in \mathbb{P}^n$, s.t. $\|f-p\|_\infty < \varepsilon$

~~No matter what f you can always find a p such that p approx f~~

Proof: Let B_n be a sequence of linear operators s.t.

1) B_n positive linear operators $C([a,b]) \to \mathbb{P}^n([a,b])$

2) $B_n q \to q$ pointwise $\forall q \in \mathbb{P}^2([a,b])$ that is only for quadratic polys

Then: **$B_n f$ converges uniformly to f $\forall f \in C^0([a,b])$**

An op is defined positive

N.B: B_n is "positive" if $q(x) \geq 0 \Rightarrow (B_n q)(x) \geq 0$ in $[a,b]$

(if $q(x) \leq 0$ it remains negative if B is positive)

Part 1:

- $\forall f \in C^0([a,b])$, $\forall x_0 \in [a,b]$:
- construct $q^\pm \in \mathbb{P}^2$ s.t. $q^-(x_0) < f(x_0) < q^+(x_0)$ $\forall x$.
- use $B_n q^\pm \to q^\pm$
- use $B_n(f-q^-)(x_0) > 0$ $B_n(q^+-f)(x_0) > 0$

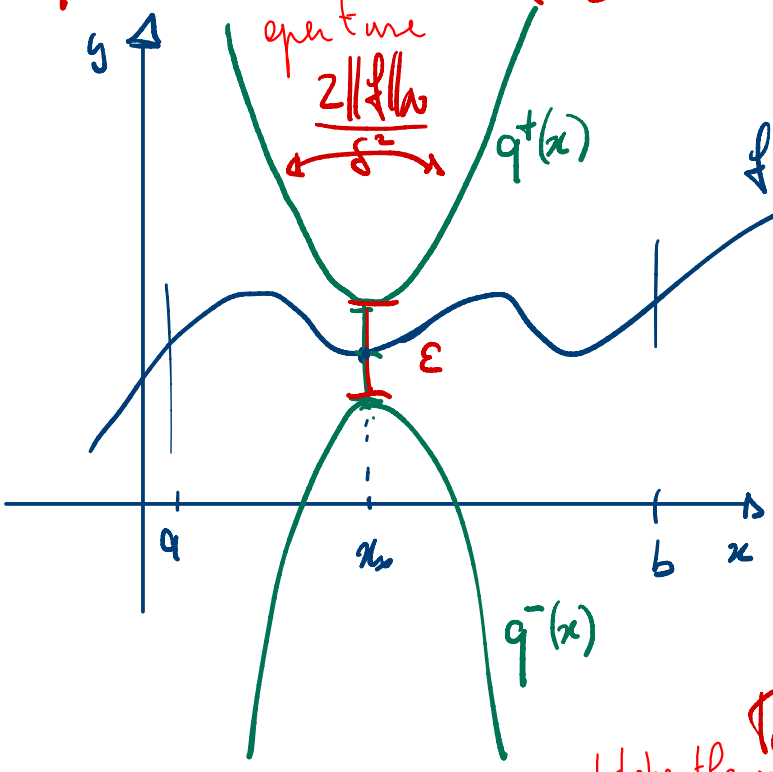
$f \in C^0([a,b]) \Rightarrow \forall \varepsilon > 0, \exists \delta > 0$

$|x_1 - x_2| \le \delta \rightarrow |f(x_1) - f(x_2)| \le \varepsilon$ } def of continuity!

Define

$$q^{\pm} := f(x_0) \pm \left(\frac{\varepsilon}{2} + \frac{2\|f\|_\infty}{\delta^2}(x - x_0)^2 \right)$$

← Constructing $q^\pm$ in this way guarantees that they are always ε/2 far from f



for varying x_0

$q^\pm(x) = a^\pm x^2 + b^\pm x + c^\pm$

$a^\pm, b^\pm, c^\pm$ depend on $x_0, \|f\|_\infty, \delta, \varepsilon$

Take $M = \max_{x_0 \in [a,b]} \left(|a^\pm|, |b^\pm|, |c^\pm| \right)$

(I take the max over the entire interval)

M depends on $\|f\|_\infty, \delta, \varepsilon$, but Not on x_0

Choose N large enough s.t. $\left\| B_n x^i - x^i \right\|_\infty \le \frac{\varepsilon}{6M}$ $\forall n > N$ for $i = 0,1,2$

($\exists N$ s.t. this is possible)

Since we might that this condition must hold for each of the two (HYPOTHESIS!)

$\Rightarrow \forall x_0$ $\left\| B_n q^\pm - q^\pm \right\| \le \frac{\varepsilon}{2}$ $\forall n \ge N$

M controls every coeff => this allows to say that $\frac{\varepsilon}{6M} \le \frac{\varepsilon}{2}$ (!)

in x_0 $f(x_0) - \varepsilon \le q^-(x_0) - \frac{\varepsilon}{2} \le B_n q^-(x) \le B_n f(x_0)$

Definition of q^- — positivity

And repeat for the reversed inequality:

$\forall x_0, \exists N$ s.t. $\forall n \ge N$ $B_n f \le B_n q^+ \le q^+ + \frac{\varepsilon}{2} \le f(x) + \varepsilon$

$$\left\| B_n f - f \right\| \le \varepsilon$$

How to define B_n ? Let $(a,b] = [0,1]$

Trick : Consider $\left((1-x)+x\right)^n = \sum_{i=0}^{n} \binom{n}{i} x^i (1-x)^{n-i}$ polynomial of degree n

$= \sum_{i=0}^{n} v_i(x)$ ($\Leftarrow 1$ defines basis functions)

$$v_i(x) = \binom{n}{i} x^i (1-x)^{n-i}$$

Bernstein polynomials.

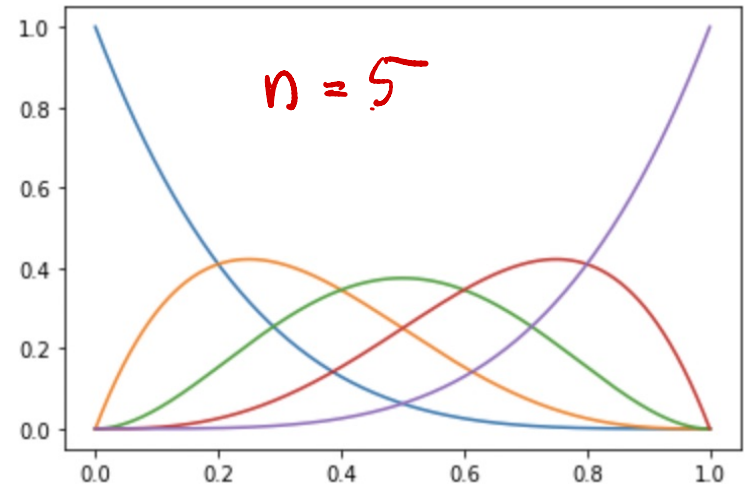
- $B_n f := \sum_{i=0}^{n} v_i(x) f\left(\frac{i}{n}\right)$ (def) — difference between interpolation and this

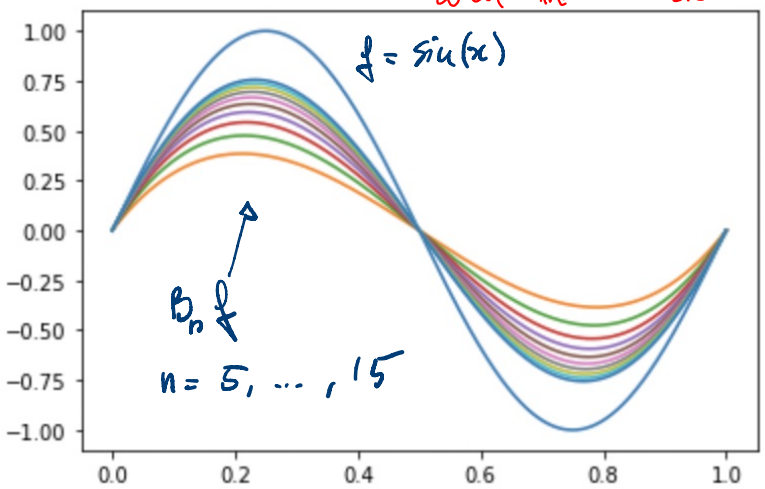
$f \geq 0 \Rightarrow B_n f \geq 0$ because v_i positive

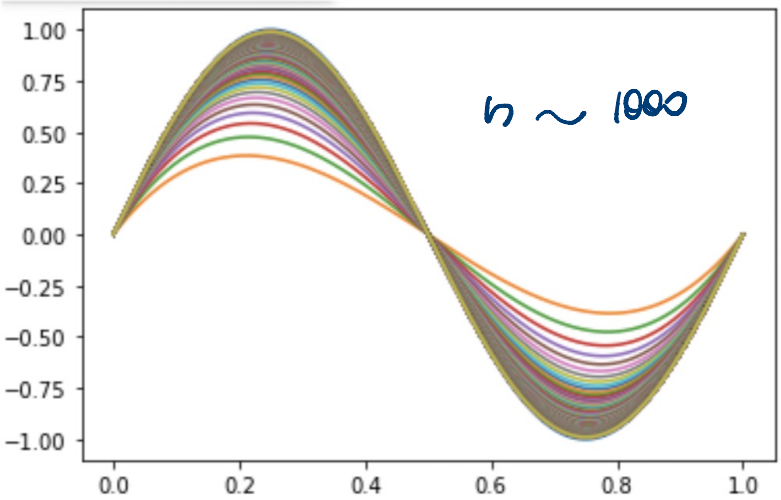
v_i always positive in $(0,1)$ but are also $\neq$ from 0 in all the interval but 0 or 1

You cannot say that the v_i are interlacing at any pt but 0 and 1

- $B_n x = x$ $\quad B_n 1 = 1$
- $B_n x^2 = \left(\frac{n-1}{n}\right) x^2 + \frac{1}{n} x \neq x^2$ for large n still $\neq x^2$ but $n \to \infty$ $B_n x^2 \to x^2$







We don't have a quick convergence

Lecture 12 — PROJECTION BASE APPROX METHOD — 10. Nov. 2020

1) Approximate and measure using L^2 norm (vs L^∞) ← derived from a scalar product

→ Scalar product : $u, v \in L^2([0,1])$,

$$(u,v) := \int_0^1 u \cdot v \, dx$$

$$\|a+b\|^2 = (a+b, a+b) = \|a\|^2 + \|b\|^2 + 2(a,b)$$

↝ $$\|u\|^2_{L^2([0,1])} \equiv \|u\|^2 := (u,u) = \int_0^1 |u|^2 dx$$

Let's assume we have $V := \text{span}\{v_i\}_{i=0}^n$, and $\|\cdot\|$.

The best approximation of $u \in L^2([0,1])$ in V satisfies:

$p \in V$ s.t. $(u-p, v) = 0 \quad \forall v \in V$

best approx

$(u-p,v) = 0 \ \forall v \in V \iff p$ is B.A. of u in V

Proof: Assume p is best approx $\Rightarrow (u-p,v) = 0 \ \forall v \in V$

by def of B.A.

$$\|u-p\|^2 \leq \|u - p + tq\|^2 \quad \forall t > 0, \ \forall q \in V$$

↑ if I move in any direction from p I get bigger distance from f to interpolant

$$\|u - p + tq\|^2 - \|u-p\|^2 \geq 0$$

$(a+b)^2 - (a-b)^2 = 4(a,b)$

$$\|\underbrace{(u-p+\tfrac{t}{2}q)}_{a} + \underbrace{(\tfrac{t}{2}q)}_{b}\|^2 - \|\underbrace{u-p}_{a-b}\|^2 \geq 0$$

$a = u - p + \frac{t}{2}q$

$b = \frac{t}{2}q$

$$2\cancel{4}\left(u - p + \tfrac{t}{2}q, \tfrac{t}{2}q\right) \geq 0$$

Linearity of scalar prod in I argument

$$0 \leq 2(u-p, q)t + t^2(q,q)$$

We have a symmetry for: $q \to -q$

$$-\frac{t}{2}\|q\|^2 \leq (u-p,q) \leq \frac{t}{2}\|q\|^2$$

$\forall t > 0$
$\forall q \in V$

$$\Rightarrow \boxed{(u-p,q) = 0}$$

Assume now $^* \; (u - p, v) = 0 \quad \forall v \in V \implies p$ is B.A.

$$\|u - v\|^2 = \|u - p + p - v\|^2 = \|u - p\|^2 + \|p - v\|^2 + 2(u-p, p-v)$$

$(u-p, p-v) \to 0$ by $*$ and the fact that $u - p \perp p$

$$\implies \|u - p\|^2 \le \|u - v\|^2 \quad \forall v \in V$$

that is p is B.A. of u in V — $(u - p, p) = 0$: the error is to be ortogonal to the BA, otherwise I can move the direction of ortogonality to improve accuracy

---

B.A. (weeny) V: Find $p \in V$ s.t.

1) $(p, v) = (u, v) \quad \forall v \in V$

you can write $p(x) = \sum p^J v_J(x)$ $\quad (\forall p \in V \;\; \exists! \{p^i\}_{i=0}^{n}$ s.t. $p = p^i v_i)$ because the space is finite dimensional and generated by basis of v_i

$\implies$ 2) $(p^J v_J, v_i) = (u, v_i) \quad i = 0, \dots, n$

MASS MATRIX

$$\underline{\underline{M}} \; \underline{p} = \underline{U}$$

$$M_{iJ} \, p^J = U_i$$

$$M_{iJ} = (v_i, v_J)$$

$$U_i = (u, v_i)$$

compute this $\implies$ to solve the probl.

$$p^J = \underline{M^{Ji}} \, U_i$$

Example:

$$V = \text{span}\{\text{pow}(x, i)\}_{i=0}^{n} \qquad p = \sum_J p^J x^{(J)} \quad \text{power basis}$$

then

$$M_{iJ} = \int_0^1 x^i \cdot x^J \, dx = \int_0^1 x^{(i+J)} \, dx = \frac{1}{i+J+1}$$

M here is called Hilbert Matrix: $\quad \text{cond.}(H) \simeq \dfrac{(1+\sqrt{2})^{4n}}{\sqrt{n}}$ $\leftarrow$ it is terribly conditioned matrix

If i or J very large $\implies$ columns or rows become similar ($i+J+1 \sim i-1+J+1 \dots$

What's the best possible "M" matrix?

$$\text{Identity}: \quad M_{iJ} = \delta_{iJ} = \begin{cases} 1 & \text{if } i = J \\ 0 & \text{if } i \neq J \end{cases}$$

Def B.A. in a space with norm defined from scalar product, select basis function and try to compute mass matrix

⇓

B.S. in a finite dim space (spanned by some basis fct) what you obtain is

$$\underline{\underline{M}}\,\underline{p} = \underline{U}$$

=> best pt is the one in which you don't have to write any matrix => possible if $\underline{\underline{M}} = \underline{\underline{\mathbb{1}}}$

=> $\varphi_i = (u, v_i)$

↓

Simplest procedure

GRAM SCHMIDT PROCEDURE

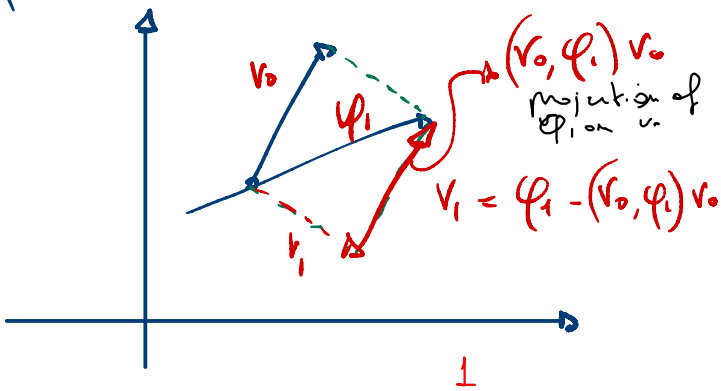
Let's try to find an orthonormal basis

Set $v_0 = 1$ (start with I el of basis) $\longrightarrow$ $\left(\int_0^1 (1)^2 dx\right)^{\frac{1}{2}} = 1$

$$\varphi_{i+1} = \hat{x}\, v_i - \sum_{j=0}^{i-1} \left(\hat{x} v_i, v_j\right) v_j$$

and normalize

$$v_{i+1} = \frac{\varphi_{i+1}}{\|\varphi_{i+1}\|}$$

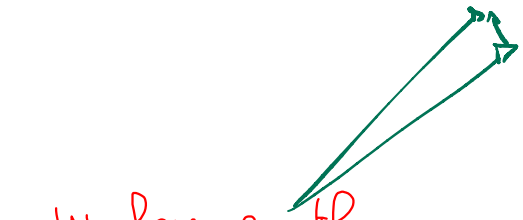


Possible problems:

$$\|\varphi_i\|^2 = \|\hat{x} v_0\|^2 + (\hat{x} v_0, v_0)^2 \underbrace{\|v_0\|^2}_{1} - 2(\hat{x} v_0, v_0)^2$$

$$= \|\hat{x} v_0\|^2 - (\hat{x} v_0, v_0)^2$$

This can be very small!!



We have another solution which does not ask same norm: $\theta_{ij} \neq \delta_{ij}$

but it is diagonal:

Bonnet recursion: $P_0 = 1 \quad P_1 = x$

$$(n+1) P_{n+1}(x) = (2n+1)\, x P_n(x) - n P_{n-1}(x)$$

(Bonnet)

→ Are orthogonal in $[-1, 1]$, and

$$P_n(1) = 1 \quad \forall n$$

(dim (1) (start from fact that P_0, P_1 are ok))

"The only" thing which is left to do is to compute

$$\int_0^1 u\, P_i\, dx$$

Approximate integrals.

Between functions you def the error as $\|p(x) - u(x)\|$ where $\|\cdot\|$ is the norm used.

Lecture 13

12.11.2020

Recap of Lec 12: Given $u \in L^2([0,1])$, find $p \in V = \text{span}\{v_i\}_{i=0}^{n}$ s.t.

$$(p, v) = (u, v) \quad \forall\, v \in V$$

$$\Rightarrow \sum_j \left(p^j v_j, v_i\right) = (u, v_i) \qquad i = 0, \dots, n$$

Rewritable as a system $\Rightarrow \underline{\underline{M}}\,\underline{p} = \underline{U}$

$$M_{ij} := (v_i, v_j)$$

$$U_i = (u, v_i)$$

$$(a,b) := \int_0^1 a \cdot b \, dx$$

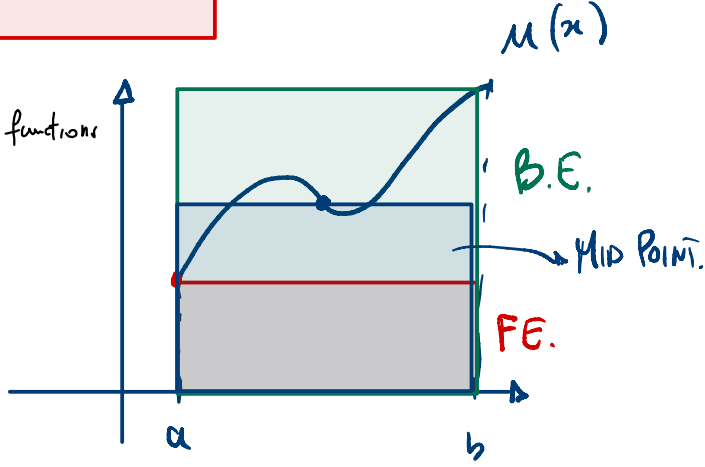
Induces a norm $\Rightarrow \|a\|^2 = (a,a) \Rightarrow \|a\| = \left(\int_0^1 a^2 dx\right)^{\frac{1}{2}}$

Today: Approximate $\int_a^b u(x)\, dx$

For now: $u \in C^0([a,b])$

Rough approx schemes for $C^0([a,b])$ functions

For example:
- FE (Forward Euler)
- BE (Backward Euler)
- MIDPOINT



We have, for each scheme

FE: $\int_a^b u(x) \simeq u(a)(b-a)$

BE: $\int_a^b u(x) \simeq u(b)(b-a)$

MIDPOINT: $\int_a^b u(x) \simeq u\left(\frac{a+b}{2}\right)(b-a)$

You don't use just one of them, but you apply all the three, one for each special case (such as particular sub interval of $[a,b]$)

Interpolatory Quadrature Rules:

$$I(u) := \int_a^b u(x)\, dx$$

$$I_n(u) := \sum_{i=0}^{n} u(q_i)\, w_i \simeq \int_a^b u(x)\, dx = I(u)$$

q_i: quadrature points; w_i: weights

if you choose correctly both q_i and w_i

If we want to integrate we can choose $\{q_i\}_{i=0}^n$ and $\{w_i\}_{i=0}^n$ — $2(n+1)$ unknowns

Most popular choices: Given $\{q_i\}_{i=0}^n$, construct interpolatory quadrature rule

Lagrange interpolation of u function → $\mathcal{L}^n u$ and integrate (exactly!) $\mathcal{L}^n u$

$$\Rightarrow \boxed{I^n(u) = \int_0^1 (\mathcal{L}^n u)(x)\,dx}$$

where $\mathcal{L}^n u = \sum_{i=0}^n u(q_i)\,\ell_i(x)$ ← choose the weights

"Bimi"

$$\ell_i = \prod_{\substack{j=0 \\ j\neq i}}^n \frac{(x-q_j)}{(q_i-q_j)}$$

$$\Rightarrow \boxed{I^n(u) = \int_0^1 \sum_{i=0}^n u(q_i)\,\ell_i(x)\,dx} = \sum_{i=0}^n u(q_i) \underbrace{\int_0^1 \ell_i(x)\,dx}_{w_i}$$

(doesn't depend on x)

number independent on the function I'm trying to integrate

$$= \boxed{\sum_{i=0}^n u(q_i)\,w_i}$$

FE, B.E., Mid Point are all interpolatory quadrature rules with $\mathbb{P}^0$ polynomial approximation

↳ that is with only 1 quadrature pt

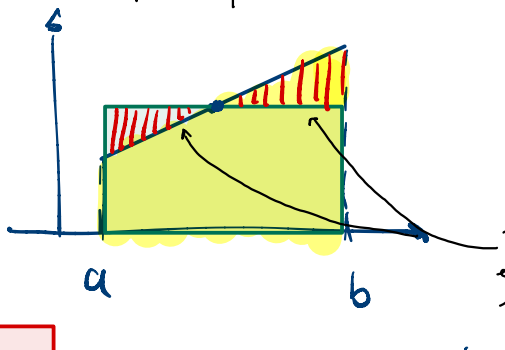
Teo 1 Interpolatory quadrature rules with $n+1$ points are exact at least for polynomials of order $\leq n$

Proof: $\forall p \in \mathbb{P}^n$ (polyn. of ord. n), $\mathcal{L}^n p = p$ by construction

$$\Rightarrow I(p) = I^n(p) \quad \forall p \in \mathbb{P}^n$$

Degree of accuracy of I^n is the maximum integer k s.t. $I(p) = I^n(p)$ $\forall p \in \mathbb{P}^k$

For the midpoint quadrature rule



$$I^0(p) = I(p) \quad \forall\, p \in \mathbb{P}^1$$

at least one case where $k > n$

Theo Given $\{q_i\}_{i=0}^{n}$, degree of accuracy is $\leq 2(n+1)$

proof: construct $\omega(x) = \prod_{i=0}^{n} (x - q_i)$ (polynomial), $\omega \in \mathbb{P}^{n+1}$

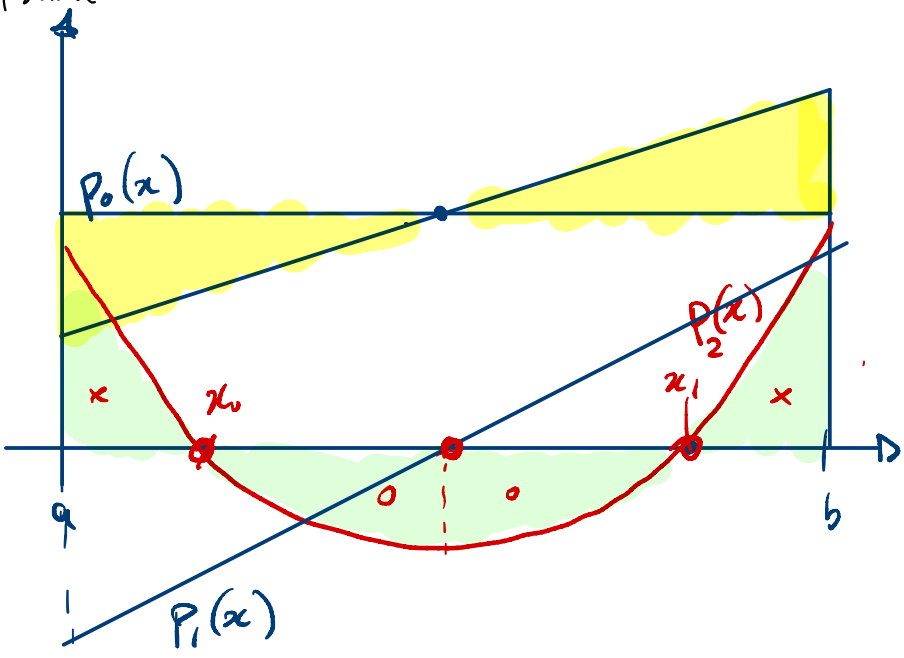
$\omega^2(x) > 0 \quad \forall x \neq q_i$, $\omega(q_i) = 0 \quad i = 0, \dots, n$

$\Rightarrow I(\omega^2) > 0$ $\quad I^n(\omega^2) = 0$ (because) by construction.

$\Rightarrow \exists\, p = \omega^2 \in \mathbb{P}^{2n+2}$ s.t. $I(p) \neq I^n(p)$

Can the degree of accuracy be $k = 2n+1$? Yes

Assume current situation



Areas marked with x and with o must be equal

equivalent of saying $\equiv$ average of $p_2(x)$ is zero

where

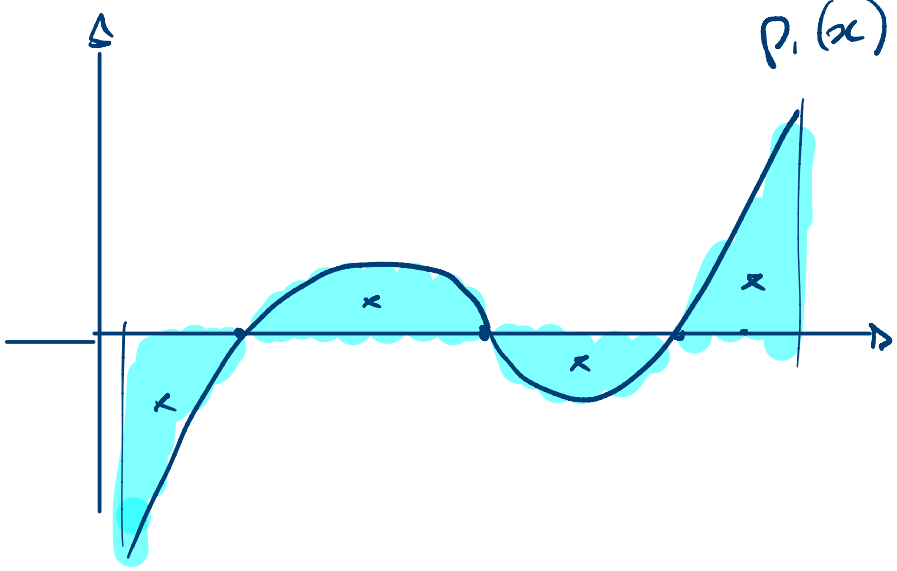
$p_0(x) = 1$

$p_1(x) = (x - 0.5)$ $\leftarrow \frac{a+b}{2}$

$p_2(x) = (x - x_0)(x - x_1)$ s.t. $\int p_2(x) = 0$

Now take the pt

$p_1(x) \cdot p_2(x) \in \mathbb{P}^3(x)$



The areas marked with x are equal

Theo

Let $u \in \mathbb{P}^{n+m}$ $\quad m \leq n+1$

then $I^n(u) = I(u)$

$\Leftrightarrow$

I^n has degree of accuracy $k = n+m$

$\Leftrightarrow$

$$\int_a^b \omega(x)\, p = 0 \qquad \forall p \in \mathbb{P}^{m-1}$$

ω can be chosen as $\perp$ to every p we are asking u to be Legendre polynomial

$$\omega = \prod_{i=0}^{n} (x - q_i) \in \mathbb{P}^{n+1}$$

Proof

Any polynomial $p \in \mathbb{P}^{n+m}$ can be written as : $\mathbb{P}^{n+1}$ $\mathbb{P}^{m-1}$ $\mathbb{P}^{m-1}$

$$p(x) = \omega(x)\, \pi(x) + q(x)$$

basically division + rest

by Ruffini's theorem

Since $q(x) \in \mathbb{P}^{m-1} \subseteq \mathbb{P}^n \quad (m \leq n+1)$

Then $\rightarrow I(q) = I^n(q)$

$$I(p) = I(\omega\pi) + I(q)$$ by linearity of interpolation

$$I^n(p) = I^n(\omega\pi) + I^n(q)$$

$I^n(\omega\pi) \rightarrow 0$

$= I(q)$

If $I(\omega\pi) = 0 = \int_0^1 \omega\pi \, dx$ then $I(p) = I^n(p)$

Main menage

Choose $\{q_i\}_{i=0}^{n}$ as the roots of Legendre basis of order $n+1$: $\int_a^b Le_{n+1} \, l_J \, dx = 0 \quad J < n+1$

Le_{n+1} ← Legendre basis of ord $n+1$

The roots of Le_{n+1} are called Gauss quadrature points. And I^n in this case is a Gauss quadrature formula, and it has degree of accuracy $k = 2n+1$

General Strategy: find $\{q_i\}, \{w_i\}$ s.t. ← have $2n+1$ pts ⇒ need $2n+1$ CNs to satisfy

$$\sum_{j=0}^{n} v_i(q_j)\, w_j = \int_a^b v_i(x)\,dx \quad \text{for } \{v_i\}_{i=0}^{2n+1} \text{ known}$$

you impose that the interpolatory quadrature formula is EXACT for a fixed set of arbitrary functions

$2(n+1)$ unknowns, in $2n+2$ equations.

NON LINER SYSTEM OF $2n+2$ equations.

if you can solve this, you win.

for $v_i = x^i$ you obtain the GAUSS QUADRATURE FORMULA

Least Squares

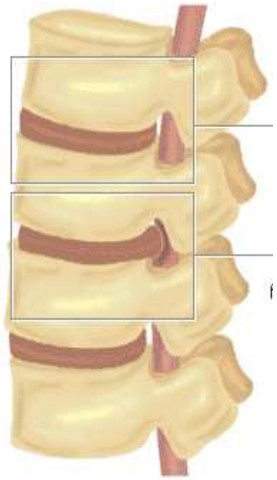
Numerical Analysis

Profs. Gianluigi Rozza- Luca Heltai

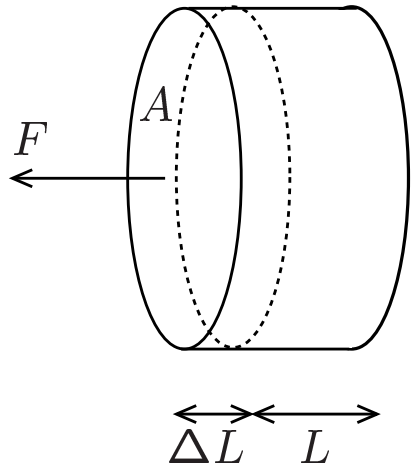
2019-SISSA mathLab Trieste

Examples and motivations

Example 1. We consider a mechanical test to establish the link between stresses ($MPa = 100N/cm^2$) and relative deformations (cm/cm) of a sample of biological tissue (an intervertebral disc, taken from P. Komarek, Chapt. 2 of *Biomechanics of Clinical Aspects of Biomedicine*, 1993, J. Valenta ed., Elsevier).



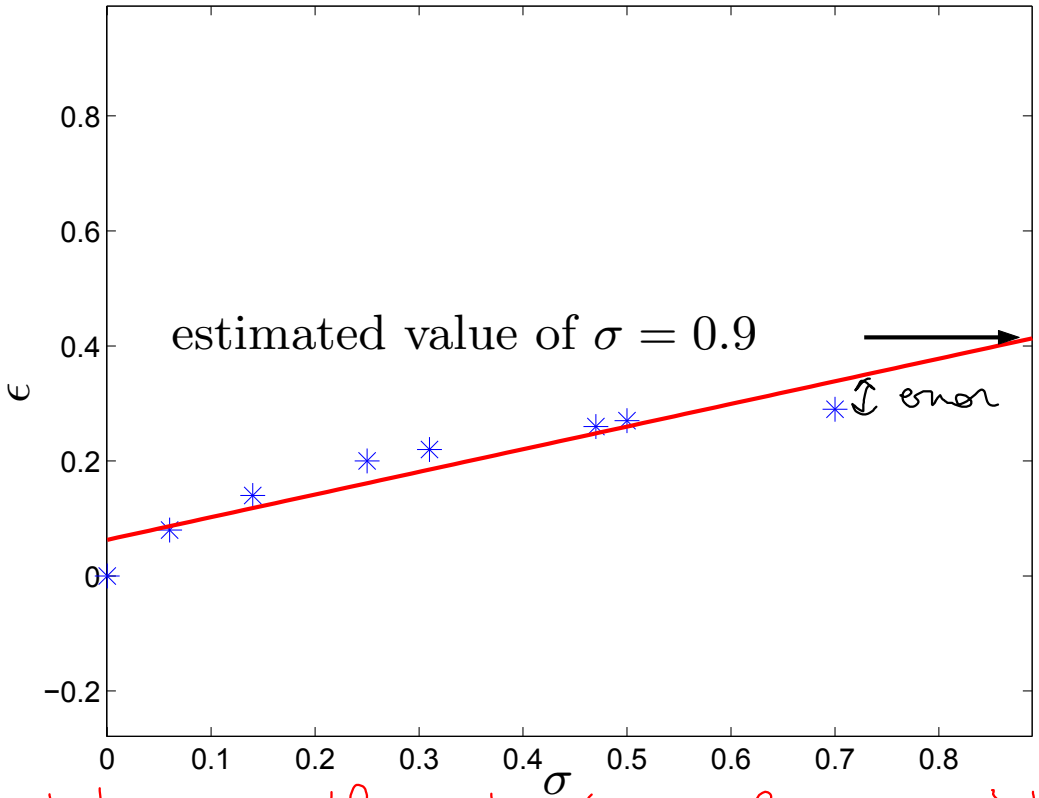
test i	pressure σ	deformation ϵ
1	0.00	0.00
2	0.06	0.08
3	0.14	0.14
4	0.25	0.20
5	0.31	0.23
6	0.47	0.25
7	0.60	0.28
8	0.70	0.29



$$\sigma = F/A$$
$$\epsilon = \Delta L/L$$

From these data, we want to estimate the deformation corresponding to a stress $\sigma = 0.9$ MPa.

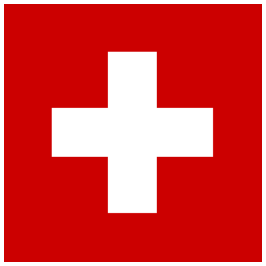
By the method of least squares, we get that best approximation for the data is $p(x) = 0.3938x - 0.0629$. The approximation can be used (called *a linear regression*) to estimate ϵ when $\sigma = 0.9$ MPa: We get $p(0.9) \simeq 0.4$.



→ we build a TREND by minimizing the distance between data and line

! If you want to approx this data (could be $10^2, 10^3$ data collected) with std interpolation you'll get a poly with high degree → NOT GOOD!

Example 2. The result of census of the population of Switzerland between 1900 and 2010 (in thousands):



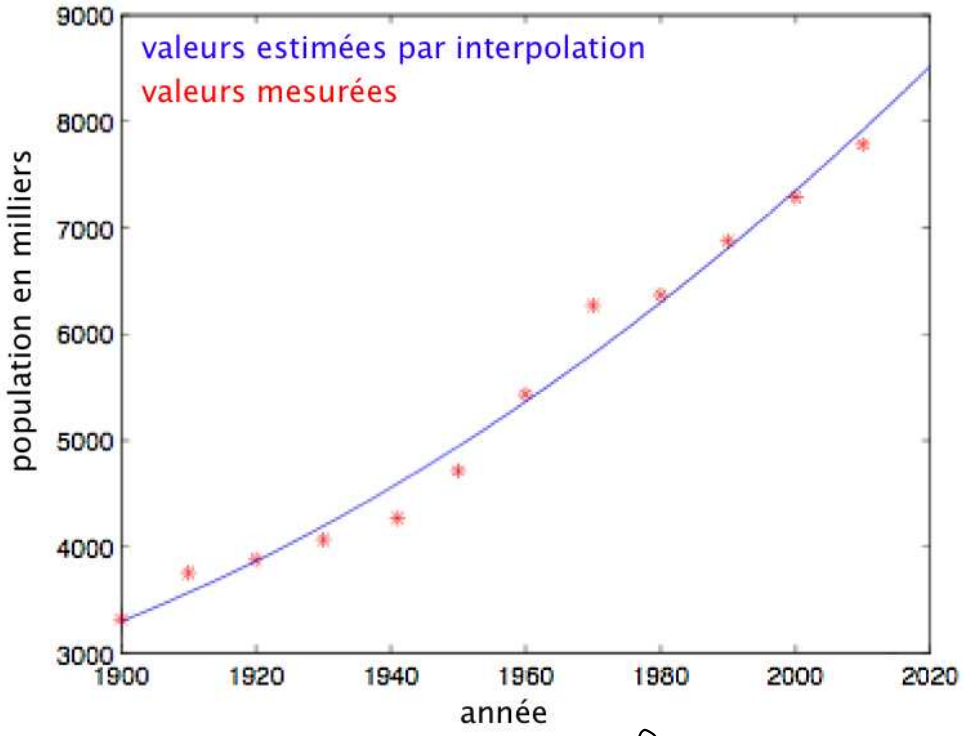
year	1900	1910	1920	1930	1941	1950
population	3315	3753	3880	4066	4266	4715

year	1960	1970	1980	1990	2000	2010
population	5429	6270	6366	6874	7288	7783

- Is it possible to estimate the number of inhabitants of Switzerland during the year when there has not been census, for example in 1945 and 1975?
- Is it possible to predict the number of inhabitants of Switzerland in 2020?

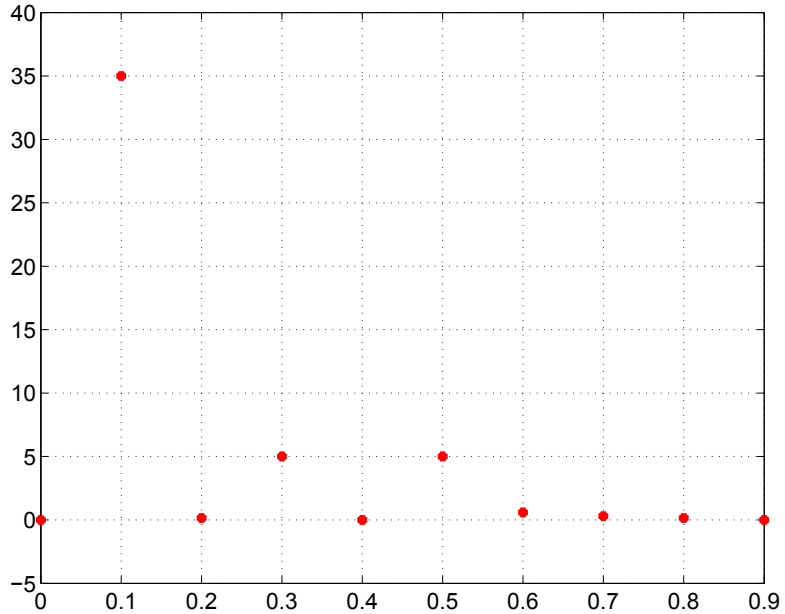
The polynomial of degree two (parabola) which approximates the data by the method of least squares is $p(x) = 0.15x^2 - 549.9x + 501600$.

↑ II ord poly. LEAST SQUARES



When fitting we should guarantee the minimization of a qty, like errors

Example 3. Points on the following figure represent the measurements of blood flow in a part of the common carotid artery during a heartbeat. The frequency of data collection is constant and equal to 10 / T where T = 1 sec. is the period of the beat.
We want to deduce from this discrete signal a continuous signal represented by a linear combination of known functions (eg. trigonometric functions - then we can adequately approximate a periodic signal).



reconstruction of the behavior of the flow rate

Let $f(t)$ be a signal that we know. $N = 10$ is a size of a sample $[f(t_0), \ldots, f(t_{N-1})]$, where $t_j = jT/N$. We are looking for $\{c_k\} \in \mathbb{C}$, $k \in [0, N-1] \subset \mathbb{N}$ such that:

vector of weights is the only thing we have to get in order to get the expression of reconstructed flow signal

basis function

$$f(t_j) = \frac{1}{N} \sum_{k=0}^{N-1} c_k \omega_N^{-kj}, \quad j = 0, \ldots, N-1, \tag{1}$$

where

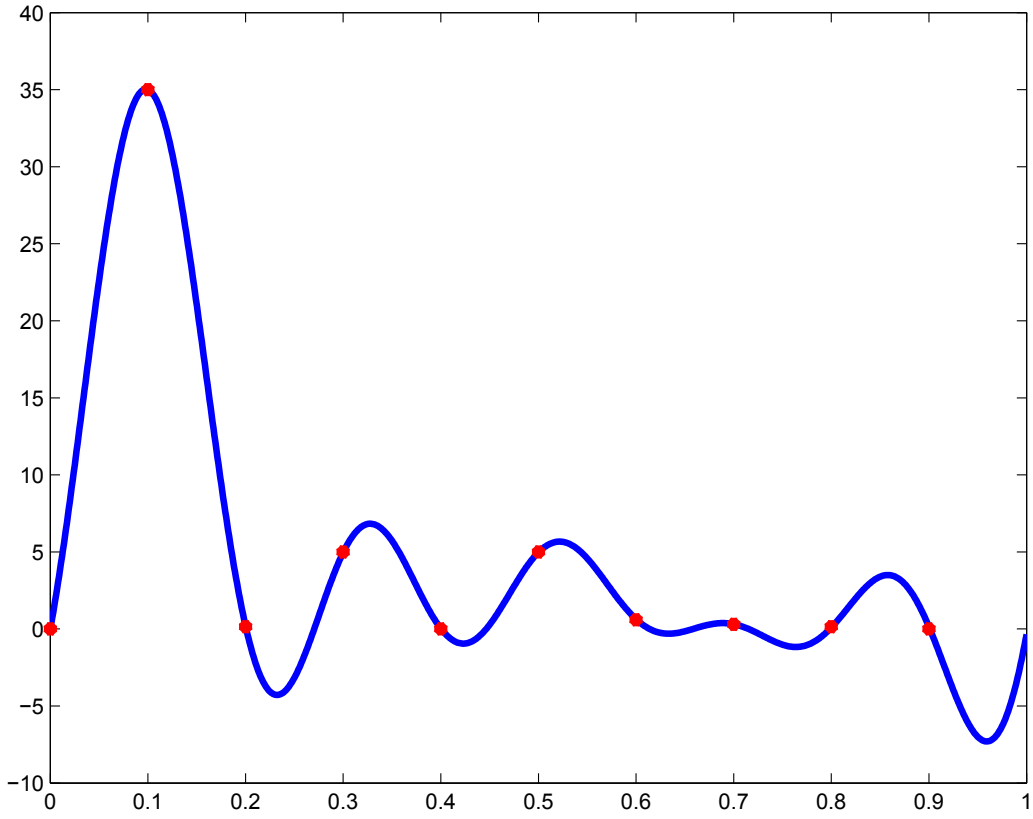
$$\omega_N = e^{(-2\pi i)/N} = \cos(2\pi/N) - i \sin(2\pi/N),$$

i is the imaginary unit. We can calculate a vector of the coefficients $\mathbf{c} = [c_1, \ldots, c_{10}]^T$ by the FFT algorithm (Fast Fourier Transform, Cooley & Tuckey, 1965), implemented in Matlab/Octave by the `fft` command.

# of data

look for this in python library

Using the formula (1), there are several techniques for obtaining the value of f in each point $t \in [0, T]$.
Using one of techniques we obtain a result that is plotted on a following figure:



If you use
Eigen latest
expect Eigen
costs; but if
you reduce it,
expect Eigen
accurate results

Approximation by the least square metho

(Chapt. 3.4 of the book)

Suppose we have $n+1$ points $x_0, x_1, \ldots, x_n$ and $n+1$ values $y_0, y_1, \ldots, y_n$.
We have seen that if n is large, the interpolating polynomial may show large oscillations (high degree!)

Instead of interpolating the values, it is possible to define a polynomial of degree $m < n$ that approximates the data "at best"

Definition 1. *We call least squares polynomial approximation of degree m the polynomial $\tilde{f}_m(x)$ of degree m such that*

$$\sum_{i=0}^{n} |y_i - \tilde{f}_m(x_i)|^2 \leq \sum_{i=0}^{n} |y_i - p_m(x_i)|^2 \qquad \forall p_m(x) \in \mathbb{P}_m$$

Remark 4. *Where $y_i = f(x_i)$ (f is a continuous function) then $\tilde{f}_m$ is called the approximation of f in the least squares sense.*

↳ minimizing the error by selecting the best polynomial of some degree

In other words, the least squares polynomial approximation is the polynomial of degree m that minimizes the distance to the data.

Let note $\tilde{f}_m(x) = a_0 + a_1 x + a_2 x^2 + \ldots + a_m x^m$ and define the function

$$\Phi(a_0, a_1, \ldots, a_m) = \sum_{i=0}^{n} \left| y_i - \left(a_0 + a_1 x_i + a_2 x_i^2 + \ldots + a_m x_i^m\right)\right|^2$$

Then the coefficients of $\tilde{f}^m$ can be determined by the relation

$$\frac{\partial \Phi}{\partial a_k} = 0, \qquad k = 0, \ldots, m, \tag{5}$$

i.e., $m+1$ linear equations in with $m+1$ unknowns a_k, $k = 0, \ldots, m$.

Example 8. Let $n = 2$ and $m = 1$, nodes $x_0 = 1$, $x_1 = 3$, $x_2 = 4$ with values $y_0 = 0$, $y_1 = 2$, $y_2 = 7$. We want to compute the (*regression line*), i.e., the the least squares polynomial approximation of degree 1, $\tilde{f}_1(x) = a_0 + a_1 x$.

We set $\Phi(a_0, a_1) = \sum_{i=0}^{2} [y_i - (a_0 + a_1 x_i)]^2$ and impose $\dfrac{\partial \Phi}{\partial a_0} = 0$ and $\dfrac{\partial \Phi}{\partial a_1} = 0$:

$$\begin{aligned}
\frac{\partial \Phi}{\partial a_0} &= -2 \sum_{i=0}^{2} [y_i - (a_0 + a_1 x_i)] = -2 \left(\sum_{i=0}^{2} y_i - 3a_0 - a_1 \sum_{i=0}^{2} x_i \right) \\
&= -2(9 - 3a_0 - 8a_1) \\
\frac{\partial \Phi}{\partial a_1} &= -2 \sum_{i=0}^{2} x_i [y_i - (a_0 + a_1 x_i)] = -2 \left(\sum_{i=0}^{2} x_i y_i - a_0 \sum_{i=0}^{2} x_i - a_1 \sum_{i=0}^{2} x_i^2 \right) \\
&= -2(34 - 8a_0 - 26a_1)
\end{aligned}$$

Hence the coefficients a_0 and a_1 are the solution of the system

$$\begin{cases} 3a_0 + 8a_1 = 9 \\ 8a_0 + 26a_1 = 34 \end{cases}$$

Generalize to odd m

Ideally, for $\tilde{f}_m(x) = a_0 + a_1 x + a_2 x^2 + \dots$ we would like to impose $\tilde{f}_m(x_i) = y_i$ pour $i = 0, \dots, n$.
This can be written as a linear system with unknowns a_k, $k = 0, \dots, m$: $B\mathbf{a} = \tilde{\mathbf{y}}$, where B is a matrix of dimension $(n+1) \times (m+1)$

dim of sol of approx

$$B = \begin{pmatrix} 1 & x_0 & \dots & x_0^m \\ 1 & x_1 & \dots & x_1^m \\ \vdots & & & \vdots \\ 1 & x_n & \dots & x_n^m \end{pmatrix}$$ dim of dataset

A rectangular B matrix is NOT solvable as a linear system

Since $m < n$, the system is oversized. The solution to (5) is equivalent to the square system (*system of normal equations*)

$$\boxed{B^T B\mathbf{a} = B^T \tilde{\mathbf{y}}.}$$

premultiply by B^T → you get a square matrix, now you can solve shit

Example 9. We have 8 measures (σ-ϵ):

```
>> sigma = [0.00 0.06 0.14 0.25 0.31 0.47 0.50 0.70];
>> epsilon = [0.00 0.08 0.14 0.20 0.22 0.26 0.27 0.29];
```

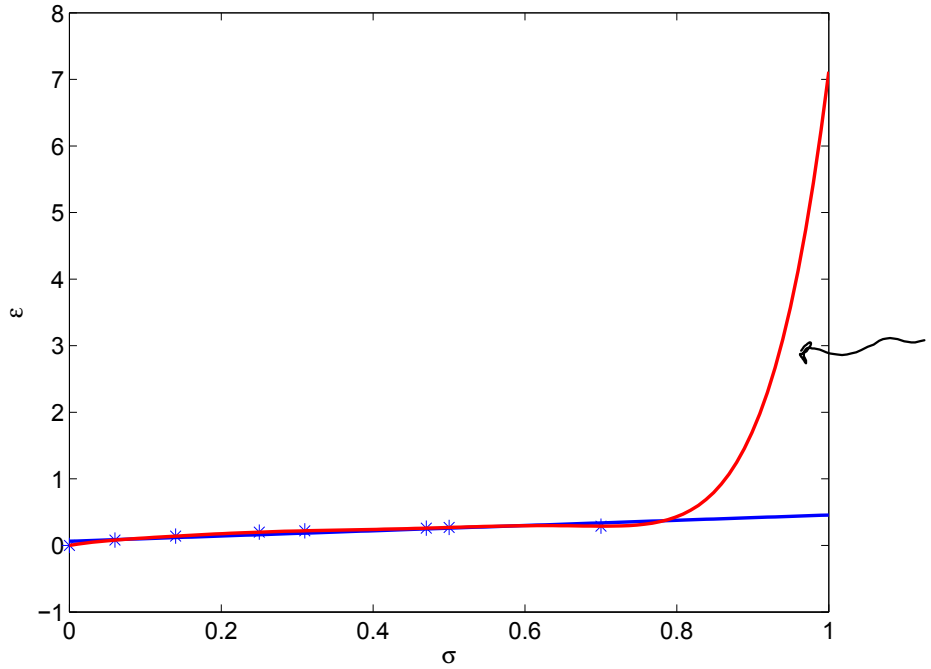
We want to extrapolate the value of ϵ for$\sigma = 0.4$. We consider two ways:

- compute the interpolating polynomial Π_7 of degree 7
- compute the least squares polynomial approximation of degree 1

On peut utiliser les commandes suivantes:

```
>>  plot(sigma, epsilon, '*'); hold on;  % plotting the known values
>>  sigma_sample = linspace(0,1.0,100);
>>  p7 = polyfit(sigma, epsilon, 7);
>>  pol = polyval(p7, sigma_sample);     % interpolating polynomial
>>  plot(sigma_sample,pol, 'r');
>>  p1 = polyfit(sigma,epsilon,1);
>>  pol_mc = polyval(p1, sigma_sample);  % least square
>>  plot(sigma_sample, pol_mc, 'g'); hold off;
```

- the interpolating polynomial Π_7 of degree 7 is in red
- the least squares polynomial approximation of degree 1 is in blue



degree 7 gives a very bad approx at the end

For $\sigma > 0.7$,the behavior of the two polynomials are very different.

In particular, for $\sigma = 0.9$ the values of $\epsilon(\sigma)$ extrapolated with the two methods are

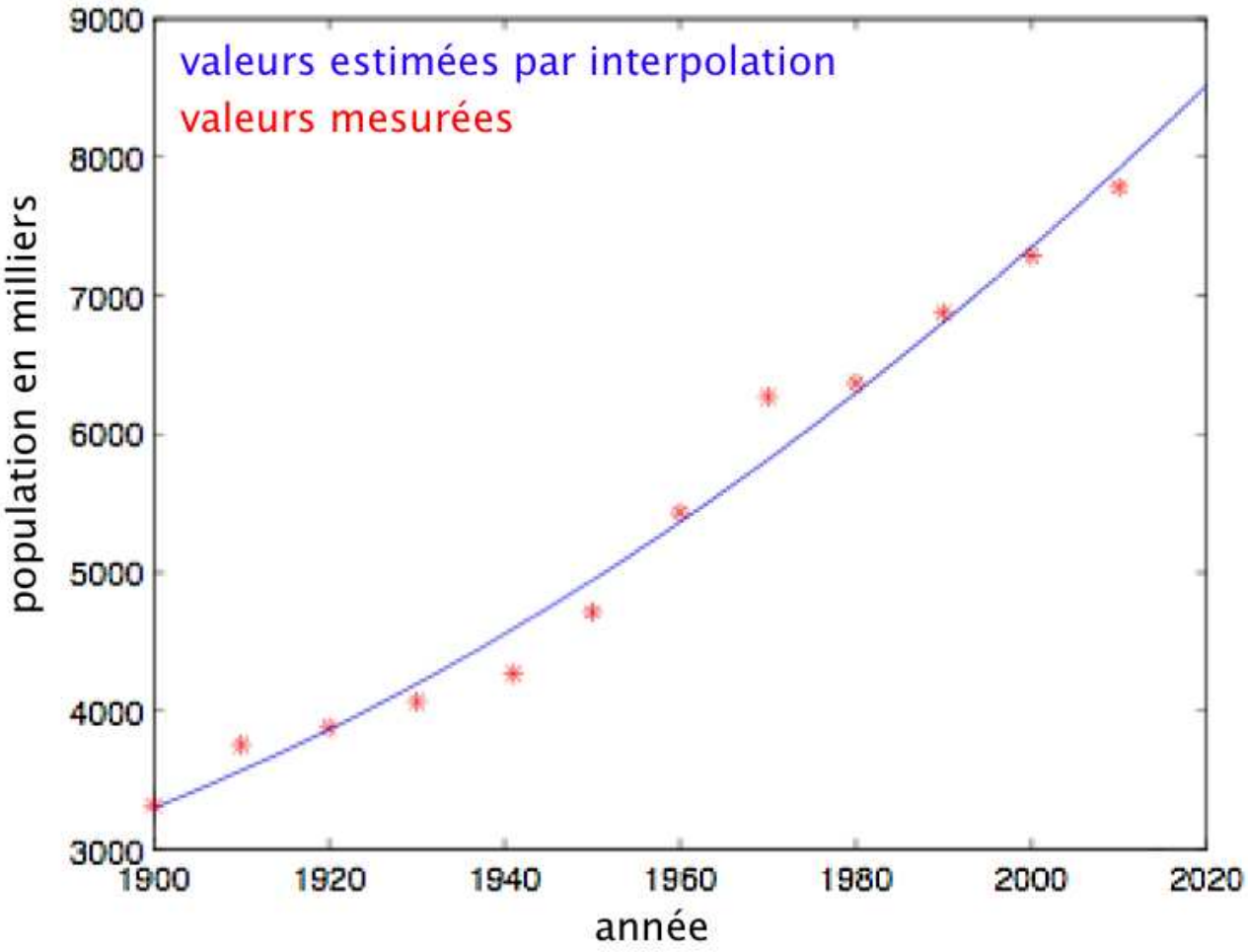
```
>> polyval(p7, 0.9)
ans =
    1.7221

>> polyval(p1, 0.9)
ans =
    0.4173
```

- The value obtained by Π_7 (172.21%) is unrealistic
- On the contrary, the value obtained with the regression line is more appropriate to compute the value at $\sigma = 0.9$.

Example 10. Swiss population Starting from the population at the 20th century decades, we extrapolate the Swiss popululation this year. We use a least square polynomial approximation of degree 2

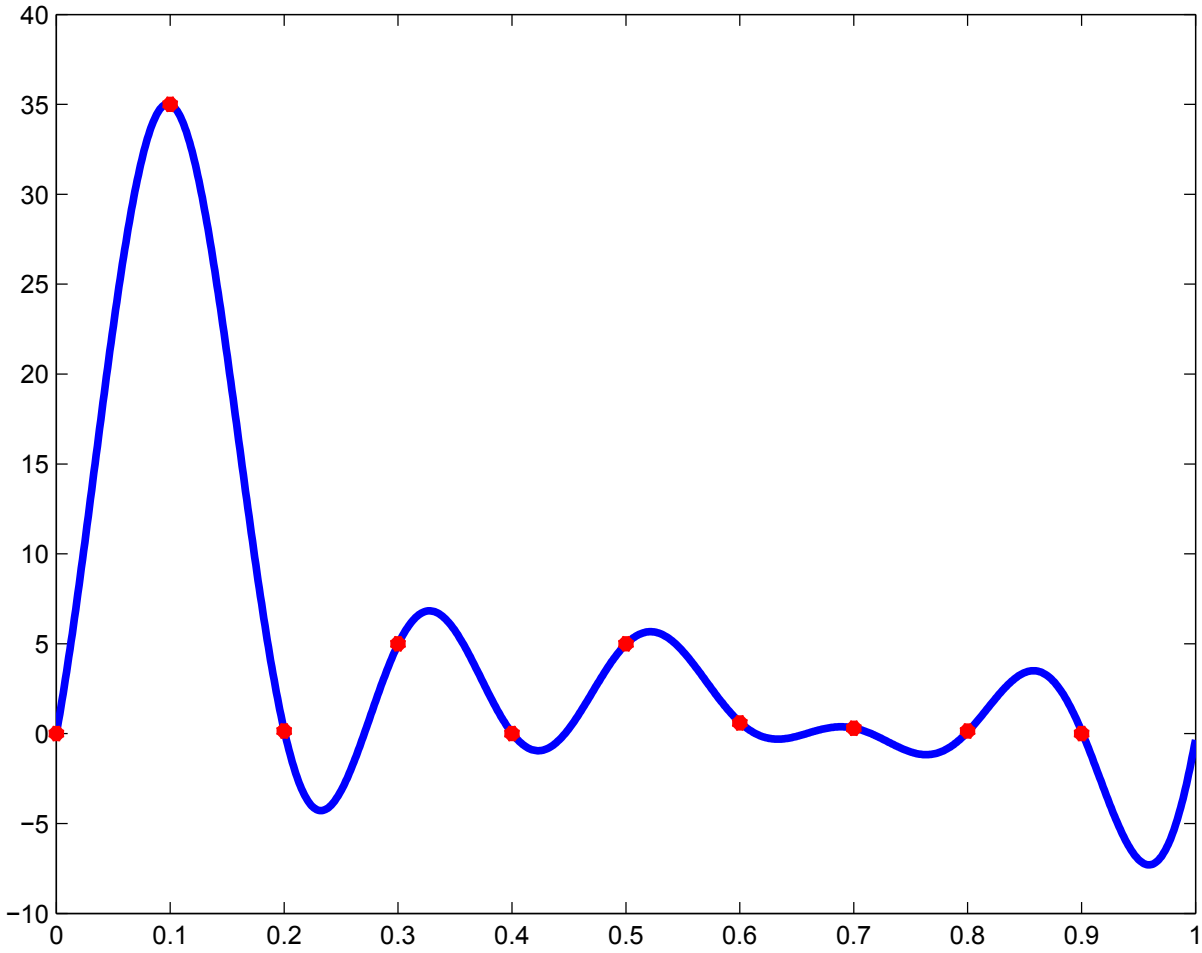
```
>> year = [1900, 1910, 1920, 1930, 1941, 1950,...
           1960, 1970, 1980, 1990, 2000];
>> population = [3315, 3753, 3880, 4066, 4266, 4715,...
           5429, 6270, 6366, 6874, 7288];
>> p2 = polyfit(year, population, 2);
>> year_sample = [1900:2:2010];
>> vp2 = polyval(p2, year_sample);
>> plot(year, population, '*r', ...
       year_sample, vp2, 'b');
```


valeurs estimées par interpolation
valeurs mesurées
population en milliers
année
9000
8000
7000
6000
5000
4000
3000
1900
1920
1940
1960
1980
2000
2020

Example. Carotide flow rate We define 10 couples of data (time vs flowrate) with the vectors **t** and **deb**. With the help of the command **interpft**, we compute the value of the interpolating function at 1000 equidistributed points in the periodicity interval [0,1]:

```
t = [0 .1 .2 .3 .4 .5 .6 .7 .8 .9];
deb = [0 35 .15 5 0 5 .6 .3 .15 0];
f = interpft(deb, 1000);
plot(linspace(0, 1, 1000), f); hold on;
plot(t, deb, 'r*')
```

interpolation function


40
35
30
25
20
15
10
5
0
−5
−10
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

Processing of polynomials

In Matlab/Octave, there are specific commands for doing calculations with polynomials. Let `x` be a vector of abscissas, `y` be a vector of ordinates and `p` (respectively $\texttt{p}_i$) be the vector of coefficients of a polynomial $P(x)$ (respectively P_i); then, we have following commands:

command	action
`y=polyval(p,x)`	`y` $=$ values of $P(x)$
`p=polyfit(x,y,n)`	`p` $=$ coefficients of the interpolating polynomial Π_n
`z=roots(p)`	`z` $=$ zeros of P such that $P(\texttt{z}) = 0$
`p=conv(`$\texttt{p}_1$`,`$\texttt{p}_2$`)`	`p` $=$ coefficients of the polynomial $P_1 P_2$
`[q,r]=deconv(`$\texttt{p}_1$`,`$\texttt{p}_2$`)`	`q` $=$ coefficients of Q, `r` $=$ coefficients of R such that $P_1 = QP_2 + R$
`y=polyderiv(p)`	`y` $=$ coefficients of $P'(x)$
`y=polyinteg(p)`	`y` $=$ coefficients of $\int P(x)\, dx$

Linear systems - Direct methods

Numerical Analysis

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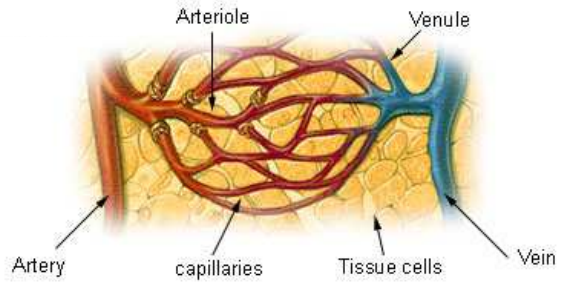
2019-SISSA mathLab Trieste

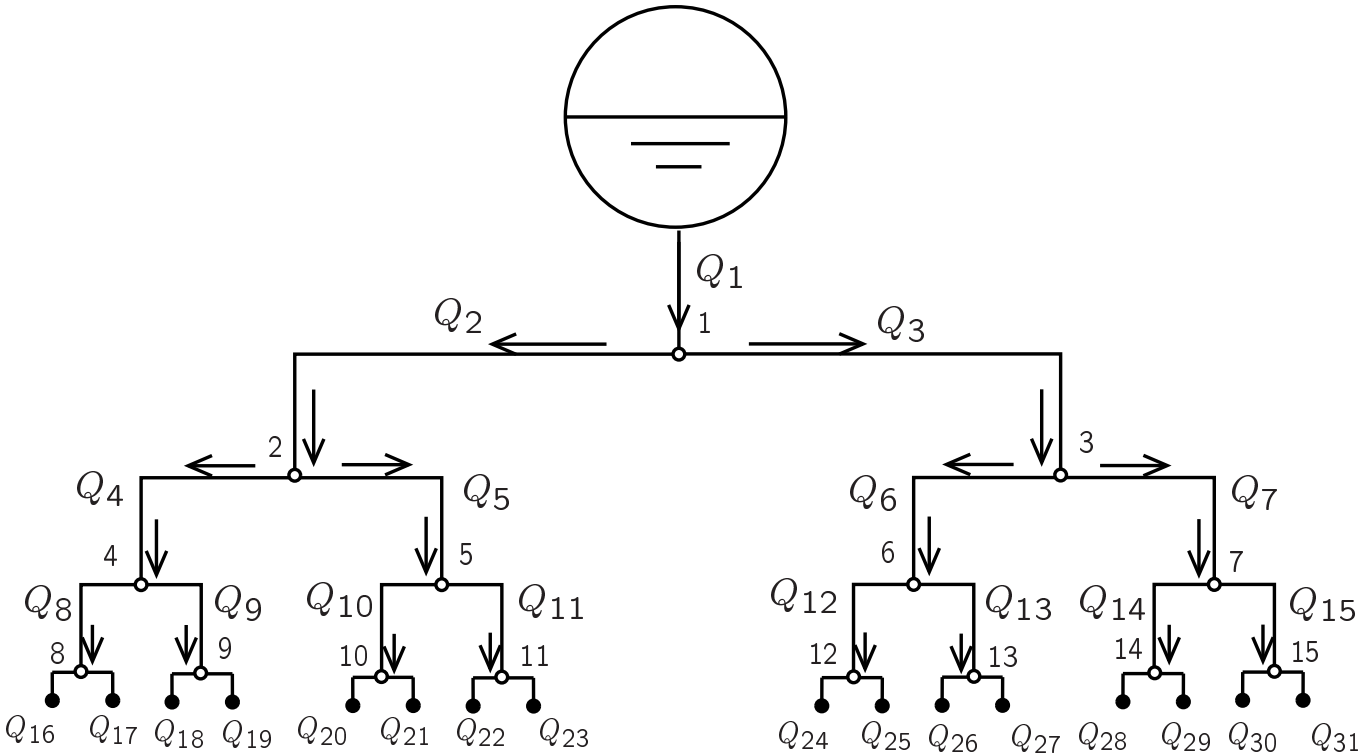
Examples and motivation

Example 1 (Capillary bed)**.** Capillaries are microscopic blood vessels, the smallest part of the circulatory system. The capillaries are grouped in networks called capillary beds, made of 10 to 100 capillaries, depending on the tissue.
Blood arrives to the capillary bed through arterioles. In the capillary bed an exchange of oxigen and waste molecules takes place.
Then, the capillaries become venules and collect the blood in veins to be transfered back to the heart.



We consider a model of capillary bed:

- We can model a certain portion of capillary system as a hydraulic network where every capillary is represented as a pipe.
- We call *nodes* (small empty circles in the figure on the next page) the points where several capillaries meet.
- The artery that feeds the system is represented as source at a constant pressure of 50mmHg.
- We suppose the blood leaves the system through the venules (small black circles in the figure) at a constant pressure (venous pressure), fixed to the reference value zero (all other pressures will be referenced to this one).
- The blood flows from the source to the sinks (we suppose in a constant way) due to the pressure gradient.


Q_1
1
Q_2
Q_3
2
3
Q_4
Q_5
Q_6
Q_7
4
5
6
7
Q_8
Q_9
Q_{10}
Q_{11}
Q_{12}
Q_{13}
Q_{14}
Q_{15}
8
9
10
11
12
13
14
15
Q_{16} Q_{17} Q_{18} Q_{19} Q_{20} Q_{21} Q_{22} Q_{23} Q_{24} Q_{25} Q_{26} Q_{27} Q_{28} Q_{29} Q_{30} Q_{31}

We want to find the pressure distribution p_j, $j = 1, \cdots, 15$, and the flows Q_m, $m = 1, \cdots, 31$, in the capillary network. To do this, we consider that:

- in every branch m of the network, $m = 1, \cdots, 31$, we have the following relation, called constitutive relation, between the blood flow Q_m (mm^3/s) and the pressure (in mmHg) in the two nodes i and j at the end-points of each capillary

$$Q_m = \frac{1}{R_m L_m}(p_i - p_j), \tag{1}$$

where R_m is the hydraulic resistance per unit length ($\text{mmHg}\,\text{s}/\text{mm}^4$) and L_m is the length of the capillary m;

- at every node j of the network, $j = 1, \cdots 15$, we impose the balance equation between inflow and outflow:

$$\left(\sum_{m \text{ entering}} Q_m \right) - \left(\sum_{m \text{ exiting}} Q_m \right) = 0,$$

where outflows have a negative value.

For example, at the node 2 in the figure, the flow Q_2 is an inflow and the flows Q_4 and Q_5 are outflows, being the balance:

$$Q_2 - Q_4 - Q_5 = 0.$$

By using for every flow the constitution relation (1) in the previous balance, we have

$$\frac{1}{R_2 L_2}(p_1 - p_2) - \frac{1}{R_4 L_4}(p_2 - p_4) - \frac{1}{R_5 L_5}(p_2 - p_5) = 0.$$

One such equation is obtained for every node in the network.
Remark: if we consider the balance for the node 1, we get

$$\frac{1}{R_1 L_1}(p_r - p_1) - \frac{1}{R_2 L_2}(p_1 - p_2) - \frac{1}{R_3 L_3}(p_1 - p_3) = 0.$$

Being the pressure p_r constant, we move it to the right-hand side.

$$-\frac{1}{R_1 L_1}p_1 - \frac{1}{R_2 L_2}(p_1 - p_2) - \frac{1}{R_3 L_3}(p_1 - p_3) = -\frac{1}{R_1 L_1}p_r.$$

In a similar way for the node 8

$$\frac{1}{R_8 L_8}(p_4 - p_8) - \frac{1}{R_{16} L_{16}} p_8 - \frac{1}{R_{17} L_{17}} p_8 = 0,$$

where we see that $p_{16} = p_{17} = 0$. Same process for the nodes $9, \cdots, 15$.

Writing the balance for every node after having substituted the constitution relation, we get a system of linear equations for the pressures:

$$A\mathbf{p} = \mathbf{b}, \tag{2}$$

A contains all the properties of our system

where $\mathbf{p} = [p_1, p_2, \cdots, p_{15}]^T$ is the unknown vector pressures at the nodes of the network, $A \in \mathbb{R}^{15\times 15}$ is the coeficient matrix of the system and $\mathbf{b} \in \mathbb{R}^{15}$ is the array of known data.

! Do evaluations of ybies you save for multiple use, in order to be more efficient and avoid "repetitivity" → save time and computational costs

Lets suppose that all capillaries have the same hydraulic resistance $R_m = R = 1$ and that capillary length halves at each bifurcation (if $L_1 = 20$, we'll have $L_2 = L_3 = 10$, $L_4 = L_5 = L_6 = L_7 = 5$ etc..), the following matrix A is generated:

$$\begin{pmatrix}
-\frac{1}{4} & \frac{1}{10} & \frac{1}{10} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{10} & -\frac{1}{2} & 0 & \frac{1}{5} & \frac{1}{5} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{10} & 0 & -\frac{1}{2} & 0 & 0 & \frac{1}{5} & \frac{1}{5} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \frac{1}{5} & 0 & -1 & 0 & 0 & 0 & 0.4 & 0.4 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \frac{1}{5} & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0.4 & 0.4 & 0 & 0 & 0 & 0 \\
0 & 0 & \frac{1}{5} & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0.4 & 0.4 & 0 & 0 \\
0 & 0 & \frac{1}{5} & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0.4 & 0.4 \\
0 & 0 & 0 & 0.4 & 0 & 0 & 0 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0.4 & 0 & 0 & 0 & 0 & -2 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0.4 & 0 & 0 & 0 & 0 & -2 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0.4 & 0 & 0 & 0 & 0 & 0 & -2 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0.4 & 0 & 0 & 0 & 0 & 0 & -2 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0.4 & 0 & 0 & 0 & 0 & 0 & 0 & -2 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0.4 & 0 & 0 & 0 & 0 & 0 & 0 & -2 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0.4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -2
\end{pmatrix}$$

and $\mathbf{b} = [-5/2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0]^T$.

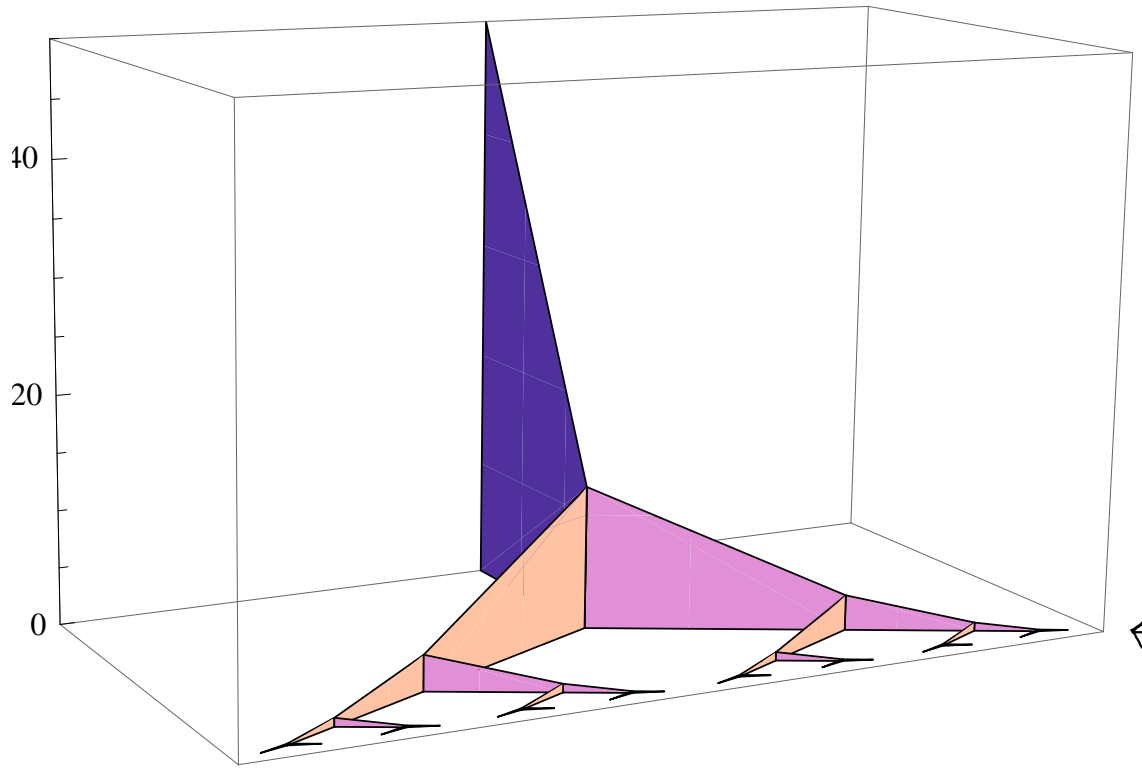
The problem of determining the pressures and flows in the network requires to solve a linear system $A\mathbf{p} = \mathbf{b}$.
In this case, the matrix A is symmetric and definite positive. This last property ensures that the matrix A is not singular and thus that the system has a unique solution.
The solution is given by the vector

$$\mathbf{p} = [12.46, 3.07, 3.07, 0.73, 0.73, 0.73, 0.73, 0.15, 0.15, 0.15, 0.15, 0.15, 0.15, 0.15, 0.15]^T.$$

Once we have the pressures, we can compute, using the relation (1), the flows:

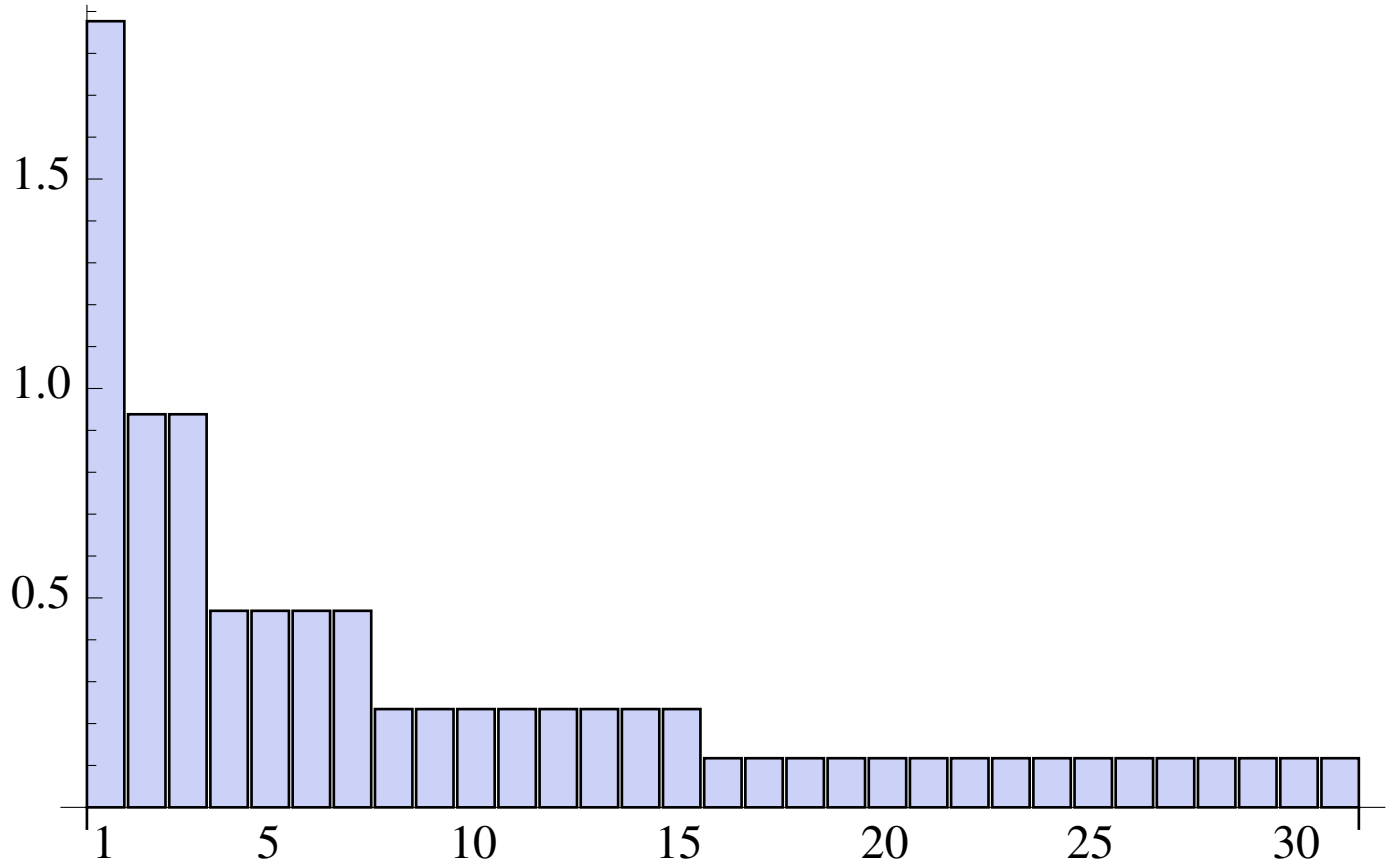
$$\begin{aligned} Q_1 &= 1.88 \\ Q_{2,3} &= 0.94 \\ Q_{4,\cdots,7} &= 0.47 \\ Q_{8,\cdots,15} &= 0.23 \\ Q_{16,\cdots,31} &= 0.12 \end{aligned}$$

Linear distribution of pressures in the capillary bed computed from the pressures at every node (solution of the system)

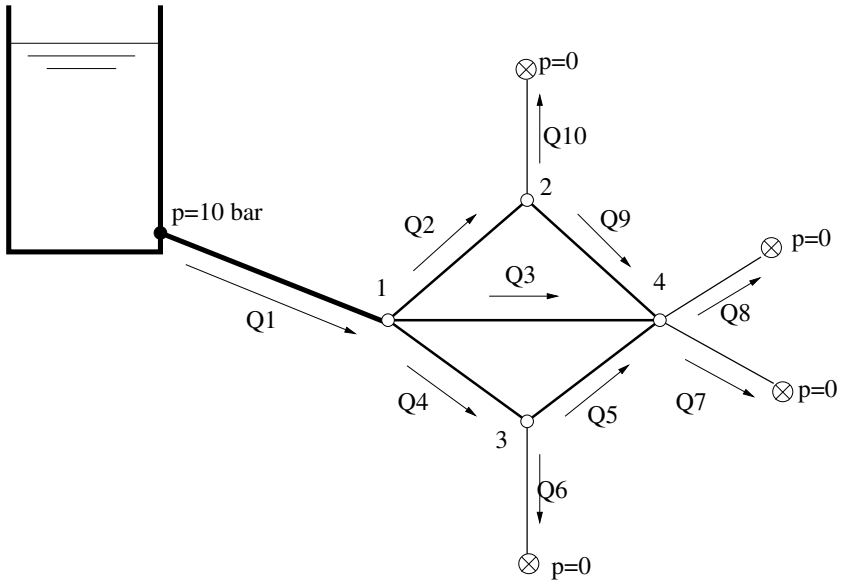


system is dissipating energy ⇓ we have a drop in pressure

Distribution of the flows in the capillary bed



Example 2 (Hydraulic network)**.** Let us consider a hydraulic network made of 10 pipes.



The network is fed by a reservoir of water at constant pressure $p_r = 10$ bar (pressure values in this exercise are the difference between the "real" pressure and the atmospheric pressure, in bar). For each pipe in the network, the following relation between the water flow Q (m^3/s) and the pressure (in bar) holds at both pipe-ends

$$Q = \frac{1}{RL}(p_{\text{in}} - p_{\text{out}}), \tag{3}$$

where R is the hydraulic resistance per unit length ((bar s)/m^4) and L is the legth (in m) of the pipeline. The resistance R depends on the pipe radius r and the dynamic viscosity μ of the liquid, following the relation $R = 8\mu/(\pi r^4)$.

At every node of the network, the balance between inflows and outflows can be set; for example for the node 2 in the figure, we have $Q_2 - Q_9 - Q_{10} = 0$ (outflows have a negative sign).

We assume atmospheric pressure at the outlets ($p = 0$ bar). A typical problem consists the pressure values and flows in the network. Using both given relations, a linear system can be built for the pressure of a form:

$$A\mathbf{p} = \mathbf{b}, \tag{4}$$

where $\mathbf{p} = [p_1, p_2, p_3, p_4]^T$ is the vector of pressures (unknown) at the 4 nodes of the network.

unknowns

The following table contains the relevant characteristics of the pipelines:

Pipe	R	L	*Pipe*	R	L	*Pipe*	R	L
1	0.2500	20	2	2.0000	10	3	1.0204	14
4	2.0000	10	5	2.0000	10	6	7.8125	8
7	7.8125	8	8	7.8125	8	9	2.0000	10
10	7.8125	8						

Correspondingly, A and $\mathbf{b}$ are:

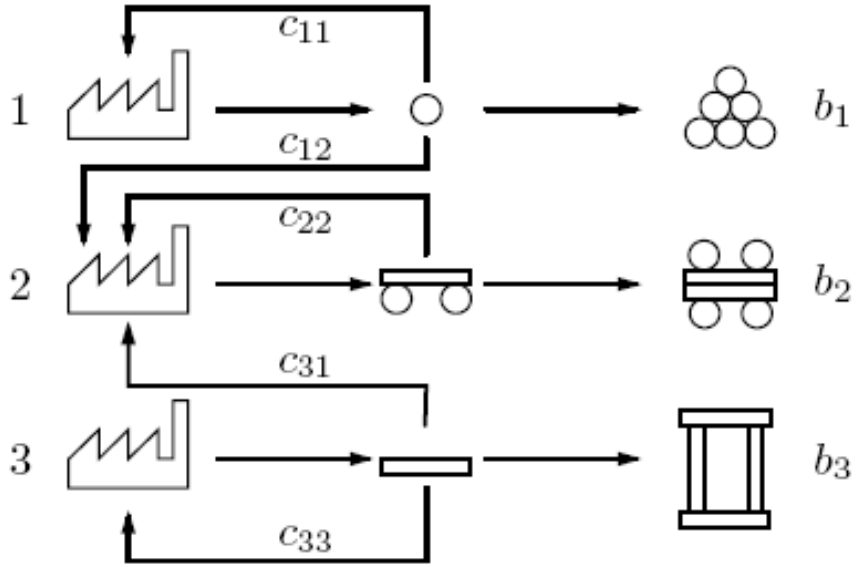
symmetrical

$$A = \begin{bmatrix} -0.370 & 0.050 & 0.050 & 0.070 \\ 0.050 & -0.116 & 0 & 0.050 \\ 0.050 & 0 & -0.116 & 0.050 \\ 0.070 & 0.050 & 0.050 & -0.202 \end{bmatrix}, \qquad \mathbf{b} = \begin{bmatrix} -2 \\ 0 \\ 0 \\ 0 \end{bmatrix}.$$

The array of pressure values at the nodes is:
$\mathbf{p} = A^{-1}\mathbf{b} = [8.1172, 5.9893, 5.9893, 5.7779]^T$. We can finally compute, using the relation (1), the flows (in m^3/s):

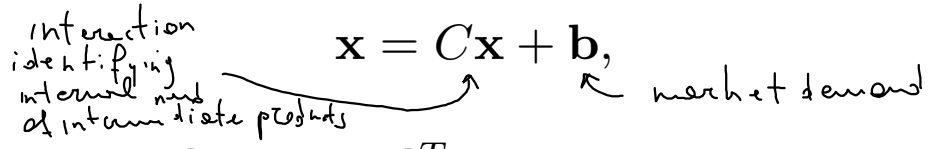
Q1	0.3766	Q2	1.0640	Q3	0.1638
Q4	0.1064	Q5	0.0106	Q6	0.0958
Q7	0.0924	Q8	0.0924	Q9	0.0106
Q10	0.0958				

Example 3 (Economy/Logistic)**.** We want to determine the situation of equilibrium between demand and offer of certain goods. Let us consider that $m >= n$ factories produce n different products. They have to adapt their productions to the internal demand (i.e. the goods needed as input by the other factories) as well as to the external demand, from the consumers.
$x_i,\ i = 1, \ldots, n$ is the total number of goods made by the factory i,
$b_i,\ i = 1, \ldots, n$ is the corresponding demand from the market and
c_{ij} the amount produced by the factory i needed for the factory j to make one unit of product.



Interaction scheme between 3 factories and the market

If we suppose that the relation between the different products is linear, the equlibrium is reached when the vector $\mathbf{x} = [x_1, \ldots, x_n]^T$ satisfies



where $C = (c_{ij})$ and $\mathbf{b} = [b_1, \ldots, b_n]^T$. Consequently, the total production $\mathbf{x}$ is solution of the linear system :

$$A\mathbf{x} = \mathbf{b}, \quad \text{where } A = I - C.$$

Formulation of the problem

We call linear system of order n (n positive integer), an expression of the form

$$A\mathbf{x} = \mathbf{b},$$

where $A = (a_{ij})$ is a given matrix of size $n \times n$, $\mathbf{b} = (b_j)$ is a given vector and $\mathbf{x} = (x_j)$ is the unknown vector of the system. The previous relation is quivalent to the n equations

$$\sum_{j=1}^{n} a_{ij} x_j = b_i, \ i = 1, \ldots, n.$$

The matrix A is called *non-singular* if $\det(A) \neq 0$; the solution $\mathbf{x}$ will be unique (for any given vector $\mathbf{b}$) if and only if the matrix associated to the linear system is non-singular.

In theory, if A is non-singular, the solution is given by the *Cramer's rule*:

$$x_i = \frac{\det(B_i)}{\det(A)}, \ i = 1, \ldots, n,$$

where B_i is the matrix by substituting the i-th column of A by the vector $\mathbf{b}$:

$$B_i = \begin{bmatrix} a_{11} & \ldots & b_1 & \ldots & a_{1n} \\ a_{21} & \ldots & b_2 & \ldots & a_{2n} \\ \vdots & & \vdots & & \vdots \\ a_{n1} & \ldots & b_n & \ldots & a_{nn} \end{bmatrix} \begin{matrix} \\ \\ \\ \\ \uparrow \\ i \end{matrix}$$

NOT EASY TO COMPUTE det(Bi) because it requires ~ N! flops (floating point operation)

=> COMPUTATIONAL COST OF CRAMER'S RULE IS of (N+1)!

↑ N=20 => you boy is FUCKED!

Unfortunately, the application of this rule is unacceptable for the practical solution of systems because the computational cost is of the order of $(n+1)!$ *floating point operations* (*flops*). In fact, every determinant requires $n!$ *flops*.

For example, the following table gives the time required by different computers to solve a linear system using the Cramer rule (o.r. stands for “out of reach”):

	Number of flops of the computer				
n	10^9 (Giga)	10^{10}	10^{11}	10^{12} (Tera)	10^{15} (Peta)
10	10^{-1} sec	10^{-2} sec	10^{-3} sec	10^{-4} sec	negligible
15	17 hours	1.74 hours	10.46 min	1 min	$6\ 10^{-2}$ sec
20	4860 years	486 years	48.6 years	4.86 years	1.7 days
25	o.r.	o.r.	o.r.	o.r.	38365 years

Alternative algorithms have to be developed. In the following sections, several methods will be analysed.

Triangular systems

A matrix $U = (u_{ij})$ is *upper triangular* if

$$u_{ij} = 0 \quad \forall i, j \ : \ 1 \leq j < i \leq n$$

and a matrix $L = (l_{ij})$ is *lower triangular* if

$$l_{ij} = 0 \quad \forall i, j \ : \ 1 \leq i < j \leq n.$$

Respectively, the system to be solved is called *upper or lower triangular system*.
Remark: If a matrix A in non-singular and triangular, knowing that

$$\det(A) = \prod_{i=1}^{n} \lambda_i(A) = \prod_{i=1}^{n} a_{ii}$$

($\lambda_i(A)$ being the i-th eigenvalue of A), we can deduce that $a_{ii} \neq 0$, for all $i = 1, \ldots, n$.

If L is lower triangular and non-singular, the linear system $L\mathbf{y} = \mathbf{b}$ corresponds to

$$\begin{cases} l_{11}y_1 & = & b_1 \\ l_{21}y_1 + l_{22}y_2 & = & b_2 \\ \vdots & & \\ l_{n1}y_1 + l_{n2}y_2 + \ldots + l_{nn}y_n & = & b_n \end{cases}$$

Thus:

$$\boxed{y_1 = b_1/l_{11}}, \qquad \text{[1 operation]}$$

and for $i = 2, 3, \ldots, n$

already computed at previous steps

$$\boxed{y_i = \frac{1}{l_{ii}}\left(b_i - \sum_{j=1}^{i-1} l_{ij}y_j\right).} \qquad \text{[} 1 + 2(i-1) \text{ operations]}$$

This algorithm is called *forward substitutions algorithm.*

The forward substitutions algorithm requires n^2 operations, whare n is the size of the system:

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

If U is upper triangular and non-singular, the system $U\mathbf{x} = \mathbf{y}$ is:

$$\begin{cases} u_{11}x_1 + \ldots + u_{1,n-1}x_{n-1} + u_{1n}x_n &= y_1 \\ \vdots & \\ u_{n-1,n-1}x_{n-1} + u_{n-1,n}x_n &= y_{n-1} \\ u_{nn}x_n &= y_n \end{cases}$$

Thus:

we proceed with inverted order

$$\boxed{x_n = y_n/u_{nn}},$$

and for $i = n-1, n-2, \ldots, 2, 1$

$$\boxed{x_i = \frac{1}{u_{ii}}\left(y_i - \sum_{j=i+1}^{n} u_{ij}x_j\right).}$$

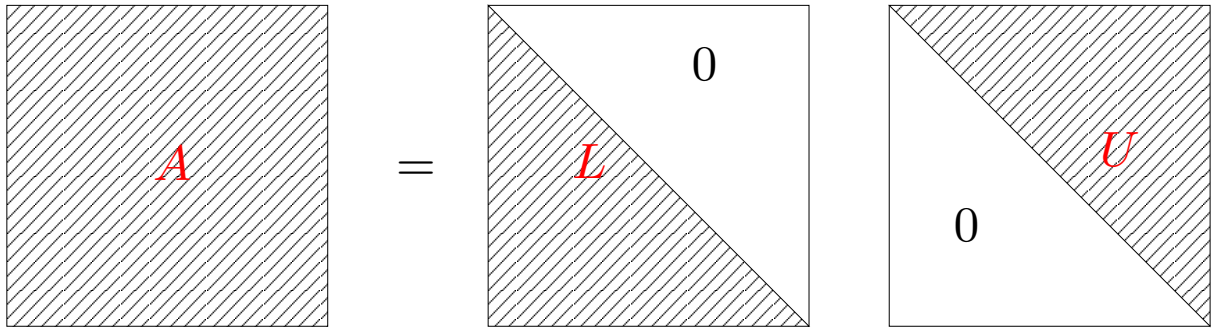
This algorithm is called *backward substitutions algorithm* The cost is, once again, n^2 operations.

The LU factorization method

(Sec. 5.3 of the book)

Let $A = (a_{ij})$ be a non-singular $n \times n$ matrix. Assume that there exist a matrix $U = (u_{ij})$, upper triangular and a matrix $L = (l_{ij})$, lower triangular such that

$$A = LU. \tag{5}$$



We call (5) a *factorization LU of A*.

If we know the factorization LU of A, solving the system $A\mathbf{x} = \mathbf{b}$ is equivalent to solving two systems defined by *triangular* matrices. Indeed,

$$A\mathbf{x} = \mathbf{b} \quad \Leftrightarrow \quad LU\mathbf{x} = \mathbf{b} \quad \Leftrightarrow \quad \begin{cases} L\mathbf{y} = \mathbf{b}, \\ U\mathbf{x} = \mathbf{y}. \end{cases}$$

We can easily calculate the solutions of both systems:

- first, we use the forward substitutions algorithm to solve $L\mathbf{y} = \mathbf{b}$ (order n^2 *flops*);
- then, we use the backward substitutions algorithm to solve $U\mathbf{x} = \mathbf{y}$ (order n^2 *flops*).

It is required to find first (if possible) the matrices L and U (what requires a number of operations of the order $\frac{2n^3}{3}$ *flops*).

Example 4. Lets try to find a factorization LU in the case case where the size of the matrix A is $n = 2$. We can write the equation (5) as

$$\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} = \begin{bmatrix} l_{11} & 0 \\ l_{21} & l_{22} \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} \\ 0 & u_{22} \end{bmatrix},$$

Or equivalently:

$$\begin{aligned} &(a) \quad l_{11}u_{11} = a_{11}, \quad &&(b) \quad l_{11}u_{12} = a_{12}, \\ &(c) \quad l_{21}u_{11} = a_{21}, \quad &&(d) \quad l_{21}u_{12} + l_{22}u_{22} = a_{22}. \end{aligned}$$

We have then a system (non-linear) with 4 equations and 6 unknowns; in order to have the same number of equations and unknowns, we fix the diagonal of L by taking $l_{11} = l_{22} = 1$. Consequently, from (a) and (b) we have $u_{11} = a_{11}$ and $u_{12} = a_{12}$; finally, if we assume $a_{11} \neq 0$, we obtain $l_{21} = a_{21}/a_{11}$ and $u_{22} = a_{22} - l_{21}u_{12} = a_{22} - a_{21}a_{12}/a_{11}$ using the equations (c) and (d).

To determine a factorization LU of the matrix A of any size n, we apply the following method.

1. The elements of L and U satisfy the non-linear system

$$\sum_{r=1}^{\min(i,j)} l_{ir}u_{rj} = a_{ij}, \quad i,j = 1,\dots,n; \tag{6}$$

2. The system (6) has n^2 equations and n^2+n unknowns. We can wipe out n unknowns if we set the n diagonal elements of L equal to 1:

we have the diagonals of L and U

$$l_{ii} = 1, \quad i = 1,\dots,n.$$

We will see that in this case there exists an algorithm (*Gauss factorization*) allowing us to efficiently compute the factors L and U.

The Gauss elimination method

The Gauss elimination method transforms the system

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

in an equivalent system (i.e. with the same solution) of the form:

$$U\mathbf{x} = \widehat{\mathbf{b}},$$

If systems have also infinite solutions!

where U is an upper triangular matrix and $\widehat{\mathbf{b}}$ is a properly modified second member.

This system can be solved by a backward substitutions method.

In the transformation, we essentially use the property that says that we do not change the solution of the system if we add to a given equation a linear combination of other equations.

Let us consider an invertible matrix $A \in \mathbb{R}^{n\times n}$ in which the diagonal element a_{11} is assumed to be non-zero. we set $A^{(1)} = A$ and $\mathbf{b}^{(1)} = \mathbf{b}$. We introduce the *multiplier*

$$l_{i1} = \frac{a_{i1}^{(1)}}{a_{11}^{(1)}}, \quad i = 2, 3, \ldots, n, \qquad A^{(1)} = \begin{bmatrix} a_{11}^{(1)} & \ldots & a_{1j}^{(1)} & \ldots & a_{1n}^{(1)} \\ \vdots & & \vdots & & \vdots \\ a_{i1}^{(1)} & \ldots & a_{ij}^{(1)} & \ldots & a_{in}^{(1)} \\ \vdots & & \vdots & & \vdots \\ a_{n1}^{(1)} & \ldots & a_{nj}^{(1)} & \ldots & a_{nn}^{(1)} \end{bmatrix}$$

where the $a_{ij}^{(1)}$ represent the elements of $A^{(1)}$. Example:

$$A = \begin{bmatrix} 2 & 4 & 6 \\ 4 & 8 & 10 \\ 7 & 8 & 9 \end{bmatrix} \quad \Longrightarrow \quad l_{21} = \frac{4}{2}, l_{31} = \frac{7}{2}.$$

The unknown x_1 can be removed from the rows $i = 2, \ldots, n$ by substracting l_{i1} times the first row and doing the same at the right-hand side.

Let us define

$$a_{ij}^{(2)} = a_{ij}^{(1)} - l_{i1}a_{1j}^{(1)}, \quad i,j = 2,\ldots,n,$$

$$b_i^{(2)} = b_i^{(1)} - l_{i1}b_1^{(1)}, \quad i = 2,\ldots,n,$$

where the $b_i^{(1)}$ are the components of $\mathbf{b}^{(1)}$ and we get a new system of the form

$$\begin{bmatrix} a_{11}^{(1)} & a_{12}^{(1)} & \ldots & a_{1n}^{(1)} \\ 0 & a_{22}^{(2)} & \ldots & a_{2n}^{(2)} \\ \vdots & \vdots & & \vdots \\ 0 & a_{n2}^{(2)} & \ldots & a_{nn}^{(2)} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1^{(1)} \\ b_2^{(2)} \\ \vdots \\ b_n^{(2)} \end{bmatrix},$$

which will be written as $A^{(2)}\mathbf{x} = \mathbf{b}^{(2)}$ and that is equivalent to the system we had at the beginning.

Once again we can transform this system by removing the unknown x_2 from the rows $3, \ldots, n$. By repeating this step we obtain a finite series of systems

$$A^{(k)}\mathbf{x} = \mathbf{b}^{(k)}, \quad 1 \leq k \leq n, \tag{7}$$

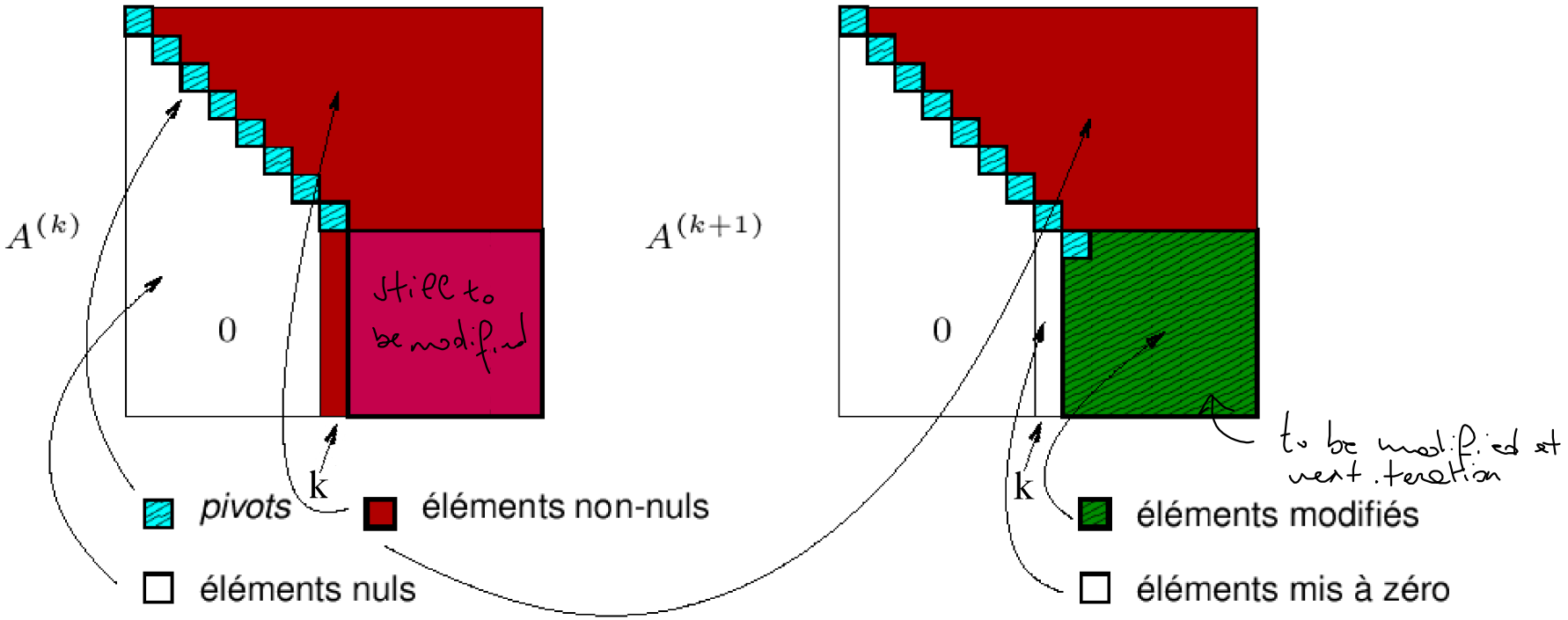
where, for $k \geq 2$, the matrix $A^{(k)}$ is of the form

$$A^{(k)} = \begin{bmatrix} a_{11}^{(1)} & a_{12}^{(1)} & \ldots & \ldots & \ldots & a_{1n}^{(1)} \\ 0 & a_{22}^{(2)} & & & & a_{2n}^{(2)} \\ \vdots & & \ddots & & & \vdots \\ 0 & \ldots & 0 & a_{kk}^{(k)} & \ldots & a_{kn}^{(k)} \\ \vdots & & \vdots & \vdots & & \vdots \\ 0 & \ldots & 0 & a_{nk}^{(k)} & \ldots & a_{nn}^{(k)} \end{bmatrix},$$

where we assume $a_{ii}^{(i)} \neq 0$ for $i = 1, \ldots, k-1$.

↳ otherwise the multiplier gives division by zero

Gauss elimination method: diagram showing how the matrix $A^{(k+1)}$ is obtained from the matrix $A^{(k)}$.



It is clear that for $k = n$ we obtain the following upper triangular system $A^{(n)}\mathbf{x} = \mathbf{b}^{(n)}$:

$$\begin{bmatrix} a_{11}^{(1)} & a_{12}^{(1)} & \dots & \dots & a_{1n}^{(1)} \\ 0 & a_{22}^{(2)} & & & a_{2n}^{(2)} \\ \vdots & & \ddots & & \vdots \\ & & & \ddots & \vdots \\ 0 & & & & \vdots \\ 0 & & & & a_{nn}^{(n)} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1^{(1)} \\ b_2^{(2)} \\ \vdots \\ \vdots \\ b_n^{(n)} \end{bmatrix}.$$

To be consistent with the previous notation, we write as U upper triangular matrix $A^{(n)}$. The elements $a_{kk}^{(k)}$ are called $pivots$ and have to be non-zero for $k = 1, \dots, n-1$.

In order to make explicit the formulae to get from the k-th systm to the $k+1$-th, for $k = 1, \ldots, n-1$, we asssume that $a_{kk}^{(k)} \neq 0$ and we define the multiplier

$$l_{ik} = \frac{a_{ik}^{(k)}}{a_{kk}^{(k)}}, \quad i = k+1, \ldots, n, \qquad [(n-k) \text{ operations}] \tag{8}$$

number of multiplies needed

we set then

$$a_{ij}^{(k+1)} = a_{ij}^{(k)} - l_{ik} a_{kj}^{(k)}, \quad i, j = k+1, \ldots, n, \qquad [2(n-k)^2 \text{ operations}]$$

$$b_i^{(k+1)} = b_i^{(k)} - l_{ik} b_k^{(k)}, \quad i = k+1, \ldots, n. \qquad [2(n-k) \text{ operations}] \tag{9}$$

Remark 1. *To perform the Gauss elimination,*

$$2\sum_{k=1}^{n-1}(n-k)^2 + 3\sum_{k=1}^{n-1}(n-k) \quad =$$

$$2\sum_{p=1}^{n-1}p^2 + 3\sum_{p=1}^{n-1}p \quad = \quad 2\frac{(n-1)n(2n-1)}{6} + 3\frac{n(n-1)}{2}$$

operations are required, plus n^2 *operations for the resolution with the backward substitutions method of the triangular system* $U\,\mathbf{x} = \mathbf{b}^{(n)}$. *By keeping only the dominant elements (of order* n^3*), we can say that the Gauss elimination method has a cost of around*

$$\frac{2}{3}n^3 \text{ operations.}$$

The following table shows the estimated computation time to solve a system using the LU factorization in different computers:

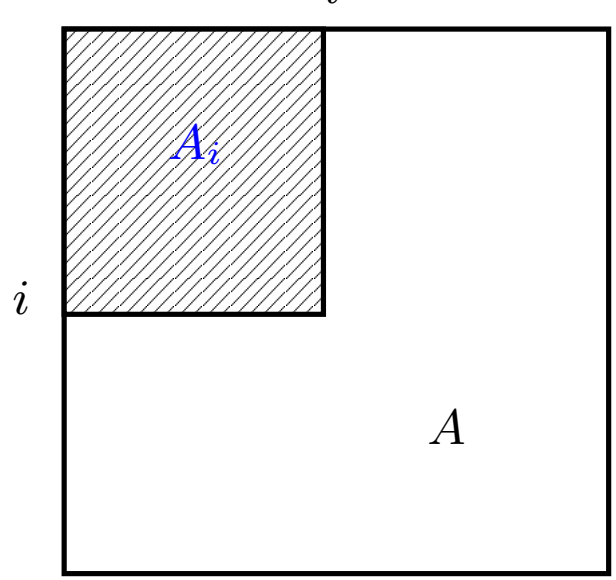
	Number of flops of the computer		
n	10^9 (Giga)	10^{12} (Tera)	10^{15} (Peta)
10^2	$7\ 10^{-4}$ sec	negligible	negligible
10^4	11 min	0.7 sec	$7\ 10^{-4}$ sec
10^6	21 years	7.7 months	11 min
10^8	o.r.	o.r.	21 years

The Gauss method is only properly defined if the pivots $a_{kk}^{(k)}$ are non-zero for $k = 1, \ldots, n-1$. Unfortunately, knowing that the diagonal elements of A are not zero is not enough to avoid null pivots during the elimination phase. For example, the matrix A in (10) is invertible and its diagonal elements are non-zero

$$A = \begin{bmatrix} 1 & 2 & 3 \\ 2 & 4 & 5 \\ 7 & 8 & 9 \end{bmatrix}, \text{ but we find } A^{(2)} = \begin{bmatrix} 1 & 2 & 3 \\ 0 & \boxed{0} & -1 \\ 0 & -6 & -12 \end{bmatrix}. \qquad (10)$$

Nevertheless, we have to stop the Gauss method at the second step, because $a_{22}^{(2)} = 0$.

Let A_i be the i-th main submatrix of A ($i = 1, \ldots, n-1$), i.e. the submatrix made of the i first rows and columns of A:



and let d_i be the principal minor of A defined as $d_i = det(A_i)$. We have the following result.

Proposition 1. *(Proposition* 5.1 *in the book) For a given matrix* $A \in \mathbb{R}^{n\times n}$, *its Gauss factorization exists and is unique iff the principal submatrices* A_i $(i = 1, \ldots, n-1)$ *are non-singular (i.e. the principal minors* d_i *are non-zero:* $d_i \neq 0$*).*

Remark: If $d_i \neq 0$ ($i = 1, \ldots, n-1$), then the pivots $a_{ii}^{(i)}$ are also non-zero.

The matrix of the previous example does not satisfy this condition because $d_1 = 1$ but $d_2 = 0$.

There are some categories of matrices for which the hypothesis of the proposition (1) are fulfilled. In particular, we mention:

1. *(Strictly >) diagonal dominant by row* matrices. A matrix A is said diagonal dominant by row if

$$|a_{ii}| \geq \sum_{j=1,\ldots,n;j\neq i} |a_{ij}|, \quad i = 1,\ldots,n.$$

2. *(Strictly >) diagonal dominant by column* matrices. A matrix A is said diagonal dominant by column if

$$|a_{jj}| \geq \sum_{i=1,\ldots,n;i\neq j} |a_{ij}|, \quad j = 1,\ldots,n.$$

Examples: $\begin{bmatrix} -4 & 1 & 2 \\ 2 & 5 & 0 \\ -2 & 1 & 7 \end{bmatrix}$ is diagonal dominant by row and by column, whereas

$\begin{bmatrix} -3 & 1 & 2 \\ 2 & 5 & 0 \\ -2 & 1 & 7 \end{bmatrix}$ is only diagonal dominant by row.

3. *Symmetric definite positive* matrices. A matrix A is symmetric if $A = A^T$; it is definite positive if all its eigenvalues are positive, i.e.:

$$\lambda_i(A) > 0, \quad i = 1, \ldots, n.$$

$\geqslant \longrightarrow$ semidefinite positiveness

Gauss $\sim LU$

We can show that the Gauss method is equivalent to the factorization $A = LU$ of the matrix A, with $L =$ multiplier matrix and $U = A^{(n)}$.

↖ now we know how to find L

More exactly:

$$A = \underbrace{\begin{bmatrix} 1 & 0 & \dots & \dots & 0 \\ l_{21} & 1 & & & 0 \\ \vdots & l_{32} & \ddots & & \vdots \\ \vdots & & \ddots & \ddots & 0 \\ l_{n1} & & & l_{n,n-1} & 1 \end{bmatrix}}_{L} \underbrace{\begin{bmatrix} a_{11}^{(1)} & a_{12}^{(1)} & \dots & \dots & a_{1n}^{(1)} \\ 0 & a_{22}^{(2)} & & & a_{2n}^{(2)} \\ \vdots & & \ddots & & \vdots \\ 0 & & & \ddots & \vdots \\ 0 & & & & a_{nn}^{(n)} \end{bmatrix}}_{U}.$$

The matrices L and U only depend on A (and not on $\mathbf{b}$), the same factorization can be resused for solving several linear systems that share the same matrix A but different vectors $\mathbf{b}$.

The number of operations is then considerably reduced, since most of the computational weight, around $\frac{2}{3}n^3 flops$, is due to the Gaussian elimination process. Indeed, let us consider the M linear systems:

$$A\mathbf{x}_m = \mathbf{b}_m \qquad m = 1, \ldots, M$$

Donc:

- the cost of the factorization $A = LU$ is $\frac{2}{3}n^3 flops$;
- the cost of the resolution of both triangular systems, $L\mathbf{y}_m = \mathbf{b}_m$ and $U\mathbf{x}_m = \mathbf{y}_m$ $(m = 1, \ldots, M)$ is $2Mn^2 flops$,

for a total of $\frac{2}{3}n^3 + 2Mn^2 flops$ which is much smaller than $\frac{2}{3}Mn^3 flops$ required to solve all the systems Gauss elimination method.

The pivoting technique

It has been already noted that the Gauss method fails if a pivot becomes zero.

In that case, we can use a technique called pivoting that consists in exchanging the rows (or the columns) of the system in such a way that no pivot is zero.

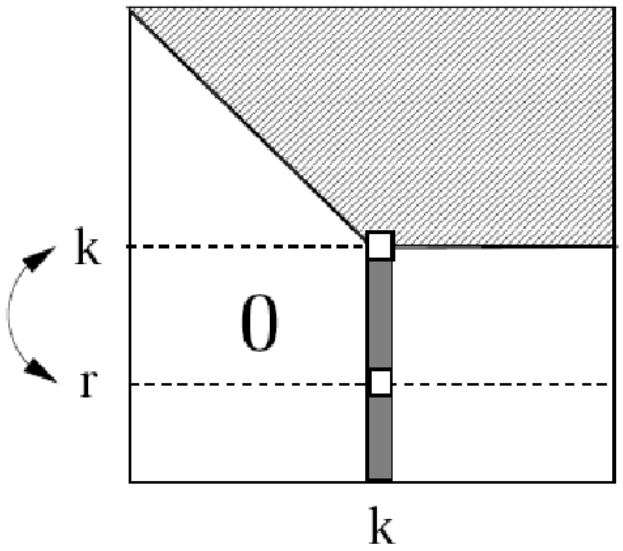
Example 5. Let us go back to the matrix (10) for which the Gauss method gives a null pivot at the second step. By just exchanging the second and the third rows, we get a non-zero pivot and can execute one step further. Indeed,

$$A^{(2)} = \begin{bmatrix} 1 & 2 & 3 \\ 0 & \boxed{0} & -1 \\ 0 & -6 & -12 \end{bmatrix} \quad \Longrightarrow \quad P_2 A^{(2)} = \begin{bmatrix} 1 & 2 & 3 \\ 0 & \boxed{-6} & -12 \\ 0 & 0 & -1 \end{bmatrix},$$

where $P_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$ is called permutation matrix.

↑ if you exchange rows
⇒ $P_2 A$: PREMULT
if column
⇒ $A P_2$: POSTMULTIPLIC

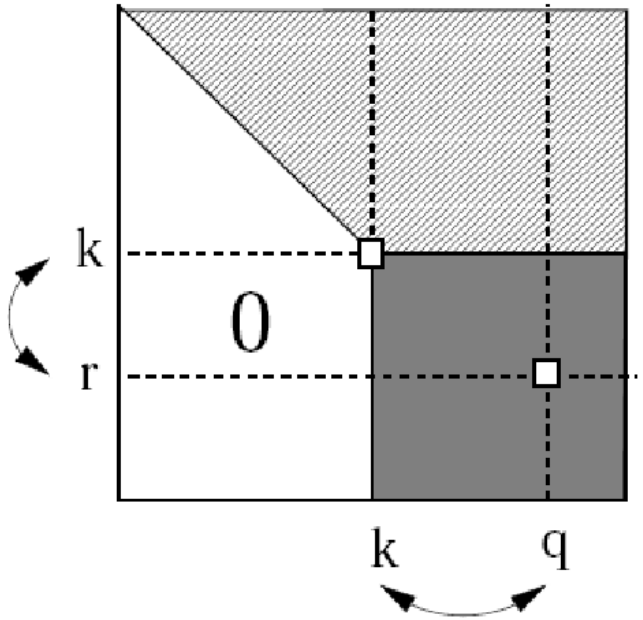
The pivoting strategy used for the example 5 can be generalized by finding, at every step k of the elimination, a non-zero pivot among the elements of the subcolumn $A^{(k)}(k:n,k)$. This is called a *partial pivot change* (by row).



From (8) we know that a big value of l_{ik} (coming for instance from a small $a_{kk}^{(k)}$) can amplify the rounding errors affecting the elements $a_{kj}^{(k)}$.

Consequently, in order to ensure a better stability, we choose as pivot the biggest element in module of the column $A^{(k)}(k:n,k)$, and the partial pivoting is performed at every step, even if it is not strictly necessary (i.e. even if the pivot is non-zero).

An alternative method consists looking for the pivot in the whole submatrix $A^{(k)}(k:n, k:n)$, performing what is called *complete pivoting*.



Remark that, whereas partial pivoting requires just an additional cost of n^2 tests, complete pivoting needs some $2n^3/3$, what considerably increases the cost of the Gauss method.

Full permutation <=> doubling of cost

In general, if at the step k we have to exchange the rows k and r, we will have to multiply $A^{(k)}$ by the following permutation matrix P_k before continuing:

$$
\begin{array}{c}
\\
k \rightarrow \\
\\
r \rightarrow \\
\\
\\
\\
\\
\\
\\
\end{array}
\begin{pmatrix}
1 & & & & & & & \\
& \ddots & & & & & & \\
& & 0 & \dots & 1 & & & \\
& & & & \vdots & & & \\
& & 1 & \dots & 0 & & & \\
& & & & & \ddots & & \\
& & & & & & 1 &
\end{pmatrix}
= P_k
$$

$$
\begin{array}{c}
\uparrow \\ r
\end{array}
\qquad
\begin{array}{c}
\uparrow \\ k
\end{array}
$$

to use on both sides of the system!

This means we will consider $P_k A^{(k)}$ insted of $A^{(k)}$.

We can prove that the result obtained is of the form:

$$\boxed{PA = LU}, \tag{11}$$

being $P = P_{n-1}P_{n-2}\dots P_2P_1$ (global permutation matrix). L is the multiplier matrix (the new ones!) and $U = A^{(n)}$.

Once the matrices L, U and P have been calculated, the resolution of the initial system is transformed into the resolution of the triangular systems

$$A\mathbf{x} = \mathbf{b} \implies PA\mathbf{x} = P\mathbf{b} \implies \begin{cases} L\mathbf{y} = P\mathbf{b}, \\ U\mathbf{x} = \mathbf{y}. \end{cases}$$

Remark that the coefficients of the matrix L have the same values as the multipliers calculated by a factorization LU of the matrix PA without pivoting.

If we use complete pivoting, it can be proved that we arrive to the following result:

$$\boxed{PAQ = LU}$$

where $P = P_{n-1} \dots P_1$ is a permutation matrix that takes into account all permutations by row, and $Q = Q_1 \dots Q_{n-1}$ is a permutation matrix that takes into account all permutations by column. By construction, la matrix L is still lower triangular, and its elements have a module lower or equal to 1.

As for the partial pivoting, the elements of L are the multipliers generated by the factorization LU of the matrix PAQ with no pivoting.

Once the matrices L, U, P and Q have been calculated, for solving the linear system we notice that we can write

$$A\mathbf{x} = \mathbf{b} \quad \Leftrightarrow \quad \underbrace{PAQ}_{LU}\underbrace{Q^{-1}\mathbf{x}}_{\mathbf{x}^*} = P\mathbf{b}\,.$$

What brings us to the resolution of triangular systems

$$\begin{cases} L\mathbf{y} = P\mathbf{b}, \\ U\mathbf{x}^* = \mathbf{y}. \end{cases}$$

and finally we compute

$$\mathbf{x} = Q\mathbf{x}^*.$$

Remark 2. *In Matlab/Octave, we can get the factorization of a matrix A with the command*

```
>> [L,U,P] = lu(A);
```

The matrix P is a permutation matrix. In the case where the matrix P is the identity, the matrices L and U are the matrices we are looking for (such that $LU = A$). Otherwise, we have $LU = PA$.

P is not needed

Example. 2 (continued) In Matlab/Octave, we first need to define the matrix `A` and the vector `b` of the linear system:

```
>> A = [-0.37, 0.05, 0.05, 0.07; 0.05, -0.116, 0, 0.05;...
        0.05, 0, -0.116, 0.05; 0.07, 0.05, 0.05, -0.202];
>> b = [-2; 0; 0; 0];
```

Then, we can use the command \ as follows:

```
>> x = A\b
x =
    8.1172
    5.9893
    5.9893
    5.7779
```

This command computes the solution of the system with *ad hoc* algorithms (it tests the matrix to choose an optimal algorithm).
Remark: the pressures at the nodes 2 and 3 are the same (by symmetry).

If we wanted to use the LU factorization:

```
>> [L,U,P] = lu(A);
>> y = L\(P*b);
>> x = U\y
x =
    8.1172
    5.9893
    5.9893
    5.7779
```

The solution is the same. We can verify that, in this case, no permutation takes place (P is the identity matrix):

```
>> P
P =
     1     0     0     0
     0     1     0     0
     0     0     1     0
     0     0     0     1
```

LU fact gives you the possibility to store LU in smarter ways

Remark 3. *Using the LU factorization, obtained by fixing the value* 1 *for the* n *diagonal elements of* L*, we can calculate the determinant of a square matrix with* $O(n^3)$ *operations, because*

binet theorem

L has diagonal elements = 1

$$\det(A) = \det(L)\det(U) = \det(U) = \prod_{k=1}^{n} u_{kk};$$

n operation

indeed, the determinant of a triangular matrix is is the product of the diagonal elements. The Matlab/Octave command `det(A)` *makes use of this.*

The inverse matrix

If A is a $n \times n$ non-singular matrix, let us call $\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(n)}$ the columns of its inverse matrix A^{-1} i.e. $A^{-1} = (\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(n)})$.
The relation $AA^{-1} = I$ can be expressed by the following n systems : for $1 \leq k \leq n$,

$$A\mathbf{x}^{(k)} = \mathbf{e}^{(k)}, \qquad (12)$$

k-th column of identity

where $\mathbf{e}^{(k)}$ is the column vector with all the elements equal to 0 except the one corresponding to the k-th row, which equals 1.
Once we know the matrices L and U that factorizes A, solving the n systems (12) defined by the same matrix A requires $2n^3$ operations.

The Cholesky factorization

In the case where the $n \times n$ matrix A is symmetric and positive definite, there exists a unique upper triangular matrix R with positive diagonal elements such that

$$\boxed{A = R^T R.}$$

This factorization is called *Cholesky factorization*. In Matlab/Octave, the command

```
>> R = chol(A)
```

can be used to compute R.

requires only 1/2 memory of LU factorization (not 2 matrices but only 1 R matrix)

upper triangular matrix and symmetric

The elements r_{ij} of R can be calculated using the expressions $r_{11} = \sqrt{a_{11}}$ and for $i = 2, \ldots, n$:

$$r_{ji} = \frac{1}{r_{jj}} \left(a_{ij} - \sum_{k=1}^{j-1} r_{ki} r_{kj} \right), \quad j = 1, \ldots, i-1, \tag{13}$$

$$r_{ii} = \sqrt{a_{ii} - \sum_{k=1}^{i-1} r_{ki}^2} \tag{14}$$

The Cholesky factorization needs around $\frac{n^3}{3}$ operations (half the operations for a LU factorization).

Example 6. In Matlab there are several families of predefined matrices (see `help gallery`). Let us consider the family of the *Lehmer* matrices, that are positive definite and thus candidates for a Cholesky factorization. We want to calculate the cost of the Cholesky factorization for matrices of size $n = 10, 20, 30, 40$ and 50.

Remark : In the version 5 of Matlab there was available the command `flops` which allowed to calculate the number of operations executed. Unfortunately, in the new version 6 of Matlab, this command has been removed (due to the integration in Matlab of certain linear algebra libraries). This example can't be executed on Matlab 6:

```
>> fl=[];
>> for n=10:10:50
    A=gallery('lehmer',n);
    flops(0)
    R=chol(A);
    fl = [fl, flops];
   end
```

We get the number of *flops* for the different sizes

```
>> fl
fl =
         385         2870         9455        22140        42925
```

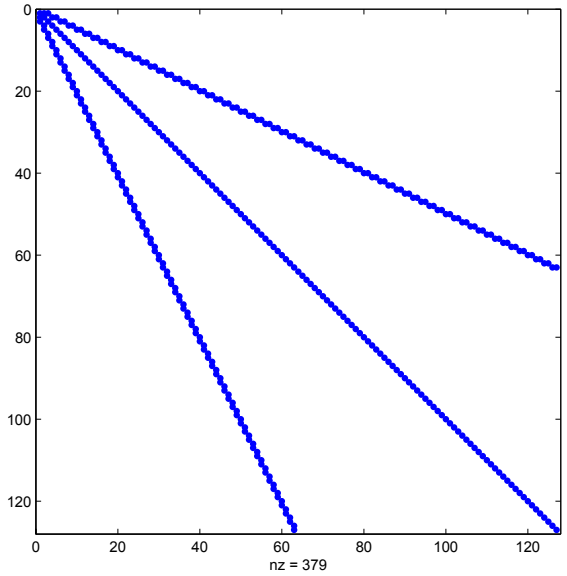
that grow proportionally to n^3. Indeed, if we calculate the ratio $fl(n)/n^3$ we find a "quasi" constant value.

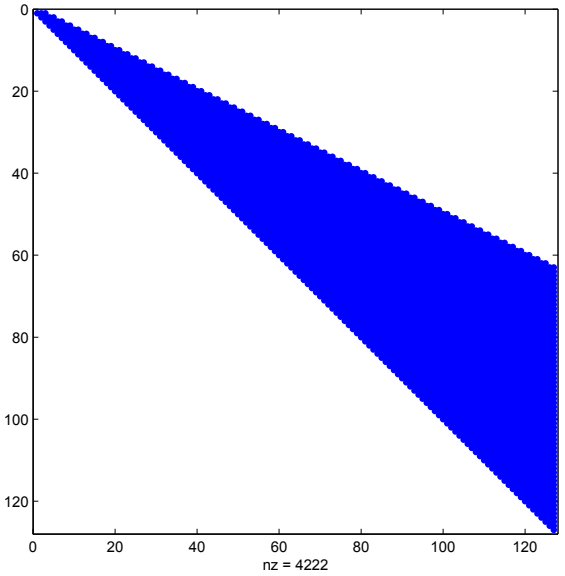
```
>> n=[10, 20, 30, 40, 50];
>> fl./(n.^3)
ans =
    0.3850    0.3588    0.3502    0.3459    0.3434
```

Remark that this value is approximately $\frac{1}{3}$. Thus, we can say that the computational cost of the Cholesky factorization is of order $\frac{1}{3}n^3$, or half the cost of the Gauss elimination method.

Memory space limitations

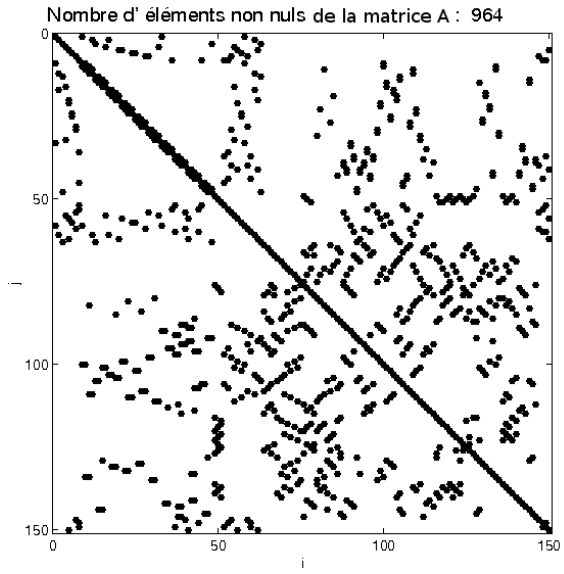
Example. 1 (continued) Let A be a matrix of size 127×127 corresponding to capillary bed with 8 bifurcation levels. This matrix is symmetric definite positive. The number of non-null entries of A is 379 and thus much smaller than $(127)^2 = 16129$. It is a *sparse* matrix. The figure on the left shows the disposition of the non-null entries of A, whereas the one on the right shows the non-null entries of the matrix R.

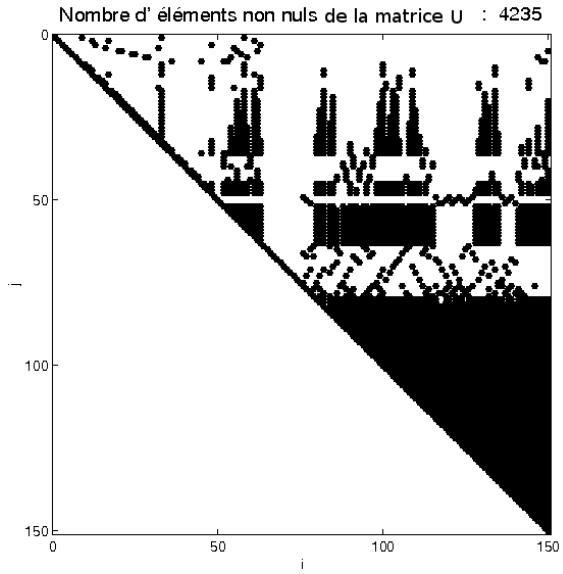




Example 7. Let us consider the problem of calculating the deformations in a structure subject to a given set of forces. The discretization using the finite elements method generates a matrix A of size 150×150. (The same matrix would have been produced by the approximation of an electric potential field.) This matrix is symmetric definite positive. The number of non-null entries of A is 964, and thus much smaller than $(150)^2 = 22500$. It is a *sparse* matrix.

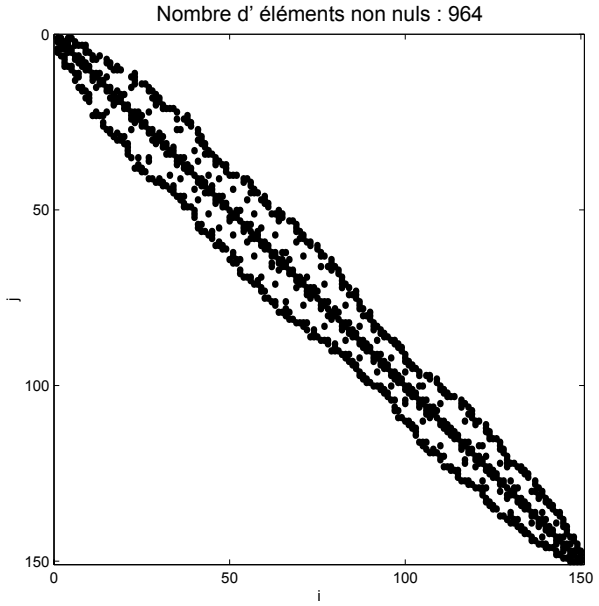
The figure on the left shows the disposition of the non-null entries of A, whereas the one on the right shows the non-null entries of the matrix R.

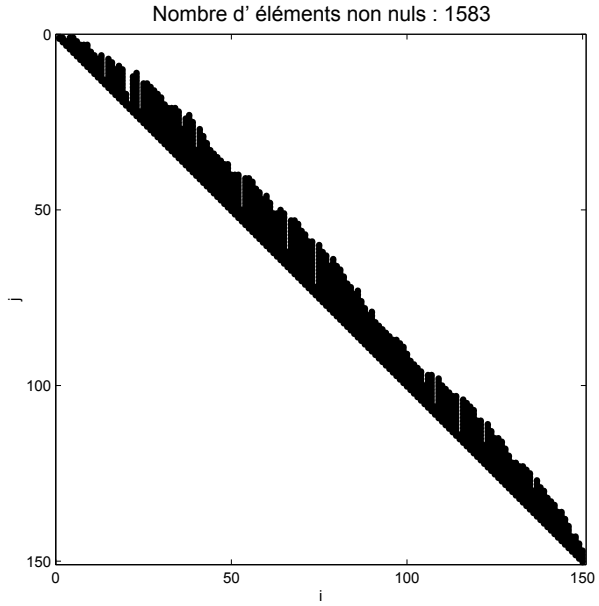




We notice that the number of non-null entries of R is much bigger than those of A (*fill-in phenomenon*). This leads to a bigger memory usage. To reduce the fill-in phenomenon, we can we can re-order rows and columns of A in a particular fashion; this is called *re-ordering* of the matrix. There are several algorithms that allow us to do this (Matlab command: `symand`).

For example, the following figure shows, on the left, one possibility of reordering A, while the one on the right shows the disposition of the non-null entries of the Cholesky factorization of the reordered matrix A.





concentrating elements around diagonals gives stability

to be defined

Precision limitations

Example 8. Rounding errors can induce important differences between the calculated solution using the Gauss elimination method (GEM) and the exact solution. This happens when the *conditioning* of the matrix of the system is very big.

The Hilbert matrix of size $n \times n$ is a symmetric matrix defined by:

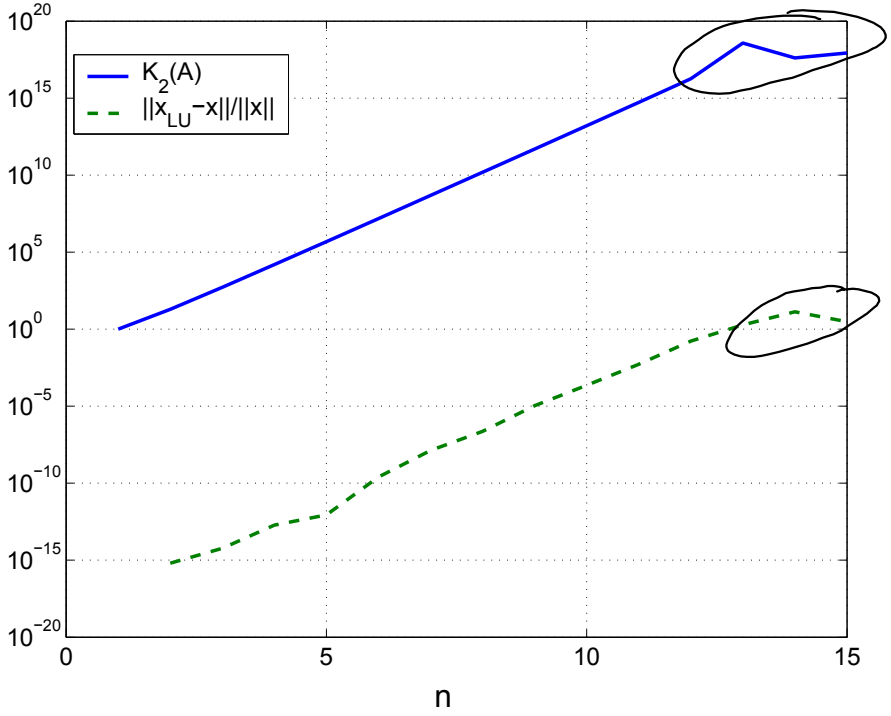
$$A_{ij} = \frac{1}{i+j-1}, \qquad i,j = 1,\ldots,n$$

In Matlab/Octave, we can build a Hilbert matrix of any size n with the command `A = hilb(n)`. For example, for $n = 4$, we get:

$$A = \begin{bmatrix} 1 & \frac{1}{2} & \frac{1}{3} & \frac{1}{4} \\ \frac{1}{2} & \frac{1}{3} & \frac{1}{4} & \frac{1}{5} \\ \frac{1}{3} & \frac{1}{4} & \frac{1}{5} & \frac{1}{6} \\ \frac{1}{4} & \frac{1}{5} & \frac{1}{6} & \frac{1}{7} \end{bmatrix}$$

We consider the linear systems $A_n \mathbf{x}_n = \mathbf{b}_n$ where A_n is the Hilbert matrix of size n with $n = 4, 6, 8, 10, 12, 14, \ldots$, whereas $\mathbf{b}_n$ is chosen such that the exact solution is $\mathbf{x}_n = (1, 1, \cdots, 1)^T$.

For every n, we calculate the conditioning of the matrix, we solve the linear system by LU factorization and we get $\mathbf{x}_n^{LU}$ as the found solution. The obtained conditioning as well as the error $\|\mathbf{x}_n - \mathbf{x}_n^{LU}\|/\|\mathbf{x}_n\|$ (where $\|\cdot\|$ is the euclidian norm of a vector, $\|\mathbf{x}\| = \sqrt{\mathbf{x}^T \cdot \mathbf{x}}$) are shown in the figure below.



tells us matrix is "uncontrollable"

relative error in order of magnitude of the solution => it is NOT reliable

Considerations on the precision (Sect. 5.5

The methods we have seen until now allow us to find the solution of a linear system in a finite number of operations. That is why they are called *direct methods*. However, there are cases where these methods are not satisfactory.

Definition 1. *We call* ***conditioning*** *of a matrix M, symmetric definite positive, the ratio between the maximum and minimum of its eigenvalues, i.e.*

$$K(M) = \frac{\lambda_{max}(M)}{\lambda_{min}(M)}$$

If h is too big => got shitty behavior

It can be shown that, the bigger the conditioning of a matrix, the worse the solution obtained by a direct method.
For example, let us consider a linear system $A\mathbf{x} = \mathbf{b}$.
If we solve this system with a computer, due to rounding errors, we will not find the exact solution $\mathbf{x}$ but an approximate solution $\hat{\mathbf{x}}$. The following relationship can be shown :

needs to be estimated because x is generally NOT known

$$\frac{\|\mathbf{x} - \hat{\mathbf{x}}\|}{\|\mathbf{x}\|} \leq K(A) \frac{\|\mathbf{r}\|}{\|\mathbf{b}\|} \tag{15}$$

where $\mathbf{r}$ is the residual $\mathbf{r} = \mathbf{b} - A\hat{\mathbf{x}}$; we write as $\|\mathbf{v}\| = \left(\sum_{k=1}^{n} v_k^2\right)^{1/2}$ the Euclidean norm of a vector $\mathbf{v}$.
Remark that, if the conditioning of A is big, the distance $\|\mathbf{x} - \hat{\mathbf{x}}\|$ between the exact solution and the numerically computed solution can be very big even if the residual is very small.

Proof for (15) : Let A be a symmetric definite positive matrix, we can consider the n eigenvalues $\lambda_i > 0$ and the associated unitary eigenvectors $\{\mathbf{v}_i\}$, $i = 1, \ldots, n$: $A\mathbf{v}_i = \lambda_i \mathbf{v}_i$, $i = 1, \ldots, n$. These vectors form an orthonormal base of $\mathbb{R}^n$, what means $\mathbf{v}_i^T \mathbf{v}_j = \delta_{ij}$ for $i, j = 1, \ldots, n$. For any $\mathbf{w} \in \mathbb{R}^n$, if we write it as

$$\mathbf{w} = \sum_{i=1}^{n} w_i \mathbf{v}_i,$$

we have

$$\begin{aligned} \|A\mathbf{w}\|^2 &= (A\mathbf{w})^T (A\mathbf{w}) \\ &= (\lambda_1 w_1 \mathbf{v}_1^T + \ldots \lambda_n w_n \mathbf{v}_n^T)(\lambda_1 w_1 \mathbf{v}_1 + \ldots \lambda_n w_n \mathbf{v}_n) \\ &= \sum_{i,j=1}^{n} \lambda_i \lambda_j w_i w_j \mathbf{v}_i^T \mathbf{v}_j = \sum_{i,j=1}^{n} \lambda_i \lambda_j w_i w_j \delta_{ij} = \sum_{i=1}^{n} \lambda_i^2 w_i^2. \end{aligned}$$

And yet, as $\|\mathbf{w}\|^2 = \sum_{i=1}^{n} w_i^2$, we get $\|A\mathbf{w}\|^2 \leq \lambda_{max}^2 \|\mathbf{w}\|^2$, i.e.
$\|A\mathbf{w}\| \leq \lambda_{max}\|\mathbf{w}\|$ where λ_{max} is the biggest eigenvalue of A.

As the eigenvalues of A^{-1} are $1/\lambda_i$, we also get
$\|A^{-1}\mathbf{w}\| \leq \frac{1}{\lambda_{min}}\|\mathbf{w}\|$ $\forall \mathbf{w} \in \mathbb{R}^n$, where λ_{min} is the smallest eigenvalue of A.
Thus, we have

$$\begin{aligned} \|\mathbf{x} - \hat{\mathbf{x}}\| &= \|A^{-1}\mathbf{r}\| \leq \frac{1}{\lambda_{min}}\|\mathbf{r}\|, \\ \|\mathbf{b}\| &= \|A\mathbf{x}\| \leq \lambda_{max}\|\mathbf{x}\|, \end{aligned}$$

from where we directly find the inequality (15). ■

Linear Systems - Iterative Methods

Numerical Analysis

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2019-SISSA mathLab Trieste

(Sec. 5.9 of the book)

Solve the linear system $A\mathbf{x} = \mathbf{b}$ using an iterative method consists in building a series of vectors $\mathbf{x}^{(k)}$, $k \geq 0$, in $\mathbb{R}^n$ that converge at the exact solution $\mathbf{x}$, i.e.:

$$\lim_{k \to \infty} \mathbf{x}^{(k)} = \mathbf{x}$$

for any initial vector $\mathbf{x}^{(0)} \in \mathbb{R}^n$.
We can consider the following recurrence relation:

$$\mathbf{x}^{(k+1)} = B\mathbf{x}^{(k)} + \mathbf{g}, \quad k \geq 0 \tag{1}$$

where B is a well chosen matrix (depending on A) and $\mathbf{g}$ is a vector (that depends on A and $\mathbf{b}$), satisfying the relation (of consistence)

$$\mathbf{x} = B\mathbf{x} + \mathbf{g}. \tag{2}$$

Given $\mathbf{x} = A^{-1}\mathbf{b}$, we get $\mathbf{g} = (I - B)A^{-1}\mathbf{b}$; the iterative method is therefore completely defined by the matrix B, known as *iteration matrix*.
By defining the error at step k as

$$\mathbf{e}^{(k)} = \mathbf{x} - \mathbf{x}^{(k)},$$

error for each iteration
$(2) - (1)$

we obtain the following recurrence relation:

$$\mathbf{e}^{(k+1)} = B\mathbf{e}^{(k)} \quad \text{and thus} \quad \mathbf{e}^{(k+1)} = B^{k+1}\mathbf{e}^{(0)}, \quad k = 0, 1, \ldots.$$

We can show that $\lim_{k\to\infty} \mathbf{e}^{(k)} = \mathbf{0}$ for all $\mathbf{e}^{(0)}$ (and thus for all $\mathbf{x}^{(0)}$) if and only if

$$\boxed{\rho(B) < 1,}$$

or $\rho(B)$ is the *spectral radius* of the matrix B, defined by

$$\boxed{\rho(B) = \max |\lambda_i(B)|}$$

and $\lambda_i(B)$ are the eigenvalues of the matrix B.

The smaller the value of $\rho(B)$, the less iterations are needed to reduce the initial error of a given factor.

Construction of an iterative method

A general way of setting up an iterative method is based on the decomposition of the matrix A:

$$A = P - (P - A)$$

where P in an invertible matrix called *preconditioner* of A.
Hence,

$$A\mathbf{x} = \mathbf{b} \quad \Leftrightarrow \quad P\mathbf{x} = (P - A)\mathbf{x} + \mathbf{b}$$

which is of the form (2) leaving

$$B = P^{-1}(P - A) = I - P^{-1}A \quad \text{and} \quad \mathbf{g} = P^{-1}\mathbf{b}.$$

We can define the corresponding iterative method

$$P(\mathbf{x}^{(k+1)} - \mathbf{x}^{(k)}) = \mathbf{r}^{(k)} \qquad k \geq 0$$

where $\mathbf{r}^{(k)}$ represents the *residual* at the iteration k: $\mathbf{r}^{(k)} = \mathbf{b} - A\mathbf{x}^{(k)}$

We can generalise this method as follows:

$$P(\mathbf{x}^{(k+1)} - \mathbf{x}^{(k)}) = \alpha_k \mathbf{r}^{(k)} \qquad k \geq 0 \tag{3}$$

where $\alpha_k \neq 0$ is a parameter that improves the convergence of the series $\mathbf{x}^{(k)}$. The method (3) is called *Richardson's method*.

The matrix P has to be chosen in such a way that renders the cost of solving (3) small enough. For example a diagonal or triangular P matrix would comply with this criterion.

Jacobi method

If the elements of the diagonal of A are non-zero, we can write

$$P = D = diag(a_{11}, a_{22}, \ldots, a_{nn})$$

D with the diagonal part of A being:

$$D_{ij} = \begin{cases} 0 & \text{si } i \neq j \\ a_{ij} & \text{if } i = j. \end{cases}$$

The Jacobi method corresponds to this choice with $\alpha_k = 1$ for all k.
We deduce:

$$D\mathbf{x}^{(k+1)} = \mathbf{b} - (A - D)\mathbf{x}^{(k)} \qquad k \geq 0.$$

By components:

$$x_i^{(k+1)} = \frac{1}{a_{ii}} \left(b_i - \sum_{j=1, j \neq i}^{n} a_{ij} x_j^{(k)} \right), \quad i = 1, \ldots, n. \tag{4}$$

NO DIAGONAL!

The Jacobi method can be written under the general form

$$\mathbf{x}^{(k+1)} = B\mathbf{x}^{(k)} + \mathbf{g},$$

with

$$B = B_J = D^{-1}(D - A) = I - D^{-1}A, \qquad \mathbf{g} = \mathbf{g}_J = D^{-1}\mathbf{b}.$$

Gauss-Seidel method

This method is defined as follows:

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

Take advantage also of partial x^{k+1} at current iteration already computed

This method corresponds to (1) with $P = D - E$ and $\alpha_k = 1$ ($\forall k \geq 0$) where E is the lower triangular matrix

D: diagonal; $-E$: lower triangular

$$\begin{cases} E_{ij} = -a_{ij} & \text{if } i > j \\ E_{ij} = 0 & \text{if } i \leq j \end{cases}$$

(lower triangular part of A without the diagonal and with its elements' sign inverted).

We can write this method under the form (3), with the iteration matrix $B = B_{GS}$ given by

$$B_{GS} = (D - E)^{-1}(D - E - A)$$

and

$$\mathbf{g}_{GS} = (D - E)^{-1}\mathbf{b}.$$

why not only E?
Library (historically)
builds matrix by block,
using also the diagonal

Example 1. Given the matrix

$$A = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 \\ 9 & 10 & 11 & 12 \\ 13 & 14 & 15 & 16 \end{pmatrix}.$$

We have then

$$D = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 6 & 0 & 0 \\ 0 & 0 & 11 & 0 \\ 0 & 0 & 0 & 16 \end{pmatrix};$$

Thus, the iteration matrix for the Jacobi method is

Not symmetric

$$B_J = D^{-1}(D - A) = I - D^{-1}A = \begin{pmatrix} 0 & -2 & -3 & -4 \\ -5/6 & 0 & -7/6 & -4/3 \\ -9/11 & -10/11 & 0 & -12/11 \\ -13/16 & -14/16 & -15/16 & 0 \end{pmatrix}.$$

For defining the matrix A and extracting its diagonal D and its lower triangular part E (without the diagonal and the sign inverted) with Matlab/Octave, we use the commands

```
>> A = [1,2,3,4;5,6,7,8;9,10,11,12;13,14,15,16];
>> D = diag(diag(A));
>> E = - tril(A,-1);
```

These allow us, for exemple, to compute the iteration matrix B_{GS} for the Gauss-Seidel method in the following way:

```
>> B_GS = (D-E)\(D-E-A);
```

We find:

$$B_{GS} = \begin{pmatrix} 0.0000 & -2.0000 & -3.0000 & -4.000 \\ 0.0000 & 1.6667 & 1.3333 & 2.0000 \\ 0.0000 & 0.1212 & 1.2424 & 0.3636 \\ 0.0000 & 0.0530 & 0.1061 & 1.1591 \end{pmatrix}.$$

Convergence

We have the following convergence results:

- (Prop 5.3) If the matrix A is strictly diagonally dominant by row, i.e.,

$$|a_{ii}| > \sum_{j=1,\ldots,n;j\neq i} |a_{ij}|, \quad i = 1,\ldots,n,$$

  then the Jacobi and the Gauss-Seidel methods converge.

- If A is symmetric positive definite, then the Gauss-Seidel method converges (Jacobi maybe not).

- (Prop 5.4) Let A be a tridiagonal non-singular matrix whose diagonal elements are all non-null. Then the Jacobi and the Gauss-Seidel methods are either both divergent or both convergent. In the latter case, $\rho(B_{GS}) = \rho(B_J)^2$.

Non zero element only on the 3 biggest "diagonals"

(≤)

! For Jacobi and Gauss-Seidel $\alpha_k = 1$ (⇒ we are NOT accelerating)

Richardson method

(Sec. 5.10)

Let consider the following iterative method:

$$P(\mathbf{x}^{(k+1)} - \mathbf{x}^{(k)}) = \alpha_k \mathbf{r}^{(k)}, \qquad k \geq 0. \tag{5}$$

If $\alpha_k = \alpha$ (a constant) this method is called stationary preconditioned Richardson method; otherwise dynamic preconditioned Richardson method when α_k varies during the iterations.

The matrix P is called preconditioner of A.

If A and P are symmetric positive definite, then there are two optimal criteria to choose α_k:

1. *Stationary case*:

$$\alpha_k = \alpha_{opt} = \frac{2}{\lambda_{min} + \lambda_{max}}, \qquad k \geq 0,$$

← from algebraic and geometrical properties

where λ_{min} and λ_{max} represent the smaller and the larger eigenvalue of the matrix $P^{-1}A$.

2. *Dynamic case*:

$$\alpha_k = \frac{(\mathbf{z}^{(k)})^T \mathbf{r}^{(k)}}{(\mathbf{z}^{(k)})^T A \mathbf{z}^{(k)}}, \qquad k \geq 0,$$

This is a lin syst

where $\mathbf{z}^{(k)} = P^{-1}\mathbf{r}^{(k)}$ is the preconditioned residual. ← it is a TRF of the residual vector

This method is also called preconditioned gradient method.

If $P = I$ and A is symmetric definite positive, we get the following methods:

- the Stationary Richardson if we choose:

$$\alpha_k = \alpha_{opt} = \frac{2}{\lambda_{min}(A) + \lambda_{max}(A)}. \tag{6}$$

$P^{-1}A = A$

- the Gradient method if :

$$\alpha_k = \frac{(\mathbf{r}^{(k)})^T \mathbf{r}^{(k)}}{(\mathbf{r}^{(k)})^T A \mathbf{r}^{(k)}}, \qquad k \geq 0. \tag{7}$$

$P^{-1}r = r$

The gradient method can be written as:
Let $\mathbf{x}^{(0)}$ be given, set $\mathbf{r}^{(0)} = \mathbf{b} - A\mathbf{x}^{(0)}$, then for $k \geq 0$,

$$
\begin{aligned}
P\mathbf{z}^{(k)} &= \mathbf{r}^{(k)} \\
\alpha_k &= \frac{(\mathbf{z}^{(k)})^T \mathbf{r}^{(k)}}{(\mathbf{z}^{(k)})^T A\mathbf{z}^{(k)}} \\
\mathbf{x}^{(k+1)} &= \mathbf{x}^{(k)} + \alpha_k \mathbf{z}^{(k)} \\
\mathbf{r}^{(k+1)} &= \mathbf{r}^{(k)} - \alpha_k A\mathbf{z}^{(k)}.
\end{aligned}
$$

We have to apply once A and inverse P at each iteration. P should then be such that the resolution of the associated system results easy (i.e. it requires a reasonable amount of computing cost). For example, we can choose a diagonal P (Like in the gradient or the stationary Richardson cases) or triangular.

Convergence of Richardson method

When A and P are s.p.d. and with the two optimal choices for α, we can show that the preconditioned Richardson Method converges to x when $k \to \infty$, and that

$$\|\mathbf{x}^{(k)} - \mathbf{x}\|_A \leq \left(\frac{K(P^{-1}A) - 1}{K(P^{-1}A) + 1} \right)^k \|\mathbf{x}^{(0)} - \mathbf{x}\|_A, \quad k \geq 0, \tag{8}$$

where $\|\mathbf{v}\|_A = \sqrt{\mathbf{v}^T A \mathbf{v}}$ and $K(P^{-1}A)$ is the condition number of $P^{-1}A$.

Remark If A et P are s.p.d., we have that

$$K(P^{-1}A) = \frac{\lambda_{max}}{\lambda_{min}}.$$

Demonstration The iteration matrix of the method is given by $R_\alpha = I - \alpha P^{-1} A$, where the eigenvalues of R_α are of the form $1 - \alpha\lambda_i$. The method is convergent if and only if $|1 - \alpha\lambda_i| < 1$ for $i = 1, \ldots, n$, therefore $-1 < 1 - \alpha\lambda_i < 1$ for $i = 1, \ldots, n$. As $\alpha > 0$, this is the equivalent to $-1 < 1 - \alpha\lambda_{max}$, from where the necessary and sufficient condition for convergence remains $\alpha < 2/\lambda_{max}$. Consequently, $\rho(R_\alpha)$ is minimal if $1 - \alpha\lambda_{min} = \alpha\lambda_{max} - 1$, i.e., for $\alpha_{opt} = 2/(\lambda_{min} + \lambda_{max})$. By substitution, we obtain

$$\rho_{opt} = \rho(R_{opt}) = 1 - \alpha_{opt}\lambda_{min} = 1 - \frac{2\lambda_{min}}{\lambda_{min} + \lambda_{max}} = \frac{\lambda_{max} - \lambda_{min}}{\lambda_{min} + \lambda_{max}}$$

what allows us to complete the proof. □

In the dynamic case, we get a result that allows us to optimally choose the iteration parameters at each step, if the matrix A is symmetric definite positive:

Theorem 1 (Dynamic case)**.** *If A is symmetric definite positive, the optimal choice for α_k is given by*

$$\alpha_k = \frac{(\mathbf{r}^{(k)}, \mathbf{z}^{(k)})}{(A\mathbf{z}^{(k)}, \mathbf{z}^{(k)})}, \qquad k \geq 0 \tag{9}$$

where

$$\mathbf{z}^{(k)} = P^{-1}\mathbf{r}^{(k)}. \tag{10}$$

Demonstration On the one hand we have

sometimes not present in literature

$$\mathbf{r}^{(k)} = \mathbf{b} - A\mathbf{x}^{(k)} = A(\mathbf{x} - \mathbf{x}^{(k)}) = A\mathbf{e}^{(k)}, \tag{11}$$

and thus, using (10),

$$P^{-1}A\mathbf{e}^{(k)} = -\mathbf{z}^{(k)}, \tag{12}$$

where $\mathbf{e}^{(k)}$ represents the error at the step k. On the other hand

$$\mathbf{e}^{(k+1)} = \mathbf{e}^{(k+1)}(\alpha) = \underbrace{(I - \alpha P^{-1}A)}_{R_\alpha}\mathbf{e}^{(k)}.$$

some kind of a (static or dynamic)

We notice that, in order to update the residual, we have the relation

$$\mathbf{r}^{(k+1)} = \mathbf{r}^{(k)} - \alpha A\mathbf{z}^{(k)} = \mathbf{r}^{(k)} - \alpha AP^{-1}\mathbf{r}^{(k)}.$$

Thus, expressing as $\|\cdot\|_A$ the vector norm associated to the scalar product $(\mathbf{x},\mathbf{y})_A = (A\mathbf{x},\mathbf{y})$, what means, $\|\mathbf{x}\|_A = (A\mathbf{x},\mathbf{x})^{1/2}$ we can write

Remember: A is symmetric

$$\begin{aligned}
\|\mathbf{e}^{(k+1)}\|_A^2 &= (A\mathbf{e}^{(k+1)},\mathbf{e}^{(k+1)}) = -(\mathbf{r}^{(k+1)},\mathbf{e}^{(k+1)}) \\
&= -(\mathbf{r}^{(k)} - \alpha AP^{-1}\mathbf{r}^{(k)}, \mathbf{e}^{(k)} - \alpha P^{-1}A\mathbf{e}^{(k)}) \\
&= -(\mathbf{r}^{(k)},\mathbf{e}^{(k)}) + \alpha[(\mathbf{r}^{(k)}, P^{-1}A\mathbf{e}^{(k)}) + (A\mathbf{z}^{(k)},\mathbf{e}^{(k)})] \\
&\quad -\alpha^2(A\mathbf{z}^{(k)}, P^{-1}A\mathbf{e}^{(k)})
\end{aligned}$$

Now we choose α as the α_k that minimises $\|\mathbf{e}^{(k+1)}(\alpha)\|_A$:

$$\frac{d}{d\alpha}\|\mathbf{e}^{(k+1)}(\alpha)\|_A\Big|_{\alpha=\alpha_k} = 0$$

We then obtain

$$\alpha_k = \frac{1}{2}\frac{(\mathbf{r}^{(k)}, P^{-1}A\mathbf{e}^{(k)}) + (A\mathbf{z}^{(k)}, \mathbf{e}^{(k)})}{(A\mathbf{z}^{(k)}, P^{-1}A\mathbf{e}^{(k)})} = \frac{1}{2}\frac{-(\mathbf{r}^{(k)}, \mathbf{z}^{(k)}) + (A\mathbf{z}^{(k)}, \mathbf{e}^{(k)})}{-(A\mathbf{z}^{(k)}, \mathbf{z}^{(k)})}$$

and using the equality $(A\mathbf{z}^{(k)}, \mathbf{e}^{(k)}) = (\mathbf{z}^{(k)}, A\mathbf{e}^{(k)})$ knowing that A is symmetric definite positive, and noting that $A\mathbf{e}^{(k)} = -\mathbf{r}^{(k)}$, we find

$$\alpha_k = \frac{(\mathbf{r}^{(k)}, \mathbf{z}^{(k)})}{(A\mathbf{z}^{(k)}, \mathbf{z}^{(k)})}$$

For the stationary case and for the dynamic one we can prove that, if A and P are symmetric definite positive, the series $\{\mathbf{x}^{(k)}\}$ given by the Richardson method (stationary and dynamic) converges towards $\mathbf{x}$ when $k \to \infty$, and

$$\|\mathbf{x}^{(k)} - \mathbf{x}\|_A \leq \left(\frac{K(P^{-1}A) - 1}{K(P^{-1}A) + 1} \right)^k \|\mathbf{x}^{(0)} - \mathbf{x}\|_A, \quad k \geq 0, \tag{13}$$

Again, K should make sense $\leftrightarrow$ A should be stable

where $\|\mathbf{v}\|_A = \sqrt{\mathbf{v}^T A \mathbf{v}}$ and $K(P^{-1}A)$ is the conditioning of the matrix $P^{-1}A$.

Remark. In the case of the gradient method or the Richardson stationary method the error estimation becomes

$$\|\mathbf{x}^{(k)} - \mathbf{x}\|_A \leq \left(\frac{K(A)-1}{K(A)+1}\right)^k \|\mathbf{x}^{(0)} - \mathbf{x}\|_A, \quad k \geq 0. \tag{14}$$

Remark. If A and P are symmetric definite positive, we have

$$K(P^{-1}A) = \frac{\lambda_{max}(P^{-1}A)}{\lambda_{min}(P^{-1}A)}.$$

The conjugate gradient method

(Sec. 5.11)

When A and P are s.p.d, there exists a very efficient and effective method to iteratively solve the system: the conjugate gradient method

Let $\mathbf{x}^{(0)}$ be given; we compute $\mathbf{r}^{(0)} = \mathbf{b} - A\mathbf{x}^{(0)}$, $\mathbf{z}^{(0)} = P^{-1}\mathbf{r}^{(0)}$, $\mathbf{p}^{(0)} = \mathbf{z}^{(0)}$,then for $k \geq 0$,

$$
\begin{aligned}
\alpha_k &= \frac{{\mathbf{p}^{(k)}}^T \mathbf{r}^{(k)}}{{\mathbf{p}^{(k)}}^T A\mathbf{p}^{(k)}} \\
\mathbf{x}^{(k+1)} &= \mathbf{x}^{(k)} + \alpha_k \mathbf{p}^{(k)} \\
\mathbf{r}^{(k+1)} &= \mathbf{r}^{(k)} - \alpha_k A\mathbf{p}^{(k)} \\
P\mathbf{z}^{(k+1)} &= \mathbf{r}^{(k+1)} \\
\beta_k &= \frac{\left(A\mathbf{p}^{(k)}\right)^T \mathbf{z}^{(k+1)}}{\left(A\mathbf{p}^{(k)}\right)^T \mathbf{p}^{(k)}} \\
\mathbf{p}^{(k+1)} &= \mathbf{z}^{(k+1)} - \beta_k \mathbf{p}^{(k)} .
\end{aligned}
$$

Now we correct also the DIRECTION. correction given by $p^{(k)}$

given as A conjugate (A orthogonal) direction wrt the direction $p^{(k-1)}$

special directions are NOT so, but only in number = to order of A matrix

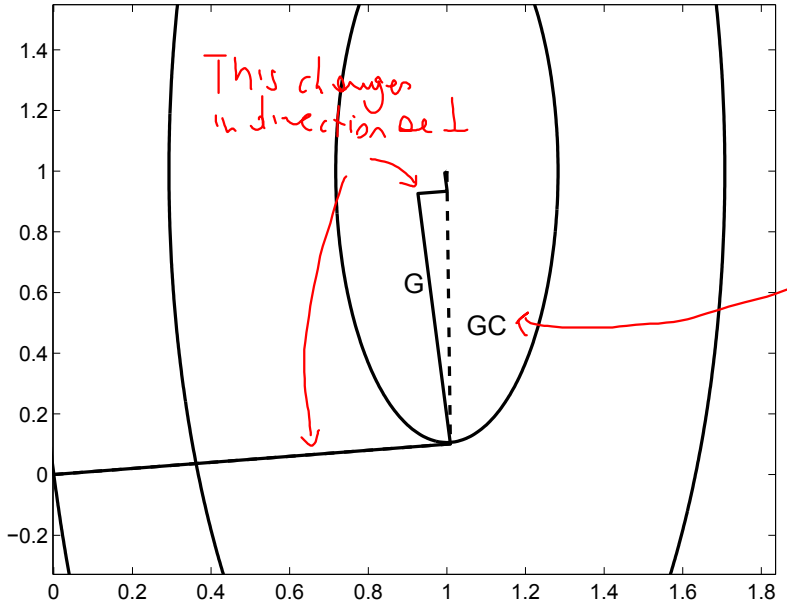
The error estimate is given by

$$\|\mathbf{x}^{(k)} - \mathbf{x}\|_A \leq \frac{2c^k}{1+c^{2k}} \|\mathbf{x}^{(0)} - \mathbf{x}\|_A , \quad k \geq 0$$

où

$$c = \frac{\sqrt{K_2(P^{-1}A)} - 1}{\sqrt{K_2(P^{-1}A)} + 1} .$$

(15)



we reach solution without changing direction because we already do it in the procedure

Example 2. Let consider the following linear system:

$$\begin{cases} 2x_1 + x_2 &= 1 \\ x_1 + 3x_2 &= 0 \end{cases} \tag{16}$$

whose matrix is $A = \begin{pmatrix} 2 & 1 \\ 1 & 3 \end{pmatrix}$ is s.p.d. The solution to this system is $x_1 = 3/5 = 0.6$ et $x_2 = -1/5 = -0.2$.

Preliminary convergence studies

- A is strictly diagonal dominant by row. Hence Jacobi and Gauss-Seidel methods converge.
- A is regular, tridiagonal with non-zero diagonal elements. Then $\rho(B_{GS}) = \rho(B_J)^2$. Therefore we expect a quicker convergence of Gauss-Seidel w.r.t. Jacobi.
- A is s.p.d., hence the gradient and the conjugate gradient methods converge. Moreover (see error estimates), the CG shall converge faster.

We want to approximate the solution with an iterative method starting with

$$\mathbf{x}^{(0)} = \begin{pmatrix} x_1^{(0)} \\ x_2^{(0)} \end{pmatrix} = \begin{pmatrix} 1 \\ \frac{1}{2} \end{pmatrix}.$$

We can see that

$$\mathbf{r}^{(0)} = \mathbf{b} - A\mathbf{x}^{(0)} = \begin{pmatrix} -\frac{3}{2} \\ -\frac{5}{2} \end{pmatrix}$$

and

$$\|\mathbf{r}^{(0)}\|_2 = \sqrt{(\mathbf{r}^{(0)})^T \mathbf{r}^{(0)}} = \frac{\sqrt{34}}{2} \approx 2.9155.$$

Jacobi method

$$\mathbf{x}^{(k+1)} = B_J \mathbf{x}^{(k)} + \mathbf{g}_J, \quad k \geq 0, \qquad \text{where } B_J = I - D^{-1}A \text{ and } \mathbf{g}_J = D^{-1}\mathbf{b}.$$

We have

$$B_J = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{3} \end{pmatrix} \begin{pmatrix} 2 & 1 \\ 1 & 3 \end{pmatrix} = \begin{pmatrix} 0 & -\frac{1}{2} \\ -\frac{1}{3} & 0 \end{pmatrix}$$

$$\mathbf{g}_J = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{3} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix}$$

and $\rho(B_J) = max|\lambda_i(B_J)| = \texttt{max(abs(eig(}B_J\texttt{)))} = 0.4082.$

For $k = 0$ (first iteration) we find:

$$\mathbf{x}^{(1)} = B_J \mathbf{x}^{(0)} + \mathbf{g}_J = \begin{pmatrix} 0 & -\frac{1}{2} \\ -\frac{1}{3} & 0 \end{pmatrix} \begin{pmatrix} 1 \\ \frac{1}{2} \end{pmatrix} + \begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{1}{4} \\ -\frac{1}{3} \end{pmatrix} \approx \begin{pmatrix} 0.25 \\ -0.3333 \end{pmatrix}.$$

Notice that

$$\mathbf{r}^{(1)} = \mathbf{b} - A\mathbf{x}^{(1)} = \begin{pmatrix} 0.8333 \\ 0.75 \end{pmatrix} \qquad \text{and } \|\mathbf{r}^{(1)}\|_2 = 1.1211.$$

Gauss-Seidel method

$$\mathbf{x}^{(k+1)} = B_{GS}\mathbf{x}^{(k)} + \mathbf{g}_{GS}, \quad k \geq 0, \quad \text{where } B_{GS} = (D-E)^{-1}(D-E-A)$$

$$\text{and } \mathbf{g}_{GS} = (D-E)^{-1}\mathbf{b}.$$

We have

$$B_{GS} = \begin{pmatrix} 2 & 0 \\ 1 & 3 \end{pmatrix}^{-1} \begin{pmatrix} 0 & -1 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & 0 \\ -\frac{1}{6} & \frac{1}{3} \end{pmatrix} \begin{pmatrix} 0 & -1 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & -\frac{1}{2} \\ 0 & \frac{1}{6} \end{pmatrix}$$

$$\mathbf{g}_{GS} = \begin{pmatrix} \frac{1}{2} & 0 \\ -\frac{1}{6} & \frac{1}{3} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} \\ -\frac{1}{6} \end{pmatrix}$$

In this case $\rho(B_{GS}) = max|\lambda_i(B_{GS})| =$ `max(abs(eig(`B_{GS}`)))` $= 0.1667$.
We can verify that $\rho(B_{GS}) = \rho(B_J)^2$.

For $k = 0$ (first iteration) we find:

$$\mathbf{x}^{(1)} = B_{GS}\mathbf{x}^{(0)} + \mathbf{g}_{GS} = \begin{pmatrix} 0 & -\frac{1}{2} \\ 0 & \frac{1}{6} \end{pmatrix} \begin{pmatrix} 1 \\ \frac{1}{2} \end{pmatrix} + \begin{pmatrix} \frac{1}{2} \\ -\frac{1}{6} \end{pmatrix} = \begin{pmatrix} \frac{1}{4} \\ -\frac{1}{12} \end{pmatrix} \approx \begin{pmatrix} 0.25 \\ -0.0833 \end{pmatrix}.$$

We have

$$\mathbf{r}^{(1)} = \mathbf{b} - A\mathbf{x}^{(1)} = \begin{pmatrix} 0.5833 \\ 0 \end{pmatrix} \qquad \text{and } \|\mathbf{r}^{(1)}\|_2 = 0.5833.$$

Preconditioned gradient method with $P = D$

We set $\mathbf{r}^{(0)} = \mathbf{b} - A\mathbf{x}^{(0)} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} - \begin{pmatrix} 2 & 1 \\ 1 & 3 \end{pmatrix} \begin{pmatrix} 1 \\ \frac{1}{2} \end{pmatrix} = \begin{pmatrix} -\frac{3}{2} \\ -\frac{5}{2} \end{pmatrix}$.

For $k = 0$, we have:

$$P\mathbf{z}^{(0)} = \mathbf{r}^{(0)} \quad \Leftrightarrow \quad \mathbf{z}^{(0)} = P^{-1}\mathbf{r}^{(0)} = \begin{pmatrix} -\frac{3}{4} \\ -\frac{5}{6} \end{pmatrix}$$

$$\alpha_0 = \frac{(\mathbf{z}^{(0)})^T \mathbf{r}^{(0)}}{(\mathbf{z}^{(0)})^T A\mathbf{z}^{(0)}} = \frac{77}{107}$$

$$\mathbf{x}^{(1)} = \mathbf{x}^{(0)} + \alpha_0 \mathbf{z}^{(0)} = \begin{pmatrix} 0.4603 \\ -0.0997 \end{pmatrix}$$

$$\mathbf{r}^{(1)} = \mathbf{r}^{(0)} - \alpha_0 A\mathbf{z}^{(0)} = \begin{pmatrix} 0.1791 \\ -0.1612 \end{pmatrix} \quad \text{and } \|\mathbf{r}^{(1)}\|_2 = 0.2410.$$

Conjugated preconditioned gradient method with $P = D$

We set $\mathbf{r}^{(0)} = \mathbf{b} - A\mathbf{x}^{(0)}$, $\mathbf{z}^{(0)} = P^{-1}\mathbf{r}^{(0)}$ and $\mathbf{p}^{(0)} = \mathbf{z}^{(0)}$. For $k = 0$, we have:

$$\alpha_0 = \frac{(\mathbf{p}^{(0)})^T\mathbf{r}^{(0)}}{(\mathbf{p}^{(0)})^T A\mathbf{p}^{(0)}} = \frac{(\mathbf{z}^{(0)})^T\mathbf{r}^{(0)}}{(\mathbf{z}^{(0)})^T A\mathbf{z}^{(0)}}$$

$$\mathbf{x}^{(1)} = \mathbf{x}^{(0)} + \alpha_0\mathbf{p}^{(0)} = \mathbf{x}^{(0)} + \alpha_0\mathbf{z}^{(0)}$$

$$\mathbf{r}^{(1)} = \mathbf{r}^{(0)} - \alpha_0 A\mathbf{p}^{(0)} = \mathbf{r}^{(0)} - \alpha_0 A\mathbf{z}^{(0)}.$$

We see that the first iteration $\mathbf{x}^{(1)}$ matches with the one obtained by the preconditioned gradient method.

We then complete the first iteration of the preconditioned conjugate gradient method:

$$P\mathbf{z}^{(1)} = \mathbf{r}^{(1)} \quad \Leftrightarrow \quad \mathbf{z}^{(1)} = P^{-1}\mathbf{r}^{(1)} = \begin{pmatrix} 0.0896 \\ -0.0537 \end{pmatrix}$$

$$\beta_0 = \frac{(A\mathbf{p}^{(0)})^T\mathbf{z}^{(1)}}{(A\mathbf{p}^{(0)})^T A\mathbf{p}^{(0)}} = \frac{(A\mathbf{z}^{(0)})^T\mathbf{z}^{(1)}}{(A\mathbf{z}^{(0)})^T\mathbf{z}^{(0)}} = -0.0077$$

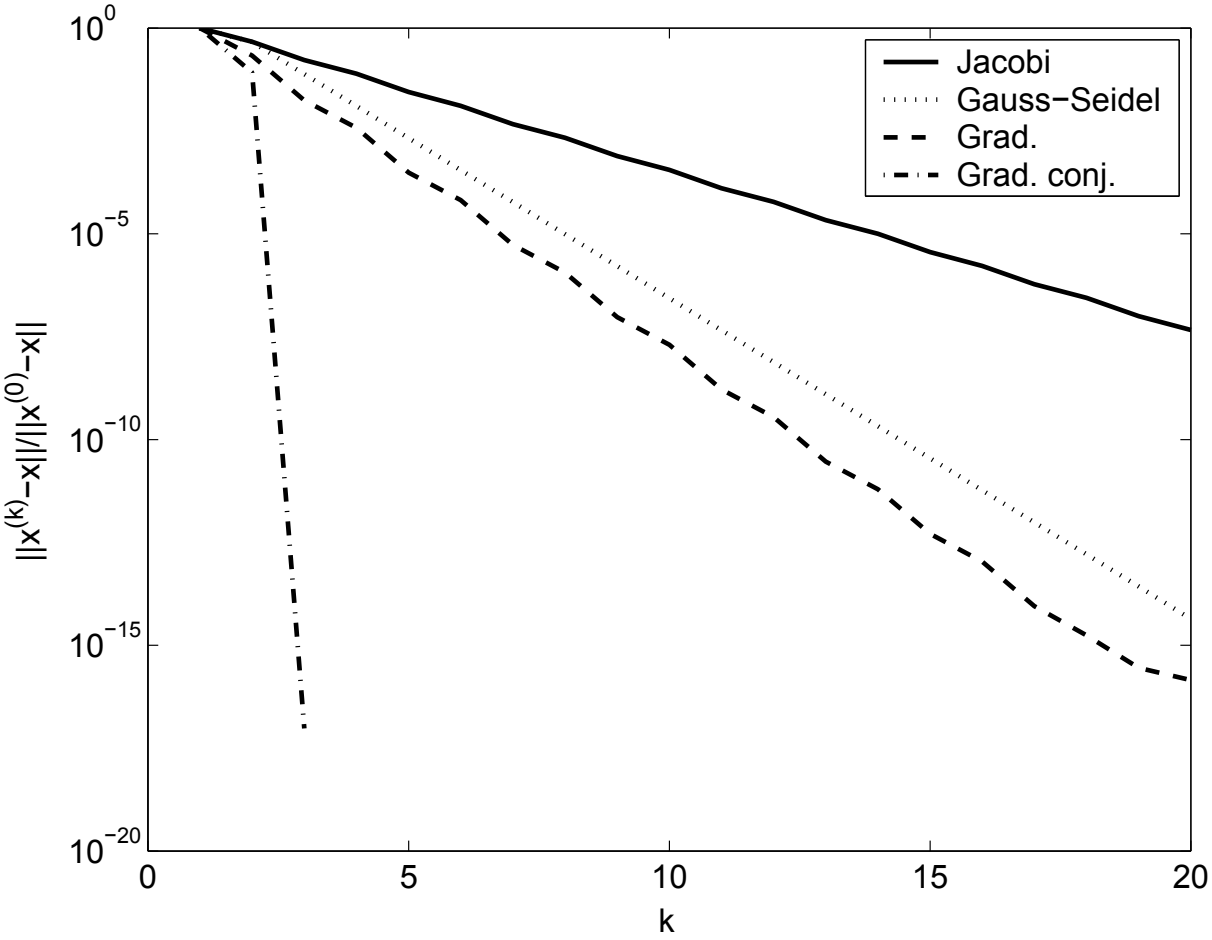
$$\mathbf{p}^{(1)} = \mathbf{z}^{(1)} - \beta_0\mathbf{p}^{(0)} = \mathbf{z}^{(1)} - \beta_0\mathbf{z}^{(0)} = \begin{pmatrix} 0.0838 \\ -0.0602 \end{pmatrix}.$$

At the second iteration, with the four different methods, we have:

Method	$\mathbf{x}^{(2)}$	$\mathbf{r}^{(2)}$	$\|\mathbf{r}^{(2)}\|_2$
Jacobi	$\begin{pmatrix} 0.6667 \\ -0.0833 \end{pmatrix}$	$\begin{pmatrix} -0.2500 \\ -0.4167 \end{pmatrix}$	0.4859
Gauss-Seidel	$\begin{pmatrix} 0.5417 \\ -0.1806 \end{pmatrix}$	$\begin{pmatrix} 0.0972 \\ 0 \end{pmatrix}$	0.0972
PG	$\begin{pmatrix} 0.6070 \\ -0.1877 \end{pmatrix}$	$\begin{pmatrix} -0.0263 \\ -0.0438 \end{pmatrix}$	0.0511
PCG	$\begin{pmatrix} 0.60000 \\ -0.2000 \end{pmatrix}$	$\begin{pmatrix} -0.2220 \\ -0.3886 \end{pmatrix} \cdot 10^{-15}$	$4.4755 \cdot 10^{-16}$

Behavior of the relative error applied to the system (16) :

Graph important for the exam



Example 3. Let now consider another example:

$$\begin{cases} 2x_1 + x_2 & = 1 \\ -x_1 + 3x_2 & = 0 \end{cases} \tag{17}$$

whose solution is $x_1 = 3/7$, $x_2 = 1/7$.

Preliminary convergence studies

The associatd matrix is $A = \begin{pmatrix} 2 & 1 \\ -1 & 3 \end{pmatrix}$. ← not symmetric => not positive definite

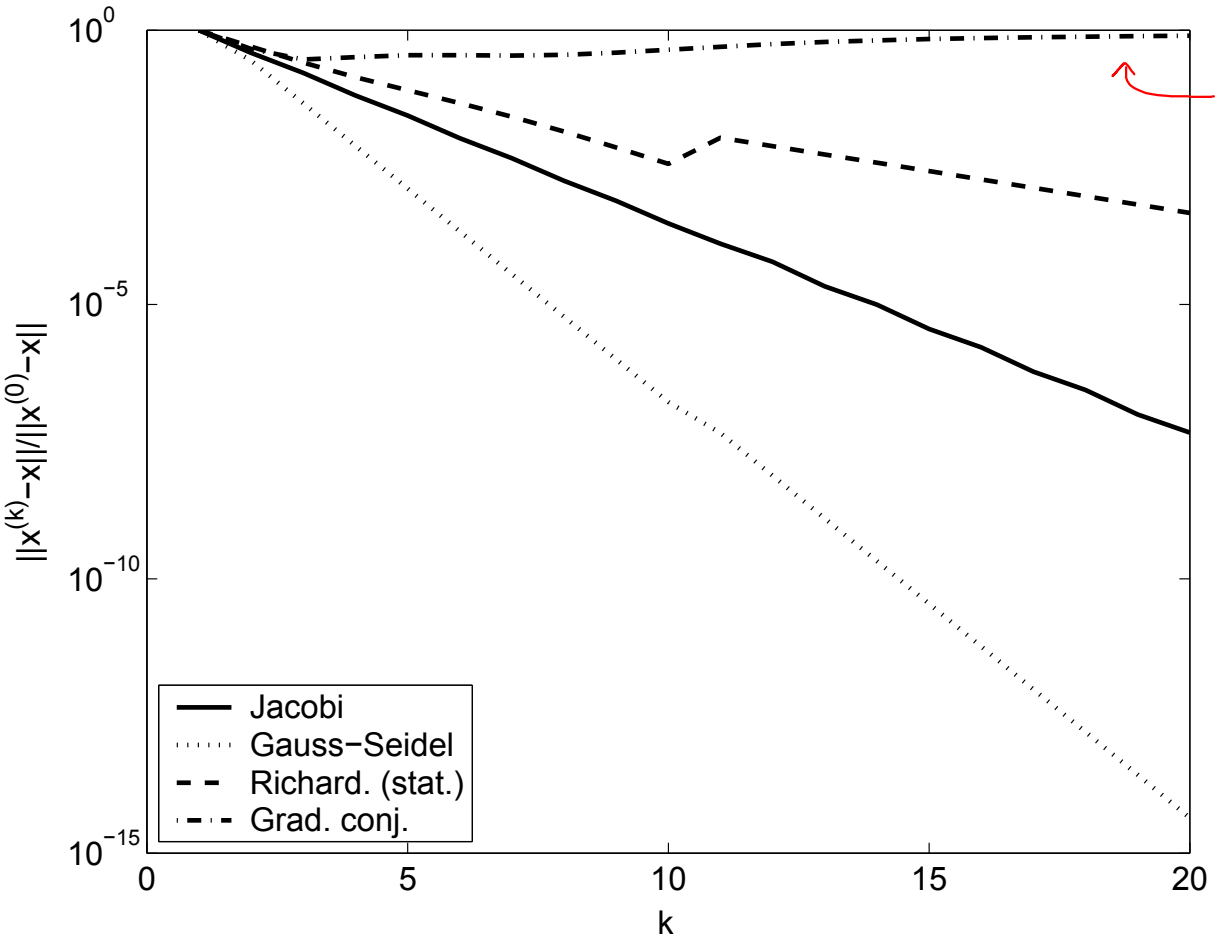
- A is strictly diagonal dominant by row. Hence Jacobi and Gauss-Seidel methods converge.
- A is regular, tridiagonal with non-zero diagonal elements. Then $\rho(B_{GS}) = \rho(B_J)^2$. Therefore we aspect a quicker convergence of Gauss-Seidel w.r.t. Jacobi.
- A **is not s.p.d.**, therefore we have no idea if the gradient or the conjugate gradient converge.

We approximate the solution with an iterative method starting from

$$\mathbf{x}^{(0)} = \begin{pmatrix} x_1^{(0)} \\ x_2^{(0)} \end{pmatrix} = \begin{pmatrix} 1 \\ \frac{1}{2} \end{pmatrix}.$$

The following figure shows the value of $\frac{\|\mathbf{x}^{(k)} - \mathbf{x}\|}{\|\mathbf{x}^{(0)} - \mathbf{x}\|}$ for the Jacobi, Gauss-Seidel, Richardson stationary (preconditioned with $\alpha = 0.5$ and $P = D = \begin{pmatrix} 2 & 0 \\ 0 & 3 \end{pmatrix}$), and the preconditioned (with $P = D$) conjugate gradient methods.
Remark that this time the preconditioned conjugate gradient method doesn't converge.

Behavior of the relative error applied to the system (17) :



why? we are applying wrong methodology, since A IS NOT SYMMETRIC

when this happens use other methods, not conjugate gradient

Convergence Criteria

(Sec. 5.12)

We have the following error bound:

If A is s.p.d, then

$$\frac{\|\mathbf{x}^{(k)} - \mathbf{x}\|}{\|\mathbf{x}\|} \leq K(A) \frac{\|\mathbf{r}^{(k)}\|}{\|\mathbf{b}\|}. \tag{18}$$

The relative error at the iteration k is bounded by the condition number of A times the residual scaled with the right hand side.

We can also use another relation in case of a preconditioned system:

$$\frac{\|\mathbf{x}^{(k)} - \mathbf{x}\|}{\|\mathbf{x}\|} \leq K(P^{-1}A) \frac{\|P^{-1}\mathbf{r}^{(k)}\|}{\|P^{-1}\mathbf{b}\|}.$$

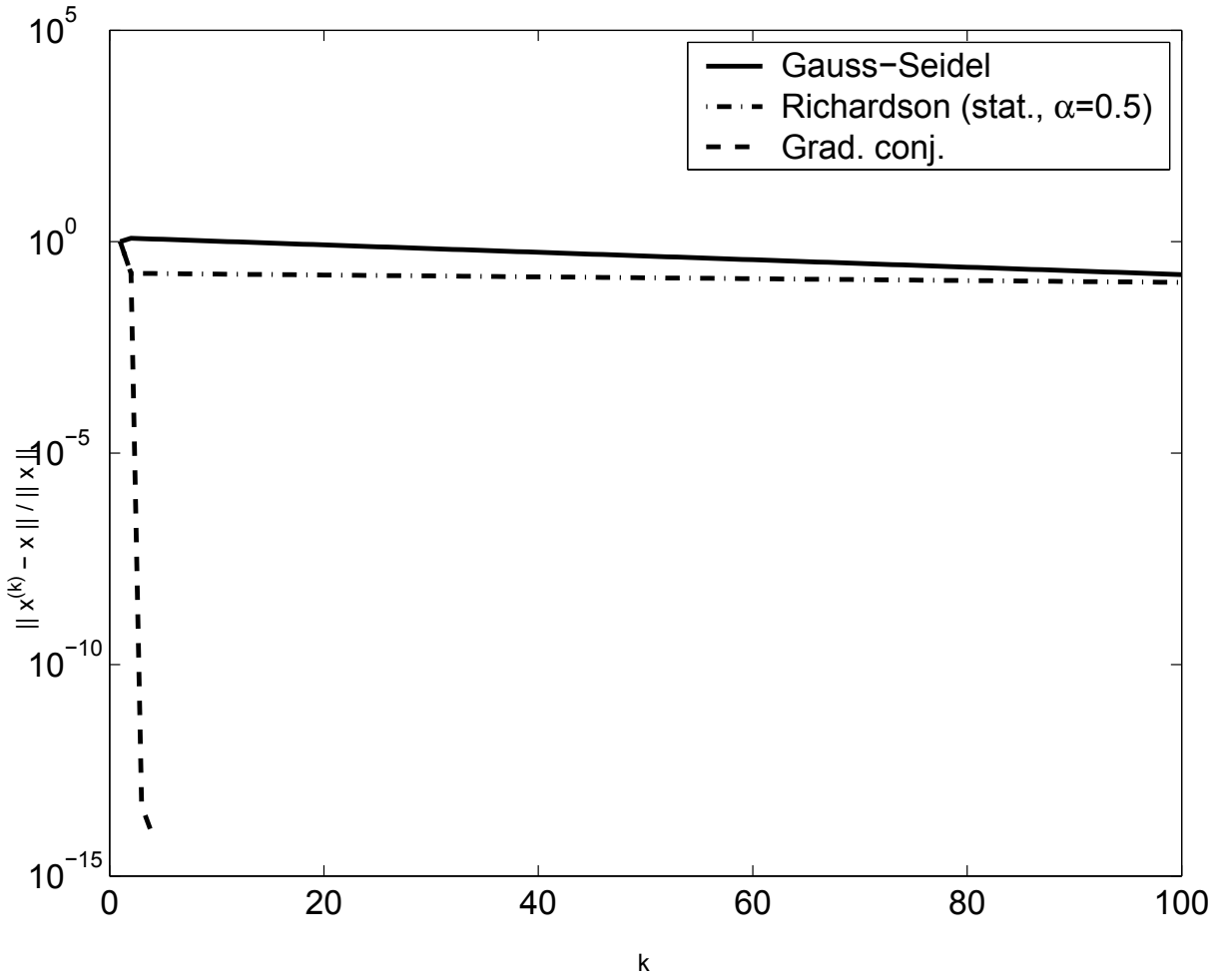
Some examples of convergence of iterative methods applied to linear systems of the kind $A\mathbf{x} = \mathbf{b}$.

Example 4. Lets start with the matrix

$$A = \begin{pmatrix} 5 & 7 \\ 7 & 10 \end{pmatrix} \tag{19}$$

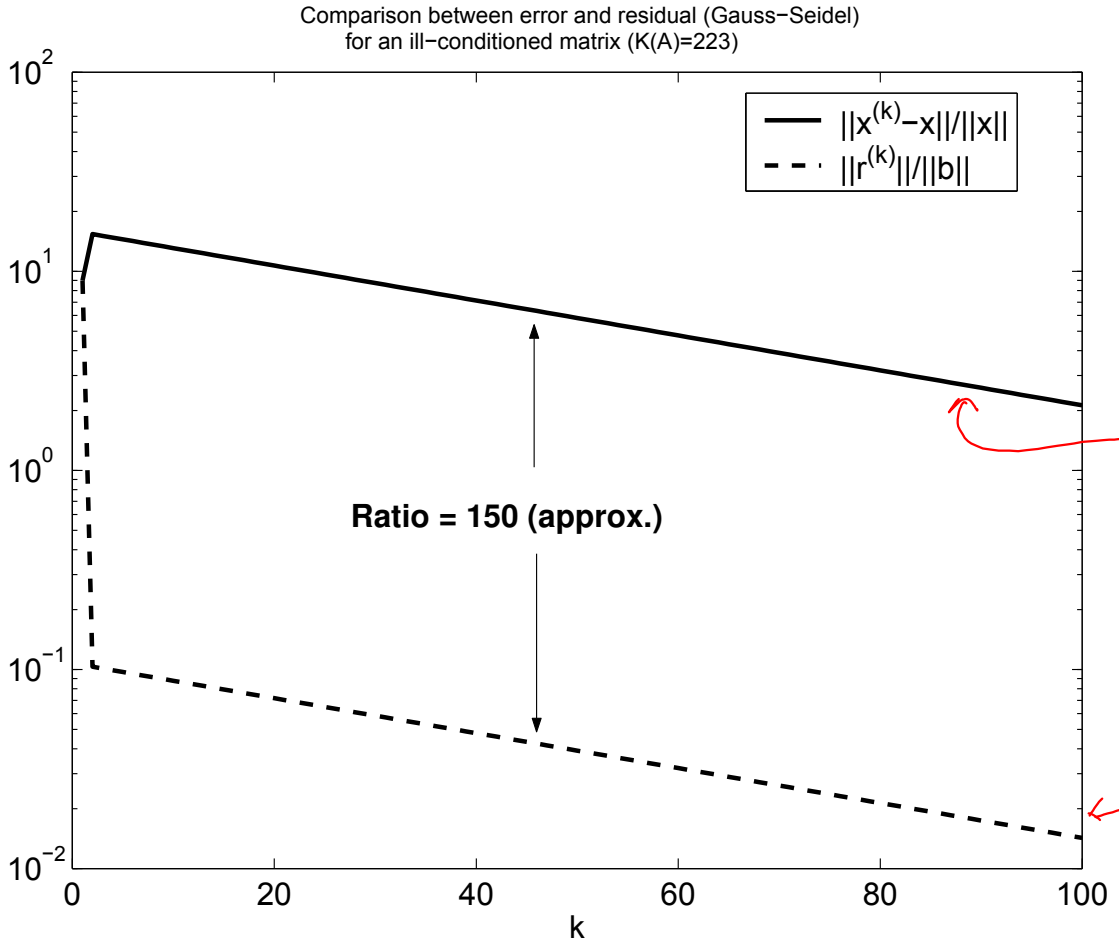
The condition number of this matrix is $K(A) \approx 223$. We consider the Gauss-Seidel method and stationary preconditioned Richardson method with $\alpha = 0.5$ and $P = \text{diag}(A)$. We have that $\rho(B_{GS}) = 0.98$ and $\rho(B_{Rich}) = 0.98$, where $B_{Rich} = I - \alpha P^{-1} A$ is the iterative matrix for the stationary Richardson method.

This figure shows the relative error behavior for Gauss-Seidel method and stationary preconditioned Richardson method and the cojugate gradient preconditioned with the same matrix



100 its for 2 x 2 matrix is UNACCEPTABLE

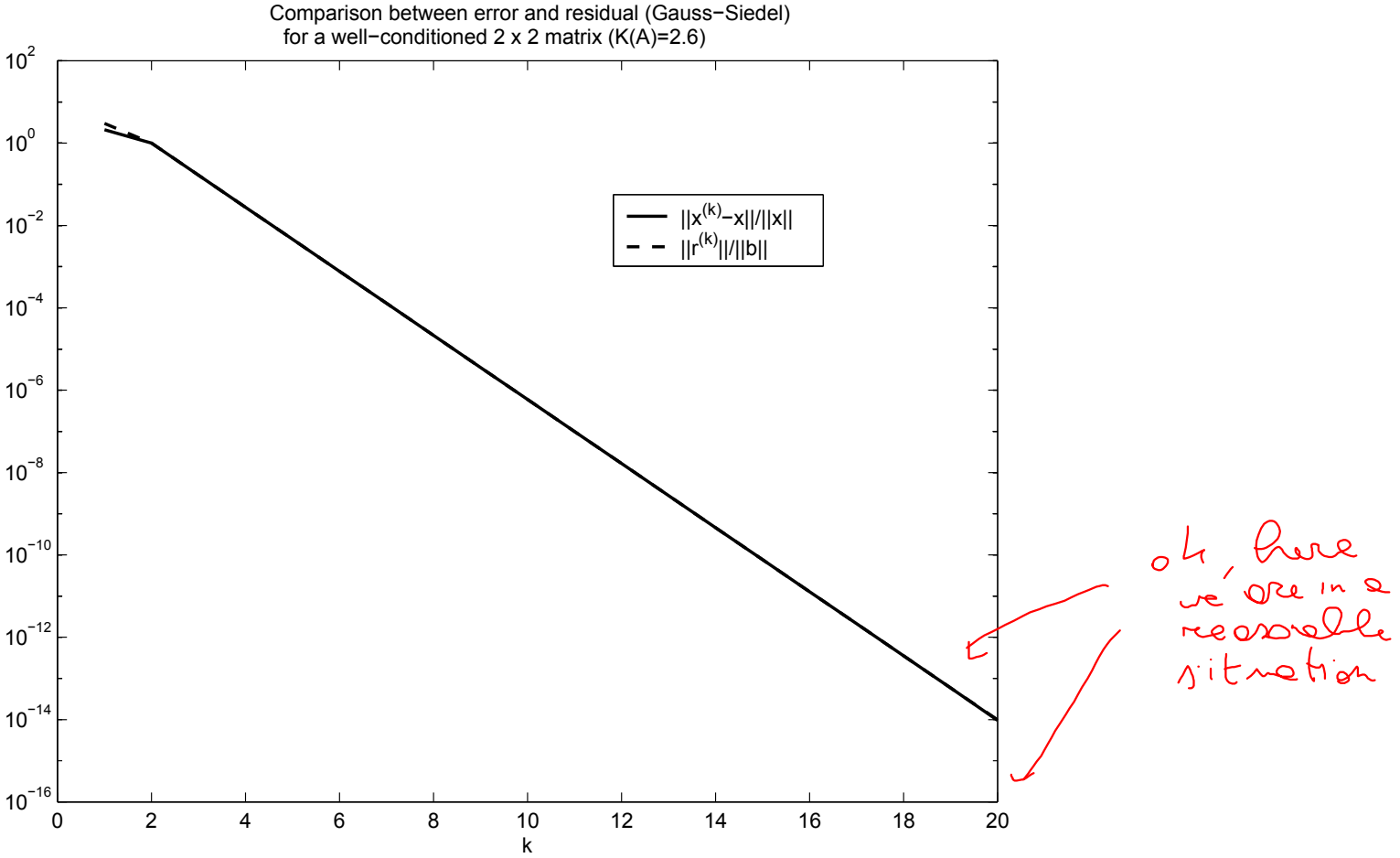
Comparison between error and residual (Gauss-Seidel) (19). Recall that $K(A) \approx 223$



LOOK AT THE 00 ORDER OF MAGNITUDE! But often this line is not available

If a metrix 2×2 requires 100 its should tell me sth is wrong

We can compare the previous figure with the same curves for well conditioned matrix 2×2 ($K(A) \approx 2.6$):



Comparison between the relative error and the residual, for a well conditioned matrix.

Example 5. We take the Hilbert matrix and we solve a linear system for different size n. We set P =diag(A) and use the preconditioned gradient method. The stoping tolerance is set to 10^-6 on the relative residual. We take $\mathbf{x}^{(0)} = \mathbf{0}$.
We evaluate the relative error

```
for j=2:7;
     n=2*j; i=j-1; nn(i)=n;
     A=hilb(n);
     x_ex=ones(n,1); b=A*x_ex;
     Acond(i)=cond(A);
     tol=1.e-6; maxit=10000;
     R=diag(diag(A));
     x0=zeros(n,1);
     [x,iter_gr(i)]=gradient(A,b,x0,maxit,tol,R);
     error_gr(i)=norm(x-x_ex)/norm(x_ex);
   end
```

For the iterative method, we set a tolerance of 10^{-6} on the relative residual. Because the matrix is ill conditioned, it is to be expected to get a relative error in the solution greater than 10^{-6} (see inequality (18)).

		Gradient method		
n	$K(A)$	Error	Iterations	Residual
4	1.55e+04	8.72e-03	995	1.00e-06
6	1.50e+07	3.60e-03	1813	9.99e-07
8	1.53e+10	6.30e-03	1089	9.96e-07
10	1.60e+13	7.99e-03	875	9.99e-07
12	1.67e+16	5.09e-03	1355	9.99e-07
14	2.04e+17	3.91e-03	1379	9.98e-07

Already a WARNING

4 OD of magnitude greater than residual → could lead to very wrong assumption on the problem you are trying to solve

Some observations

Memory and computational costs

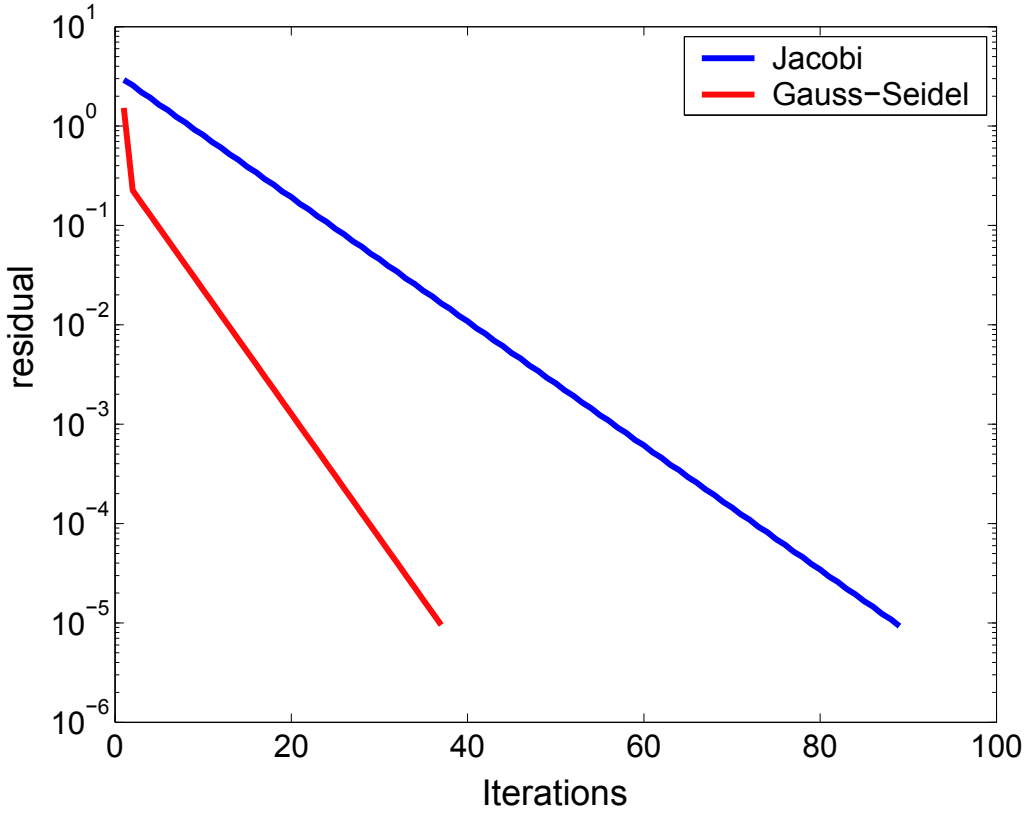
Computational cost (*flops*) and used memory (*bytes*): we consider the Cholesky an the conjugate gradient methods for sparse matrices of size n (originated in the approximation of solutions to the Poisson equation in the finite elements method) with m non zero elements.

		Cholesky		Conjugate gradient		flops(Chol.)/	Mem(Chol.)/
n	m/n^2	flops	Memory	flops	Memory	flops(GC)	Mem(GC)
47	0.12	8.05e+03	464	1.26e+04	228	0.64	2.04
83	0.07	3.96e+04	1406	3.03e+04	533	1.31	2.64
150	0.04	2.01e+05	4235	8.86e+04	1245	2.26	3.4
225	0.03	6.39e+05	9260	1.95e+05	2073	3.27	4.47
329	0.02	1.74e+06	17974	3.39e+05	3330	5.15	5.39
424	0.02	3.78e+06	30815	5.49e+05	4513	6.88	6.83
530	0.01	8.31e+06	50785	8.61e+05	5981	9.65	8.49
661	0.01	1.19e+07	68468	1.11e+06	7421	10.66	9.23

conjugate gradient saves 10 times the bytes and flops than the cholesky method

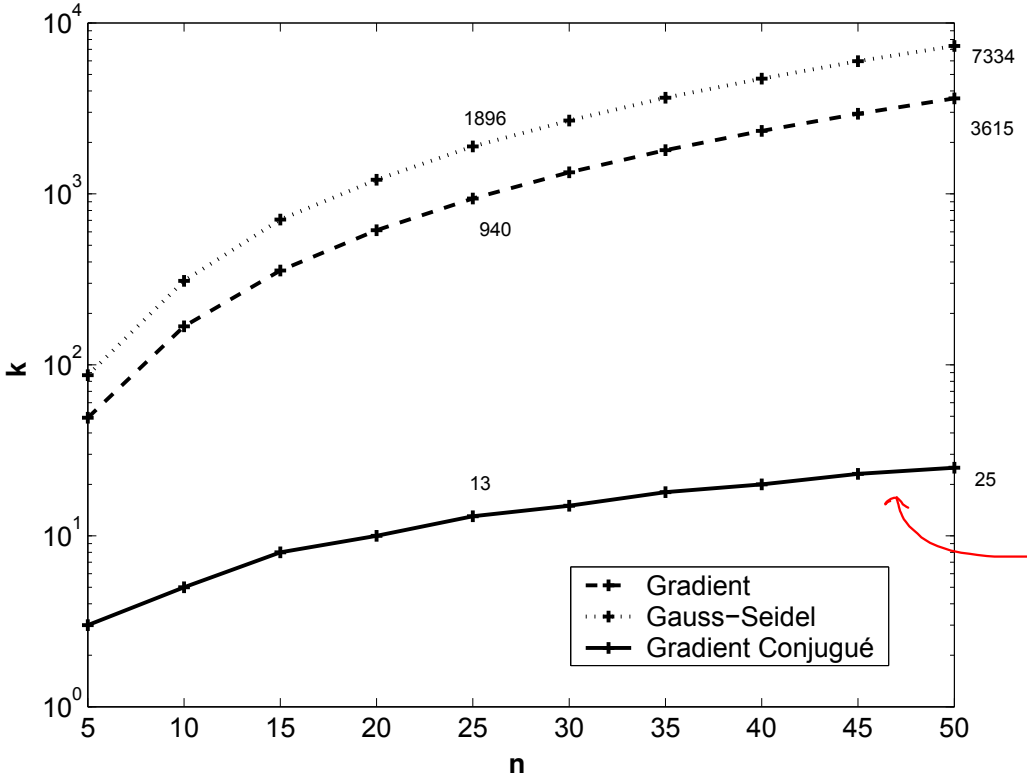
Iterative methods: Jacobi, Gauss-Seidel

Behaviour of the error for a well conditioned matrix ($K = 20$)



Iterative methods: G-S, Gradient, Gradient Conjugate

Number of iterations as function of the size n of a stiffness matrix, tolerance 10^{-6}

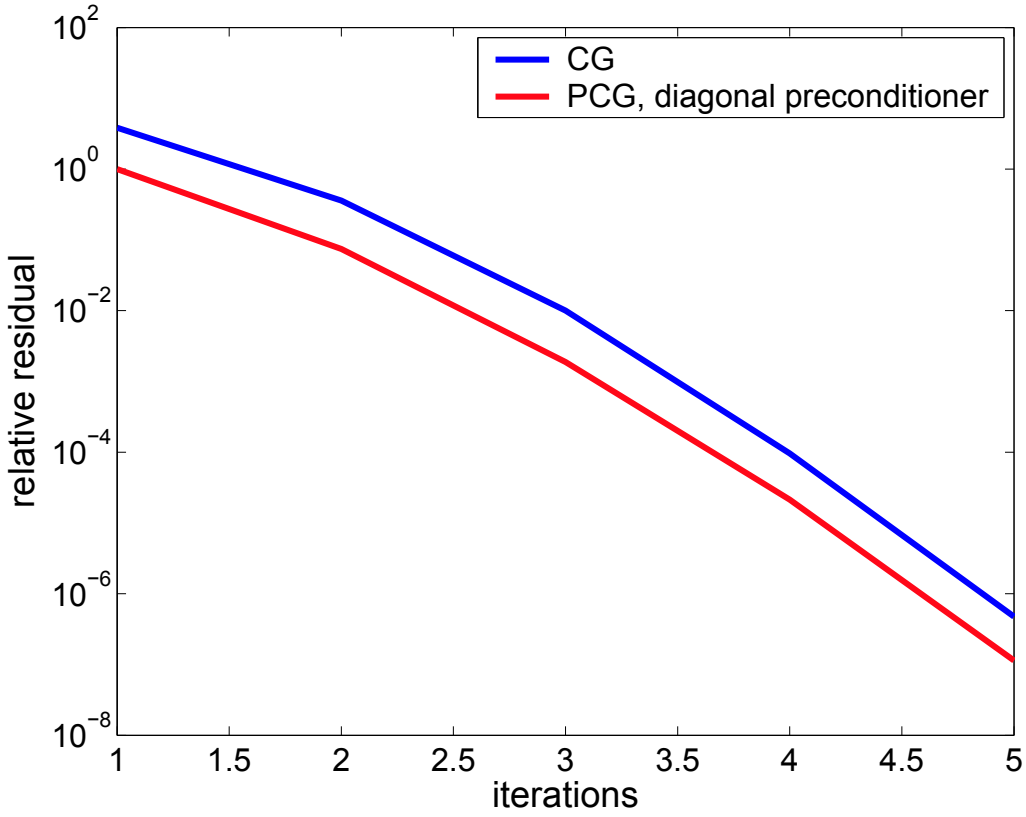


# of iteration

conjugate gradient requires less since the # of A orthogonal direction is equal to the order of the matrix

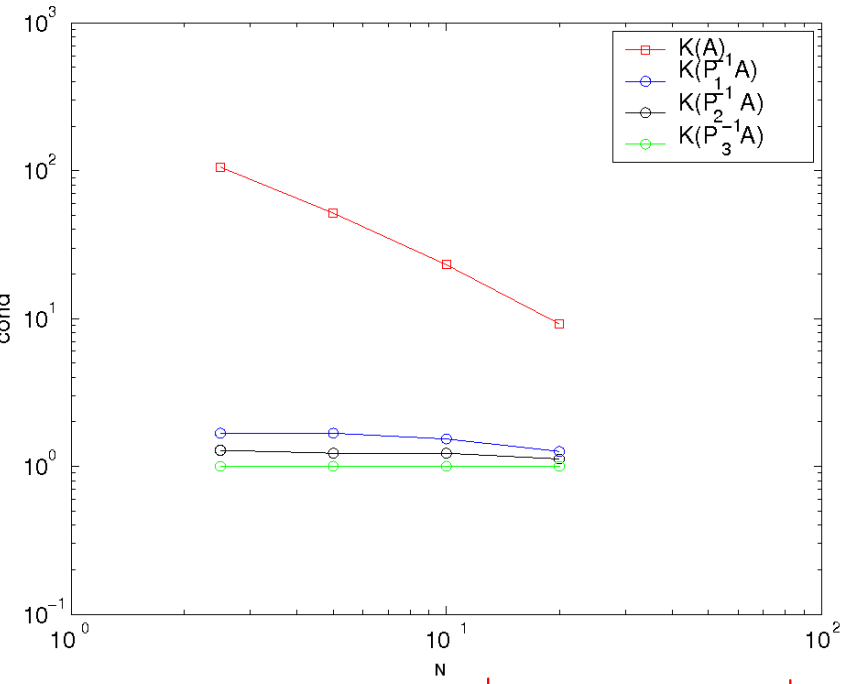
Preconditioning

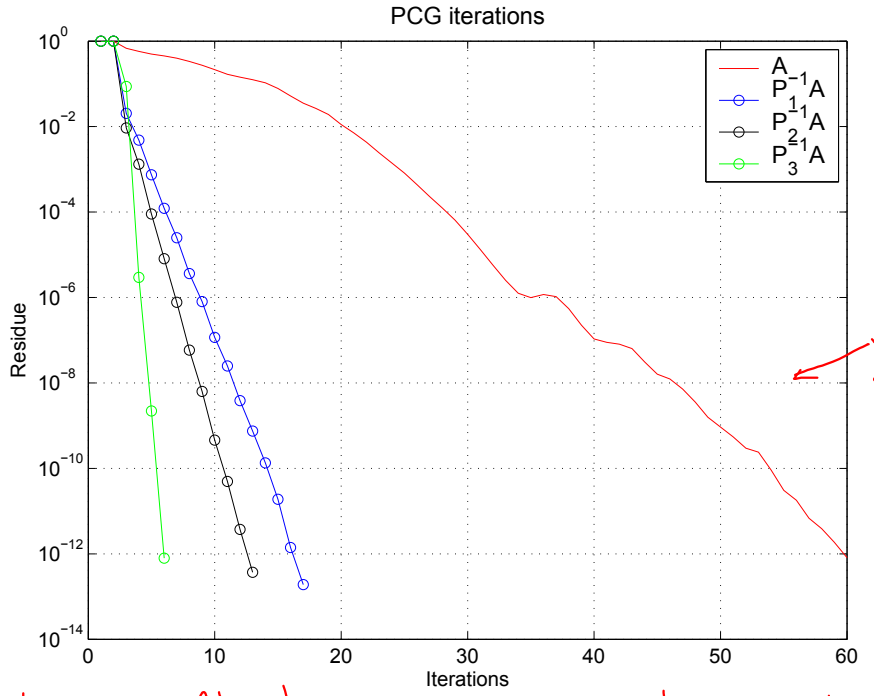
The convergence conjugate gradient and the preconditioned conjugate gradient methods with a diagonal preconditioner ($K = 4 \cdot 10^8$)



Preconditioning

Role of the preconditioning over the condition number of a matrix (approximation by the finite element method of the Laplacian operator)



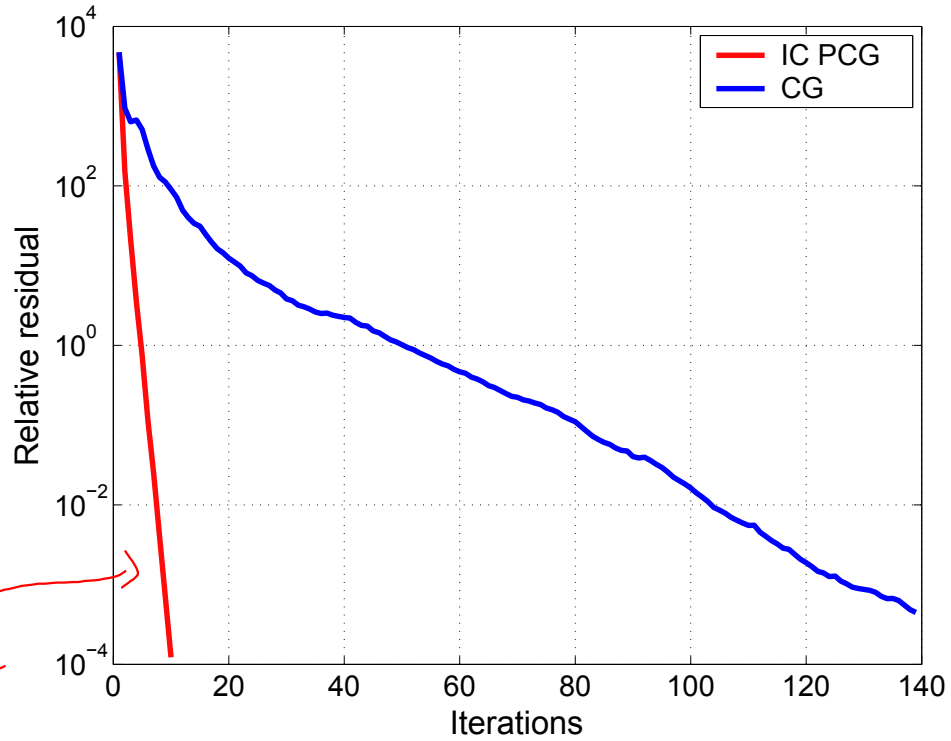


preconditioning SPEEDS UP convergence

Question: do you know which matrix could be preconditioned and which isn't? If K ~ 1 could be preconditioned. If K is high, is likely not preconditioned

Preconditioning

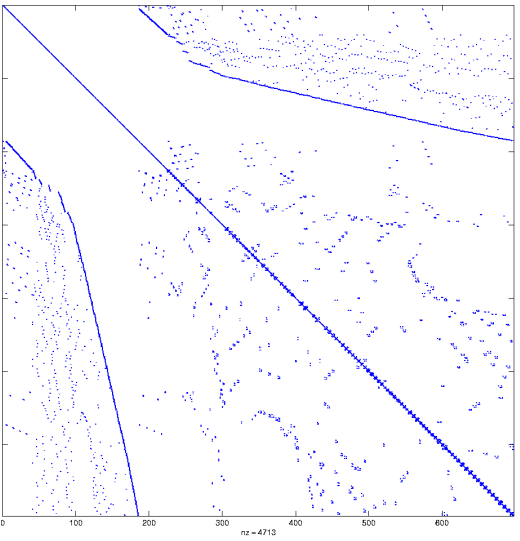
The convergence of the conjugate gradient method and the preconditioned conjugate gradient method with a preconditioner based on an Cholesky incomplete decomposition for a sparse matrix originated from the finite element method ($K = 1.5 \cdot 10^3$)



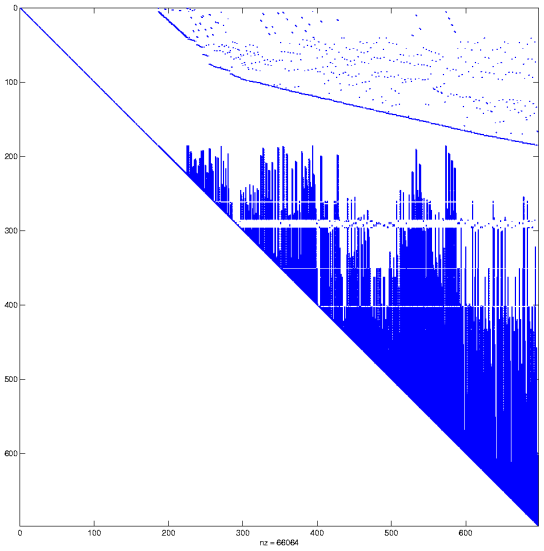
Cholesky as preconditioner

Pre-conditioning

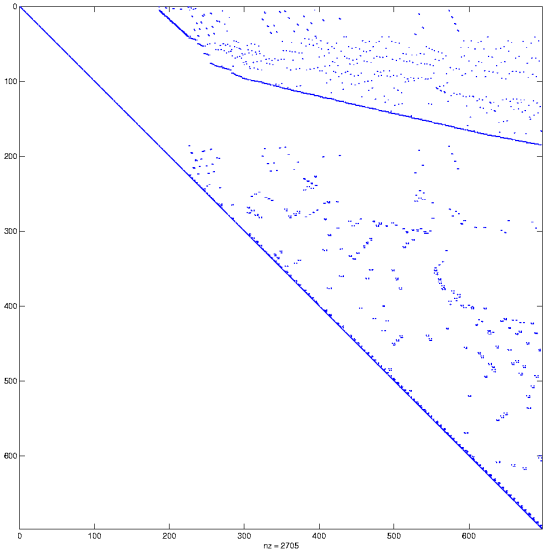
Comparison between the non zero elements of the sparse matrix A from the previous example, its Cholesky factor R and the matrix $\tilde{R}$ obtained by the Cholesky incomplete decomposition:



A



R



$\tilde{R}$

Non-linear systems

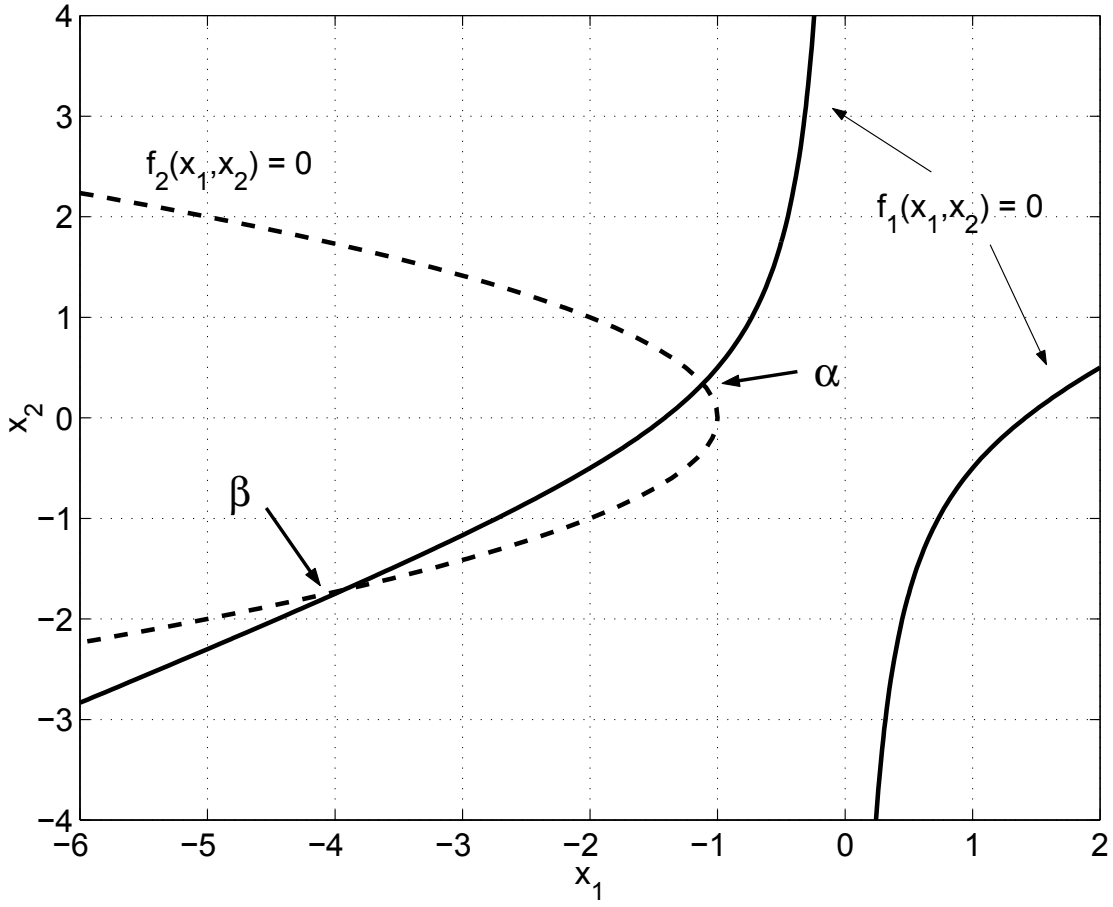
Example 6. Lets consider the following system of non-linear equations:

$$\begin{cases} x_1^2 - 2x_1x_2 = 2 \\ x_1 + x_2^2 = -1. \end{cases} \tag{20}$$

This system can be written in the form:

$$\mathbf{f}(\mathbf{x}) = \mathbf{0} \qquad \text{i.e.} \qquad \begin{cases} f_1(x_1, x_2) = 0 \\ f_2(x_1, x_2) = 0 \end{cases}$$

where $\mathbf{f} = (f_1, f_2)$, $f_1(x_1, x_2) = x_1^2 - 2x_1x_2 - 2$ and $f_2(x_1, x_2) = x_1 + x_2^2 + 1$.



Curves $f_1 = 0$ *and* $f_2 = 0$ *in the square* $-6 \leq x_1 \leq 2$, $-4 \leq x_2 \leq 4$

We want to generalise the Newton method for the case of non-linear systems. To do this, we define the *Jacobian* matrix of the vector $\mathbf{f}$:

$$J_{\mathbf{f}}(\mathbf{x} = (x_1, x_2)) = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} \end{bmatrix} = \begin{bmatrix} 2x_1 - 2x_2 & -2x_1 \\ 1 & 2x_2 \end{bmatrix}.$$

If $J_{\mathbf{f}}(\mathbf{x}^{(k)})$ is invertible, the Newton method for non linear systems is written : *Let* $\mathbf{x}^{(0)} = (x_1^{(0)}, x_2^{(0)})$, *we compute for* $k = 0, 1, 2, \ldots$

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - [J_{\mathbf{f}}(\mathbf{x}^{(k)})]^{-1}\mathbf{f}(\mathbf{x}^{(k)}), \quad k = 0, 1, 2 \ldots . \tag{21}$$

We can write (21) as

{ in place of 1/f' of Newton method, we put the Jacobian at -1 (inverse of Jacobian)

$$[J_{\mathbf{f}}(\mathbf{x}^{(k)})](\mathbf{x}^{(k+1)} - \mathbf{x}^{(k)}) = -\mathbf{f}(\mathbf{x}^{(k)}), \quad k = 0, 1, 2 \ldots . \tag{22}$$

↑ quasi-Newton methods update Jacobian every m iteration with m > 1

Description of the first step of the algorithm: given the vector $\mathbf{x}^{(0)} = [1, 1]^T$.
We calculate:

$$J_{\mathbf{f}}(\mathbf{x}^{(0)}) = \begin{bmatrix} 0 & -2 \\ 1 & 2 \end{bmatrix}.$$

We determine $\mathbf{x}^{(1)}$ as solution of the equation :

$$[J_{\mathbf{f}}(\mathbf{x}^{(0)})](\mathbf{x}^{(1)} - \mathbf{x}^{(0)}) = -\mathbf{f}(\mathbf{x}^{(0)}).$$

And we continue with (22).

Lecture 21 — Solution of prototypical PDE in dimension 1. — 10/12/2020

Prototypical problem

Given f (regular enough) find u s.t.

$$\begin{cases} -u'' = f & \text{in } [0,1] \\ u(0) = u(1) = 0 \end{cases}$$

(unknown of the problem is a ft; $u(0) = u(1) = 0$: boundary CNs)

Problems like this can be found:
- Heat conduction
- Elasticity
- Maxwell equations

Requirement for WELL POSEDNESS: $f \in C^0([0,1])$, and $u \in C^2([0,1])$

Strong formulation

First approach

FINITE DIFFERENCES.

This prob will be well posed if the final linear system is invertible (det of matrix is $\neq 0$)

Approximate the differential operators using the incremental definition of the derivative:

$$u'(x) := \lim_{h \to 0} \frac{u(x+h) - u(x)}{h}$$

Forward difference — FD

$$u'(x) := \lim_{h \to 0} \frac{u(x) - u(x-h)}{h}$$

backward — BD

(can do also for u'')

$$u'(x) := \lim_{h \to 0} \frac{u(x+h) - u(x-h)}{2h}$$

centred — CD

for C^1 fts these are $(\Rightarrow$ for $h \to 0$

Then the FINITE DIFFERENCE scheme is:

Fix h, and define Du as

$$D^F u = \frac{u(x+h) - u(x)}{h} \qquad \text{FD}$$

$$D^B u = \frac{u(x) - u(x-h)}{h} \qquad \text{BD}$$

$$D^C u = \frac{u(x+h) - u(x-h)}{2h} \qquad \text{CD}$$

Assume $u \in C^\infty(I(x))$ in an open set of x $I(x)$

then a taylor expansion

$$u(x+h) = u(x) + u'(x)h + \frac{u''}{2}(x)h^2 + \frac{u'''}{6}(x)h^3 + \frac{u''''}{24}(x)h^4 + \dots + \frac{u^{(n)}h^n}{n!}$$

$$u(x-h) = u(x) - u'(x)h + \frac{u''}{2}(x)h^2 - \frac{u'''}{6}(x)h^3 + \frac{u''''}{24}(x)h^4 + \dots + \frac{u^{(n)}(-h)^n}{n!}$$

Theorem Given $u \in C^\infty([a,b])$, $x \in (a,b)$, then $\forall k > 0$

$\exists \xi \in (x, x+h)$

equality EXACT

$$u(x+h) = \left(\sum_{i=0}^{k-1} \frac{u^{(i)}(x)}{i!} h^i \right) + \frac{u^{(k)}(\xi)}{k!} h^k$$

You can truncate expansion at any para and what you find is the value of the ft at one point in $(x, x+h)$

Truncation Error of Finite Difference schemes:

! At point 1 for truncating, I have to use the ξ point, by previous theorem

because I divide by h

FD $$\frac{u(x+h) - u(x)}{h} = u'(x) + \frac{u''(\xi)}{2}h$$ 1st order scheme

BD $$\frac{u(x) - u(x-h)}{h} = u'(x) - \frac{u''(\xi)}{2}h$$ 1st order scheme

CD $$\frac{u(x+h) - u(x-h)}{2h} = u'(x) + \frac{u'''(\xi)}{6}h^2$$ 2nd order scheme

Use low order (I ord) if ft is not regular (maybe u'' doesn't exist) and low h, while high order if u is regular, and high h

CFD^{II} Central finite diff of II ord

$$\frac{u(x-h) - 2u(x) + u(x+h)}{h^2} = u''(x) + \frac{u''''(\xi)}{12}h^2$$

I want II derivative

2nd order scheme for 2nd derivative

Apply CFD II to $-u'' = f$, $u(0) = u(1) = 0$ in $[0,1]$

Split the interval $[0,1]$ into $N-1$ subintervals (N points)

$$\{x_i\}_{i=0}^{N-1} = \left\{0, \frac{1}{N-1}, \frac{2}{N-1}, \dots, \frac{N-1}{N-1}=1\right\} = \left\{\frac{i}{(N-1)}\right\}_{i=0}^{N-1} = \{i \cdot h\}_{i=0}^{N-1}$$

$$h = \frac{1}{(N-1)} \qquad \text{set } u^i := u(x_i)$$

$$\{u_i\}_{i=0}^{N-1} \in \mathbb{R}^N$$

For $i = 1$ to $N-2$ write: (For all i)

$$\frac{1}{h^2}\underbrace{\left[-u^{i-1} + 2u^i - u^{i+1}\right]}_{\simeq -u''} = f_i \equiv \underline{\underline{A}}\,\underline{u} = \underline{f}$$

system of equations

$$A \in \mathbb{R}^{N\times N}, \quad u, f \in \mathbb{R}^N$$

$$\sum_{J=0}^{N-1} A_{iJ}\, u^J = f_i$$

$$A_{iJ} = \frac{1}{h^2}\begin{cases} -1 & \text{when } J = i-1 \text{ or } i+1 \\ 2 & \text{when } J = i \\ 0 & \text{otherwise} \end{cases} \qquad \text{and } i \in [1, N-2]$$

$$\begin{matrix} 0 \\ 1 \\ \\ \\ \\ N-2 \\ N-1 \end{matrix} \begin{pmatrix} \cdots & & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & -1 & \\ & & \ddots & \ddots & \ddots \\ & & & -1 & 2 & -1 \\ & & & & \cdots \end{pmatrix} \cdot \frac{1}{h^2}$$

$$f_i = f(x_i) \qquad i = 1, \dots, N-2$$

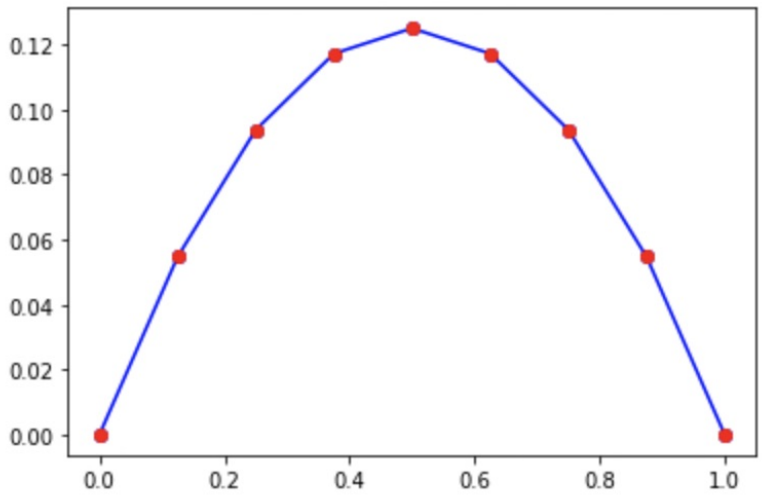
What about I and last columns?

For $i = 0$, $i = N-1$ we impose ← we set the BOUNDARY CONDITION

$$u^0 = 0 \quad \rightarrow \quad A_{00} = 1 \qquad f_0 = 0$$

$$u^{N-1} = 0 \quad \rightarrow \quad A_{N-1,N-1} = 1 \qquad f_{N-1} = 0$$

! The more the points the higher the CN NUMBER => more ill-conditioned



Example of solution to

$$-u'' = 1$$

$$u(0) = u(1) = 0$$

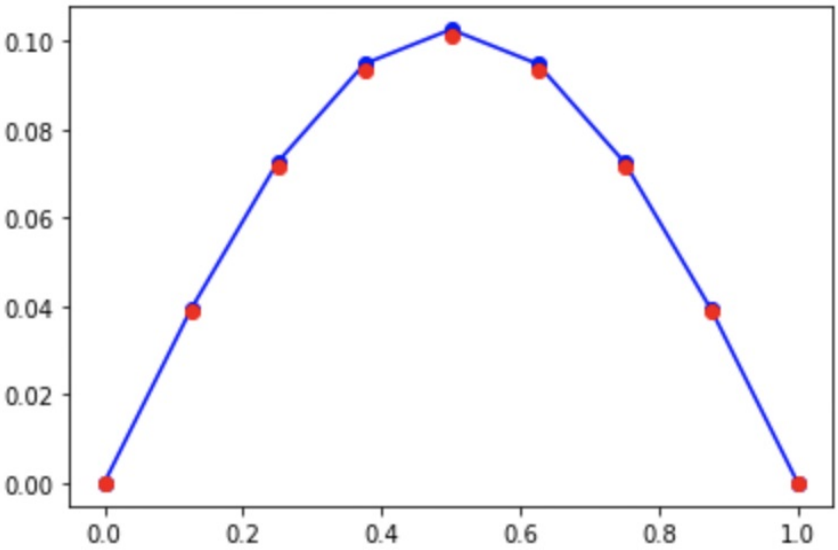
with $N = 9$

the red dots are the exact solution.

$$u_{exact} = \frac{x(1-x)}{2}$$ ← exact function

We have error zero (blue overlap red) because error is up to u'''', but u'''' of a parabola is zero!

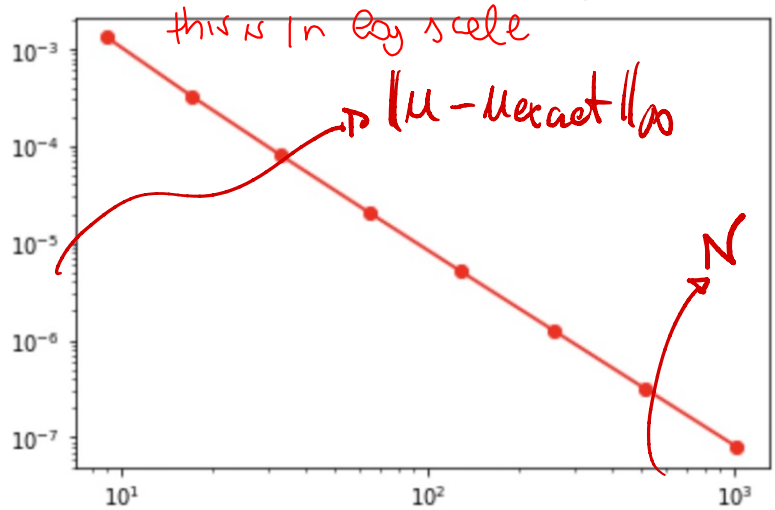
Same thing with $f(x) = \sin(\pi x)$



Here the error is not zero, because

$$u'''' = -f'' \neq 0$$

Plot the error $\|u - u_{exact}\|_\infty = \max_{i \in [0, N-1]} |u^i - u(x_i)|$



Straight line:

$$E = c h^k$$

$$= c \left(\frac{1}{N-1}\right)^k$$

what is k?

inclination of line (with minus sign) in LOG SCALE (→ found $\log E$)

How to measure the rate k ?

Two options: 1) we know the exact solution

2) we do <u>not</u> know the exact solution

Case 1

Hypothesis: C is indep. of h_i and h → target

$$E_1 = \|u_{h_1} - u_{exact}\|_\infty \simeq C h_1^k$$

$$E_2 = \|u_{h_2} - u_{exact}\|_\infty \simeq C h_2^k$$

same k for the 2 cases

$$\frac{E_1}{E_2} \simeq \left(\frac{h_1}{h_2}\right)^k$$

we need at least 2 measurements

$$k = \frac{\log(E_1/E_2)}{\log(h_1/h_2)} = \frac{\log(E_1) - \log(E_2)}{\log(h_1) - \log(h_2)}$$

Case 2

Make sure we reduce h by a constant factor θ, and use at least 3 approx solutions.

$h_{i+1} = \theta h_i$

$$\|u_{h_2} - u_{h_1}\|_\infty \leq \|u_{h_2} - u_{exact}\|_\infty + \|u_{h_1} - u_{exact}\|_\infty$$

$$\simeq C h_1^k + C h_2^k$$

$$\simeq C h_1^k + C \theta^k h_1^k$$

$$\simeq \underbrace{C(1+\theta^k)}_{C_2} h_1^k$$

$$\frac{\|u_{h_1} - u_{h_2}\|_\infty}{\|u_{h_2} - u_{h_3}\|_\infty} \sim \frac{C_2 h_1^{\,k}}{C_2 h_2^{\,k}} = \theta^{-k}$$

$h_2 = \theta h_1$

$h_3 = \theta h_2$

← I do a third measurement and I do the same, by the fact that 2 consecutive stv do the same in terms of error

$$k = \frac{\log\left(\|u_{i+2} - u_{i+1}\|_\infty\right) - \log\left(\|u_{i+1} - u_i\|_\infty\right)}{\log(\theta)}$$

I remember that we had $u_i, u_{i\pm 1}$, that are 3 consecutive approximate solutions

Lecture 22 LH

PDE - 1D - FEM ← Finite Elements Method

15.12.2020

$$\text{(1)} \begin{cases} -u'' = f & \text{in } [0,1] \\ u(0) = u(1) = 0 \end{cases}$$

We tried to:

⇝ approximate u''

- split $[0,1]$ in $N-1$ intervals with size $h = \frac{1}{(N-1)}$
- define approx of u'' on each $x_i = ih \qquad i = 0, \dots, N-1$

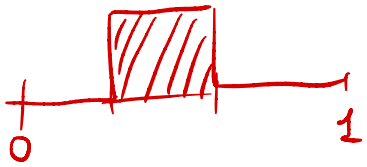
$$-u^{i-1} + 2u^i - u^{i+1} = f_i$$

- issues: i) u'' is defined if $u \in C^2([0,1])$

  ii) ($f \in C^0([0,1])$)

excluded situations:

f:



iii) truncation error: ← defines the order by which I approximate u''

$$u'' = CD^{II}(u) + O(\|u''''\|_\infty h^2)$$

SOLUTION: rewrite the problem (1) in weak form

Let's see a special case

- Let v be a smooth function: $v : [0,1] \to \mathbb{R}$

Multiply (1) by v and integrate on $[0,1]$

$$\int_0^1 -u'' \cdot v = \int_0^1 f \cdot v \qquad \forall\, v \text{ "smooth enough"}$$

Let's further assume that $v(0) = v(1) = 0$ ← v satisfies boundary CNs of problem

→ Integrate by parts: $\int_0^1 u'v' - u'v\Big|_0^1$ → 0 because $v(0) = v(1) = 0$

$$(wv)' = w'v + wv' \qquad w = u'$$

so the problem is now:

Find u in V s.t.

$$\text{(2)} \quad \int_0^1 u'v' = \int_0^1 fv \qquad \forall\, v \in V$$

Weak formulation of (1) $(-u'' = f)$

← This is weaker: we are only asking u to have only one degree of continuity (FIRST DERIVATIVE not even needed)

What's the "right" space V for (2) to make sense?

i) V must incorporate that $v(0) = v(1) = 0 \quad \forall v \in V$

ii) (2) must make sense $\forall u, v \in V$

in particular

$\rightarrow v = u \Rightarrow \int_0^1 (u')^2 = \int_0^1 fu$

$\Rightarrow$ It only makes sense if $\int_0^1 (u')^2 < +\infty$

So it must be

$\Rightarrow V = \{ v \text{ s.t. } \int_0^1 (v')^2 < +\infty \;/\; v(0) = v(1) = 0 \}$

(V is the Sobolev space $H_0^1([0,1])$ ← means: "first derivatives")

space of ft that are in L^2 and whose first derivatives are in L^2

V is the space of functions whose first derivative is in L^2, and that are zero on $\{0, 1\}$

A solution to (1) is a solution to (2) (always true!)

↓ sum

$(wv)' = w'v + wv'$

$\Rightarrow \int_0^1 (wv)' = \int_0^1 w'v + \int_0^1 wv'$

$wv\Big|_0^1 = \int_0^1 w'v + \int_0^1 wv'$

$\Rightarrow \int_0^1 w'v = -\int_0^1 wv' + wv\Big|_0^1$

stronger in weak sense, but not the contrary in general

$$\boxed{\int_0^1 -u''v = \int_0^1 u'v' + u'v\Big|_0^1}$$

? 0 because $v(0) = v(1) = 0$

"weak" solution

$\not\Leftarrow$ false: $-u'' = f \Rightarrow \int_0^1 u'v' = \int_0^1 fv \quad \forall v \in V$

You def the WEAK vf of pb as the solution of this problem

$V \equiv H_0^1([0,1]) := \{ v \in L^2, \ v' \in L^2, \ v(0) = v(1) = 0 \}$

f must be s.t. $\int_0^1 fv < +\infty \quad \forall v \in H_0^1([0,1])$

true if $f \in L^2$

but also if f is less reg. than L^2, but such that $\int_0^1 f \cdot v < +\infty \quad \forall v \in H_0^1([0,1])$

$f \in V^*$ ← dual space of V ← what is that!

↳ for example Dirac δ is not in L^2, but this works anyway

Weak derivative:

$Du(x) = u'(x) \quad \forall u \in C^1([0,1]), \forall x \in [0,1]$

$Du(x)$ is ← weak derivative s.t. $-\int_0^1 u \varphi' = \int_0^1 Du \, \varphi \quad \forall \varphi \in C_0^\infty((0,1))$

By construction, if $u \in C^1([0,1]) \Rightarrow$

$-\int_0^1 u \varphi' \overset{\text{integration by part}}{=} \int u' \varphi = \int_0^1 Du \, \varphi \Rightarrow Du = u'$

↑ True only if $u \in C^1$, but then can be def whenever $\int u \varphi'$ exist

$D^\alpha u = u^{(\alpha)}$ if $u \in C^\alpha([0,1])$

D^α is a weak derivative of u if ← this is satisfied

$$\int_0^1 D^\alpha u, \varphi = (-1)^\alpha \int_0^1 \varphi^{(\alpha)} Du \quad \forall \varphi \in C_0^\infty((0,1))$$

where $C_0^\infty((0,1)) := \{ \varphi \in C^\infty([0,1]) \text{ s.t. } \varphi^{(\alpha)}(0) = \varphi^{(\alpha)}(1) = 0 \ \forall \alpha \in \mathbb{N}_0 \}$

The final weak form of our problem is

Given $f \in L^2([0,1])$ (could be $(H_0^1([0,1]))^*$ dual of $H_0^1([0,1])$)

Find $u \in H_0^1([0,1])$ s.t.

$$\int_0^1 u' v' = \int_0^1 f v \qquad \forall\, v \in H_0^1([0,1])$$

$$H_0^1([0,1]) := \{ v \in L^2([0,1]),\ v' \in L^2([0,1]),\ v(0) = v(1) = 0 \}$$

Assume that we have $V_h \subset V \equiv H_0^1(\Omega)$

$V_h = \text{span}\{ v_i \}_{i=0}^{N-1}$ $\quad \dim(V_h) = N$ ← finite dim

Write a approximate problem:

find $u_h \in V_h$ s.t. $\quad \left(u_h(x) = \sum_{J=0}^{N-1} u^J v_J(x) \right)$

$$\int_0^1 u_h' v_i' = \int_0^1 v_i f \qquad i = 0, \dots, N-1$$

← that is for ALL basis functions

$$\rightarrow \sum_{J=0}^{N-1} \int_0^1 u^J v_J' v_i' = \int_0^1 v_i f$$

$$A u = F$$

$$A_{iJ} := \int_0^1 v_J' v_i' \qquad F_i = \int_0^1 v_i f$$

I DO NOT CHANGE WAY IN WHICH I COMPUTE DERIVATIVES: I will choose basis so I can compute derivative exactly

Define V_h piecewise polynomial and $C^0([0,1])$

Select N points that define $N-1$ intervals

$$\{x_i\}_{i=0}^{N-1} = ih = \frac{i}{(N-1)}$$

the intervals are $[x_i, x_{i+1}]$ $i = 0, \dots, N-2$

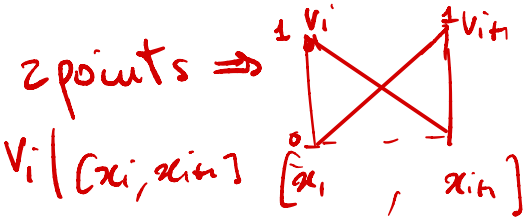
poly of order k

$$V_h^k := \{ v \in \mathbb{P}^k([x_i, x_{i+1}]) \mid v(0) = v(1) = 0 \quad v \in C^0([0,1]) \}$$

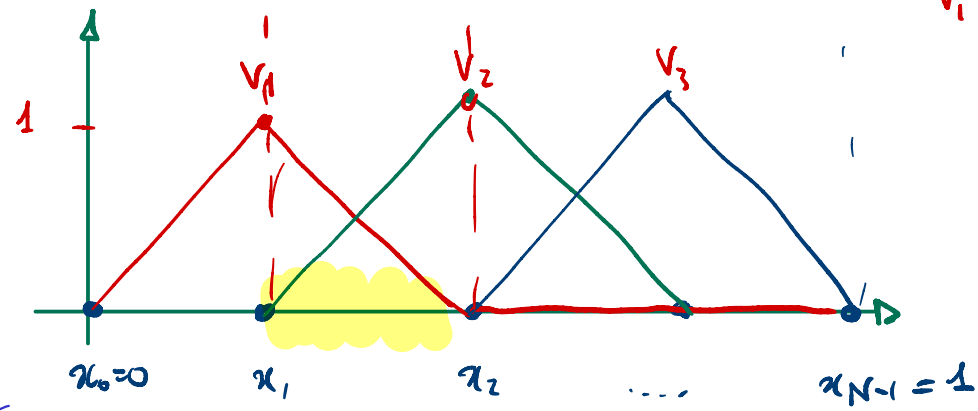
Continuous piecewise polynomial of order k.

Example $k = 1 \Rightarrow \mathbb{P}^1([x_i, x_{i+1}])$

we choose Lagrange basis of order 1 in $[x_i, x_{i+1}]$ with support points $\{x_i, x_{i+1}\}$ 2 points $\Rightarrow$



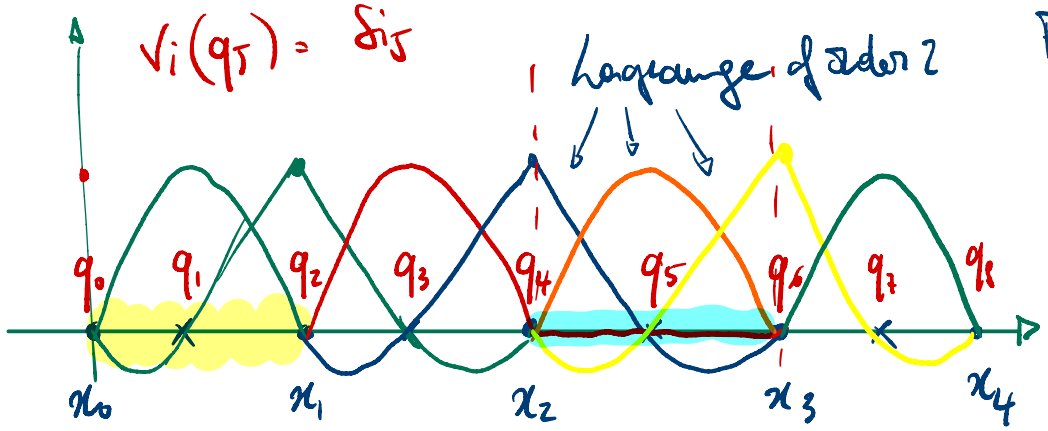
$v_i | [x_i, x_{i+1}]$ $[x_i, x_{i+1}]$



$q_i = x_i$ for linear polynomials.

For example, choose

$$v_i(x_j) = \delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}, \quad v_i \in V_h^1$$



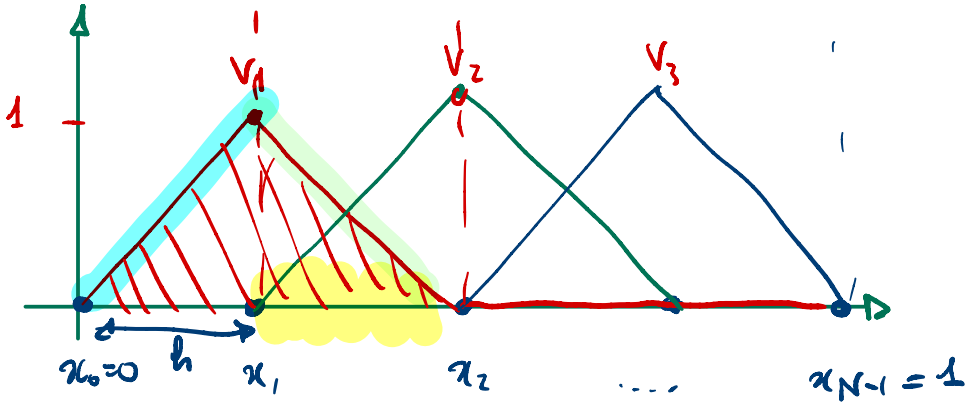
For polynomials of order 2, choose

$$\{q\}_{i=0}^{(N-1)+(N-2)} = \{x_i\}_{i=0}^{N-1} \cup \left\{\frac{x_i + x_{i+1}}{2}\right\}_{i=0}^{N-2}$$

union

Consider

1D case linear

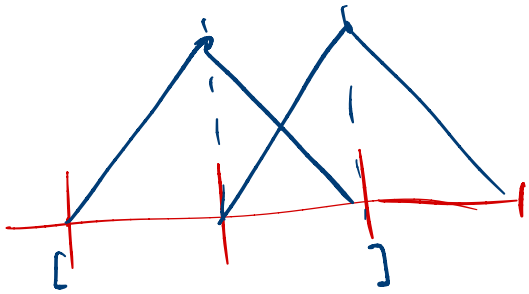


$$\dim(V_h) = N-2$$

$$V_i = \begin{cases} \dfrac{(x - x_{i-1})}{h} & x \in [x_{i-1}, x_i] \\ \dfrac{(x_{i+1} - x)}{h} & x \in [x_i, x_{i+1}] \\ 0 & \text{elsewhere} \end{cases}$$

$i = 1, \dots, N-2$

$$V_i' = \begin{cases} \dfrac{1}{h} & \text{in } [x_{i-1}, x_i] \\ -\dfrac{1}{h} & \text{in } [x_i, x_{i+1}] \\ 0 & \text{elsewhere} \end{cases}$$



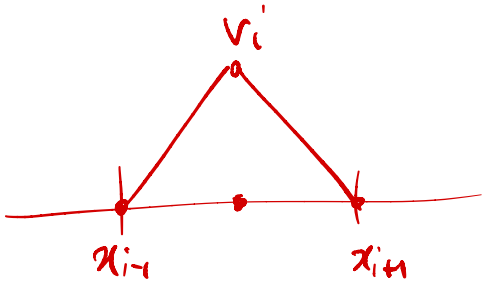
$$A_{ij} := \int_0^1 V_i' V_j' \begin{cases} \neq 0 & \text{if } i = j, j-1, j+1 \\ 0 & \text{elsewhere} \end{cases}$$

$$A_{ij} = \begin{cases} \displaystyle\int_{x_{i-1}}^{x_{i+1}} \left(\frac{1}{h}\right)^2 = 2\frac{1}{h} & \text{if } i = j \\ \displaystyle\int_{x_i}^{x_{i+1}} -\left(\frac{1}{h}\right)^2 = -\frac{1}{h} & \text{if } i = j-1 \text{ or } i = j+1 \end{cases}$$

$$A_{ij} := \begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \end{pmatrix} \frac{1}{h}$$

Same matrix as FD ($\frac{1}{h}$!)

$$F_i = \int_{x_{i-1}}^{x_{i+1}} f(x)\, v_i(x)\, dx$$



$$\approx f(x_i) \cdot h$$ using trapez rule (same as FD with h)

since integral of v_i between x_{i-1}, x_{i+1} is 1/2 of the whole rectangle of height $1/h$

proof:

$$\int_{x_{i-1}}^{x_i} v_i(x) f(x) + \int_{x_i}^{x_{i+1}} v_i(x) f(x)$$

$$h\left[\frac{1}{2} v_i(x_{i-1}) f(x_{i-1}) + \frac{1}{2} v_i(x_i) f(x_i)\right] + h\left[\frac{1}{2} v_i(x_i) f(x_i) + \frac{1}{2} v_i(x_{i+1}) f(x_{i+1})\right]$$

($v_i(x_{i-1}) = 0$, $v_i(x_{i+1}) = 0$)

$$= f(x_i)\, h$$

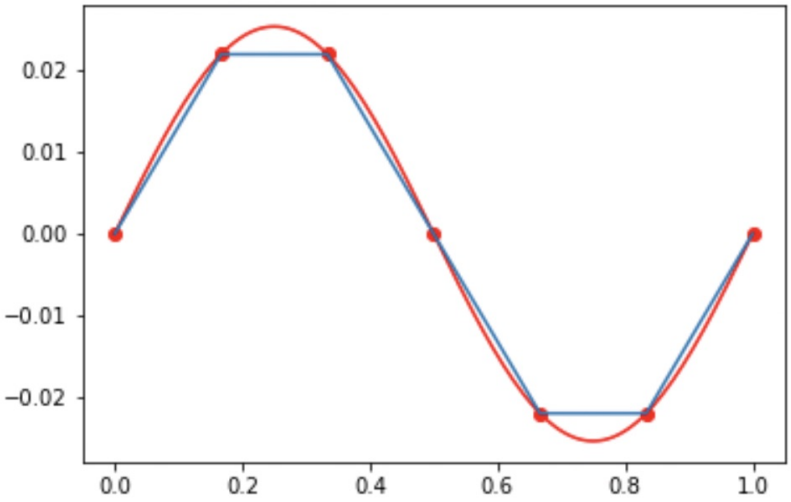
Approximation property of FEM:

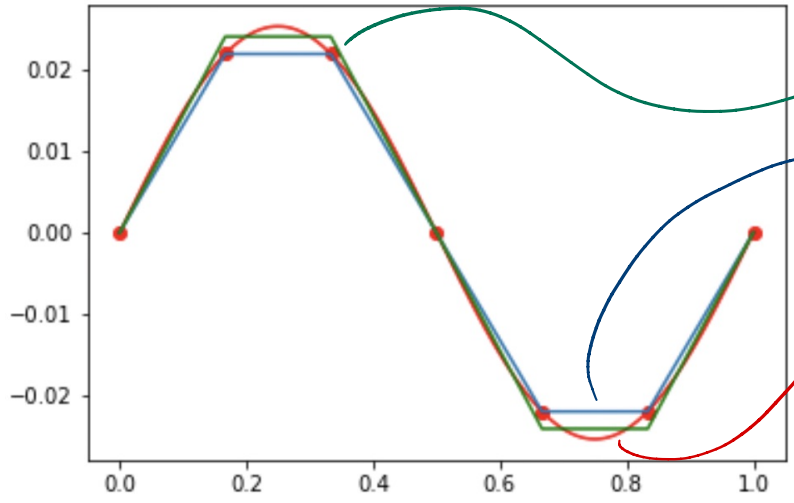
$$\int_0^1 u' v_h' = \int_0^1 f v_h \qquad \forall v_h \in V_h$$

$$\int_0^1 u_h' v_h' = \int_0^1 f v_h \qquad \forall v_h \in V_h \subset V$$

$$\int_0^1 (u' - u_h') v_h' = 0 \qquad \forall v_h \in V_h \subset V$$

orthogonality of the error





FD

FE

Exact

In 1D, the FEM solution coincides with the exact solution at the nodes (while FD does not)

but it depends on the partial diff equation and IT IS EXACT FOR ANY SYMMETRIC POSITIVE DEFINITE SYSTEM (when you can construct a norm with differential operators)

FD is special case of FEM, but it is the "prototipo figurato" of FEM

Lecture 23 LH — Abstract setting of FEM — 17.12.2020

Small recap of necessary concepts of functional analysis

Given V, W normed vector spaces (on the real field $\mathbb{R}$)

Define $\mathcal{L}(V,W)$ the space of linear functions from V to W:

$$f \in \mathcal{L}(V,W) \qquad f : V \longrightarrow W$$

i) $\forall u, v \in V$, $\forall \alpha, \beta \in \mathbb{R}$ $\quad W \ni f(\alpha u + \beta v) = \alpha f(u) + \beta f(v)$

ii) $\forall u \in V \quad \|f(u)\|_W \leq \|f\|_* \, \|u\|_V$

$$\|f\|_* := \sup_{0 \neq v \in V} \frac{\|f(v)\|_W}{\|v\|_V}$$

Special cases:

$$\mathcal{L}(V,\mathbb{R}) \equiv V^* \quad \text{the dual space of } V$$

$$f \in V^* \rightarrow f : V \longrightarrow \mathbb{R}, \quad v \longrightarrow f(v) \equiv \underbrace{{}_{V^*}\langle f, v \rangle_V}_{\text{just notation for now}} \in \mathbb{R}$$

you define

$$\|f\|_{V^*} = \|f\|_* = \sup_{0 \neq v \in V} \frac{|f(v)|}{\|v\|_V} = \sup_{0 \neq v \in V} \frac{|{}_{V^*}\langle f, v \rangle_V|}{\|v\|_V}$$

Bilinear forms: $a : V \times V \longrightarrow \mathbb{R}$

$$a(u,v) \equiv \langle Au, v \rangle \qquad \forall\, u, v \in V$$

where

$$A \in \mathcal{L}(V, V^*) \qquad A : V \longrightarrow V^*$$

$$(Au)(v) \in \mathbb{R}$$

(Au: this is an object in V^*)

$a(\cdot,\cdot)$ is a bilinear form if it is a function from $V \times V$ to $\mathbb{R}$ which is linear in both arguments separately

$$\forall\, u, v, w, z \in V \qquad \alpha, \beta, \gamma, \theta \in \mathbb{R}$$

Linearity in both arguments:

$$a(\alpha u + \beta v, \gamma w + \theta z) = \gamma\alpha\, a(u,w) + \alpha\theta\, a(u,z) \ldots.$$

$$|a(u,v)| \leq \|A\|_* \, \|u\|_V \, \|v\|_V \qquad \forall\, u, v \in V$$

where

$$\|A\|_* := \sup_{0 \neq u \in V} \frac{\|Au\|_{V^*}}{\|u\|_V} = \sup_{0 \neq u,v \in V} \frac{|\langle Au, v \rangle|}{\|u\|_V \, \|v\|_V} = \sup_{0 \neq u,v \in V} \frac{|a(u,v)|}{\|u\| \, \|v\|}$$

if $\|A\|_*$ is $< +\infty$ $\longrightarrow$ then $a(u,v)$ is bounded

Finite element method:

- Take the strong form of the PDE (1)
- Look for a solution in a vector space V
- multiply (1) by test functions in V and integrate on the domain Ω of the PDE
- integrate by parts until you cannot reduce any more the order of the differential op.

$\Rightarrow$ you end up with:

i) a bilinear form in $V \times V$

ii) a linear operator in V^*

Example

new notation for II derivatives

① $\begin{cases} -\Delta u = f & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega \end{cases}$

② Take u in V (V contains the condition $u=0|_{\partial\Omega}$)

③ $\int_\Omega -\Delta u \cdot v = \int_\Omega f v$

$-\Delta u \to -\operatorname{div}(\nabla u)$

④ Integration by part

$\int_\Omega \operatorname{div}(w) = \int_{\partial\Omega} w \cdot n$

$v = 0|_{\partial\Omega}$

0

$\int_\Omega \nabla u \cdot \nabla v - \int_{\partial\Omega} \nabla u \cdot n \, v = \int_\Omega f v$

⑤ $a(u,v) = \int_\Omega \nabla u \nabla v$

$f(v) := \int_\Omega f v$

$f \in V^*$

Consider the case where V is Hilbert,

i) $(u,v)_V$ is its scalar product

ii) $\|u\|_V^2 := (u,u)_V$

Example for FEM of Poisson Problem

$V \equiv H_0^1(\Omega) := \{ v \in L^2(\Omega),\ \nabla v \in L^2(\Omega),\ v|_{\partial\Omega} = 0 \}$

$$(u,v)_V \overset{\text{definition}}{=} \int_\Omega uv + \int_\Omega \nabla u \cdot \nabla v$$

$$\Rightarrow \|u\|_V = \|u\|_1 := \left(\int_\Omega u^2 + \int |\nabla u|^2 \right)^{\frac{1}{2}}$$

A scalar product is a BILINEAR FORM

Abstract setting. V Hilbert (not only H_0^1, but any Hilbert)

Lax Milgram Lemma:

Let

1) a: bilinear, bounded operator

2) a: coercive

1) $a(u,v) \leq \|A\|_* \|u\|_V \|v\|_V \quad \forall u,v \in V$

2) $a(u,u) \geqslant \alpha \|u\|_V^2 \quad \forall u \in V$

Then $\forall f \in V^*$, $\exists!$ solution $u \in V$ to

① $a(u,v) = f(v) = \langle f, v \rangle \quad \forall v \in V$

this it has the property:

And $\|u\| \leq \frac{1}{\alpha} \|f\|_*$ ← solution is BOUNDED with respect to "data"

Since ① is true for every $v \in V$, and $u \in V$ then:

$$\alpha \|u\|^2 \leq a(u,u) = \langle f, u \rangle = f(u) \leq \|f\|_* \|u\|$$

$$\rightarrow \quad \|u\| \leq \frac{1}{\alpha} \|f\|_*$$

Proof of Lax Milgram

2 ingredients
1) Riesz Theorem
2) Contraction theorem (fixed points)

Riesz theorem (1): (Riesz operator $\tau : V^* \rightarrow V$)

$$\forall \; f \in V^* \;, \quad \exists! \; \tilde{f} \in V \quad \text{s.t.}$$

i) $(\tilde{f}, v)_V = \langle f, v \rangle = f(v)$

ii) $\|\tilde{f}\|_V = \|f\|_*$ $\qquad \tilde{f} = \tau f$

Contraction Theorem

Let $T : V \longrightarrow V$ be a contraction, i.e:

$\exists L < 1$ s.t.

$$\|T(u) - T(v)\|_V \leq L \|u - v\|$$

Then $\exists!$ φ fixed point of T: $T(\varphi) = \varphi$

↓ proof of contraction theorem

Let $u^0 \in V$, and define $u^{k+1} = T(u^k)$

$$\rightarrow \|u^{k+1} - u^k\|_V = \|T(u^k) - T(u^{k-1})\| \leq L \|u^k - u^{k-1}\|$$

$$\rightarrow \|u^{k+1} - u^k\| \leq L^k \|T(u^0) - u^0\|$$

$$|L| < 1 \Rightarrow \|u^{k+1} - u^k\| \rightarrow 0$$

$$\Rightarrow \exists!\ u \text{ s.t. } u^k \rightarrow u$$

Proof of Lax Milgram

$$\langle Au, v \rangle = \langle f, v \rangle \qquad \forall v \in V$$

$$a(u, v) = f(v)$$

$$\langle \underbrace{Au - f}_{V^*}, v \rangle \qquad \forall v \in V$$

Riesz repr. theorem

$$(z(Au - f), v)_V \qquad \forall v \in V$$

Construct a fixed point iteration (for $\rho \in \mathbb{R}$)

$$T_\rho(v) := v - \rho z(Av - f) \qquad T_\rho : V \rightarrow V$$

↑ How we see this is a contraction!

$$\|T_\rho(v) - T_\rho(w)\|_V^2 = \|v - w - \rho z A(v - w)\|_V^2$$

$$\|T_\rho(v)-T_\rho(w)\|_V^2 = \|v-w\|_V^2 + \rho^2\|A(v-w)\|_V^2 - 2\rho(A(v-w), v-w)_V$$

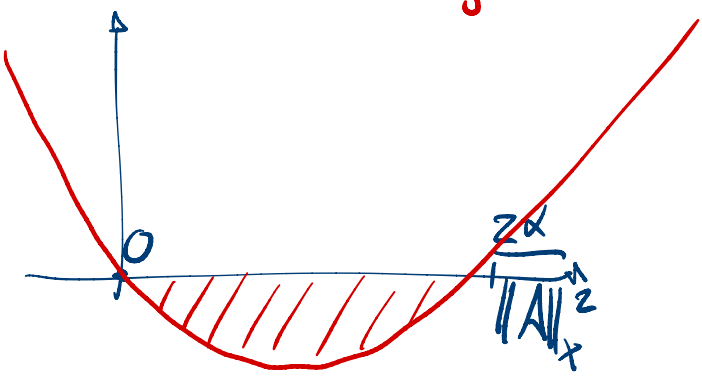
$$= \|v-w\|_V^2 + \rho^2\|A(v-w)\|_{V^*}^2 - 2\rho\langle A(v-w), v-w\rangle$$

$$\leq \|v-w\|^2 + \rho^2\|A\|_*^2\|v-w\|_V^2 - 2\rho\alpha\|v-w\|_V^2$$

$$\|T_\rho(v)-T_\rho(w)\|^2 \leq \underbrace{\left(\rho^2\|A\|_*^2 - 2\rho\alpha + 1\right)}_{<1}\|v-w\|_V^2$$

Can we choose ρ s.t. $\rho^2\|A\|_*^2 - 2\rho\alpha + 1 < 1$?

$$\rho\left(\rho - \frac{2\alpha}{\|A\|_*^2}\right) < 0$$



If $\rho \in \left(0, \frac{2\alpha}{\|A\|_*^2}\right)$ then T is a contraction

$\Rightarrow \exists! u \mid T(u) = u \Rightarrow$ $u = u - \rho z(Au - f)$

$\Rightarrow Au = f$

Galerkin methods:

Choose $V_h = \text{span}\{v_i\}_{i=0}^{N-1}$ s.t. $V_h \subset V$

→ Find $u_h \in V_h$ ⇒ $u_h = \sum_{J=0}^{N-1} u^J v_J$ s.t.

$$\langle A u_h, v_i \rangle = \langle f, v_i \rangle = f(v_i) \qquad i = 0, \dots, N-1$$

$$\sum_J \langle A u^J v_J, v_i \rangle = \langle f, v_i \rangle = f(v_i)$$

$$A_{iJ} := \langle A v_J, v_i \rangle$$

$$\underline{\underline{A}}\,\underline{u} = \underline{f} \qquad \underline{f}_i := f(v_i)$$

1): $\langle A u_h, v_h \rangle = \langle f, v_h \rangle \quad \forall v_h \in V_h$

$\langle A u, v_h \rangle = \langle f, v_h \rangle \quad \forall v_h \in V_h$

I'm saying that the error is A CONJUGATE wrt V_h

$\langle A(u - u_h), v_h \rangle = 0 \quad \forall v_h \in V_h$

The pic above etc

Cea's Lemma (orthogonality of error)

coercivity:

$$\alpha \|u - u_h\|^2 \leq \langle A(u - u_h), u - u_h \rangle = \quad \text{Cea's lemma} \quad \forall v_h \in V_h$$

$$= \langle A(u - u_h), u - v_h \rangle \leq \|A\|^* \|u - u_h\| \, \|u - v_h\|$$

$$\|u - u_h\|_V \leq \frac{\|A\|_*}{\alpha} \inf_{v_h \in V_h} \|u - v_h\|_V$$

← Infimum

A priori error estimate

Trick: Make $\text{dist}(V_h, V)$ small!

$$\text{dist}(V_h, V) := \sup_{u \in V} \inf_{v_h \in V_h} \|u - v_h\|$$

if you can $\text{dist}(V_h, V) < \varepsilon$ ⇒ V is ε approximable by V_h

For Lagrangian Finite elements of order k we bound $u - I(u)$ in terms of Sobolev norms of u:

If $I(u)$ is Lagrange interpolation of u, then

$$\|u - I(u)\|_{m,T} < c\, h_T^{k+1-m} |u|_{k+1,T}$$

T ← "intervals" or "elements"; h_T ← measure of the element

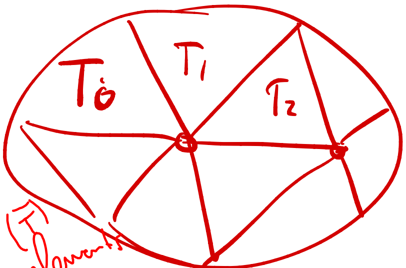
on each "element" T of Ω_h, discretization of Ω.

1D: $\Omega = [0,1]$ $\quad T = [x_i, x_{i+1}]$

$h_T = (x_{i+1} - x_i)$

$$\Omega_h = \overset{\circ}{\overline{\bigcup_{i=1}^{M} \overline{T_i}}}$$

↑ internal part ($\circ$) of the union of all the closures ($\overline{T}$) of the elements



$$|u|_{\alpha,T} := \left(\sum_{|m|=\alpha} \int_T \left(D^m u \right)^2 \right)^{\frac{1}{2}}$$

$D^m u$: weak derivative of order m

$$\|u\|_{\alpha,T} := \left(\sum_{|m|\le\alpha} |u|^2_{\alpha,T} \right)^{\frac{1}{2}}$$

m is multi index $m_1, m_2, \dots, m_d$ in dimension d

and $|m| = \sum_{i=1}^{d} |m_i|$

in 1D: $|u|_{\alpha,T} := \left(\int_T \left(u^{(\alpha)} \right)^2 \right)^{\frac{1}{2}}$

Exercise

we try to approx a finite dim space V, with a smaller finite dim space V_h

$V = \mathbb{R}^n \qquad V_h = \text{span}\{v_i\}_{i=0}^{m-1} \qquad m \le n \qquad v_i \in \mathbb{R}^n \ (\equiv V)$

$$(u, v) := \sum_{i=0}^{n-1} u^i v^i$$

$$\|u\| := \left(\sum_{i=0}^{n-1} (u^i)^2 \right)^{\frac{1}{2}}$$

Apply Galerkin to this problem:

$$a : V \times V \longrightarrow \mathbb{R}$$

$$\underline{\underline{A}} : V = \mathbb{R}^n \longrightarrow V^* \ (\equiv V) = \mathbb{R}^n$$

$\underline{\underline{A}}$ is a $\mathbb{R}^{n\times n}$ matrix, SPD, v_i are $\mathbb{R}^n$ vectors

Galerkin approx:

$$\langle \underline{\underline{A}} \, u^j \underline{v}_j, \underline{v}_i \rangle = \langle \underline{f}, \underline{v}_i \rangle \qquad i = 0, \dots, m-1$$

Should give me a $\mathbb{R}^{m\times m}$ matrix A

$$A_{ij} = \langle \underline{\underline{A}} \underline{v}_j, \underline{v}_i \rangle = \underline{v}_i^T \underline{\underline{A}} \underline{v}_j$$

$$F_i = \langle \underline{f}, \underline{v}_i \rangle = \underline{v}_i^T \underline{f}$$

$V_{id} := (\underline{v}_d)_i \qquad V \in \mathbb{R}^{n \times m}$

Matrix containing the basis $\{\underline{v}_d\}_{d=0}^{m-1}$

$$\boxed{V^T \underline{\underline{A}} V u = V^T \underline{f}}$$

$$A u = F$$

$V \in \mathbb{R}^{n \times m} \qquad \underline{\underline{A}} \in \mathbb{R}^{n \times n} \qquad \underline{f} \in \mathbb{R}^n$

$u \in \mathbb{R}^m$

If we manage to construct $V^T A V = \underline{Id}$ (what I wish to get is)

then $u = V^T f$ (nothing has to be inverted here) $\qquad u \simeq V V^T f$

$V u \simeq \underline{u} \qquad u_0 = 0$

Start with $\varphi_0 = r_0 = A u_0 - f = -f$

$\varphi_0^T \underline{\underline{A}} \varphi_0 := \beta_0^2 \longrightarrow v_0 = \frac{\varphi_0}{\beta_0}$

$\longrightarrow v_0^T \underline{\underline{A}} v_0 = 1$

construct v_{k+1} s.t. $\boxed{v_{k+1}^T A v_j = 0 \quad \forall j \leq k}$

and $\boxed{v_{k+1}^T A v_{k+1} = 1}$

$\Rightarrow$ at most after n iteration $u = V^T V f$

And you get exact for the CG method

Lecture 29 - LA

FEM / FDM 2D

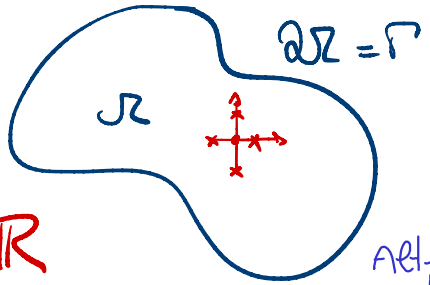
14.01.2021

One problem formulation is

1) $-\Delta u = f$ in Ω

$u = 0$ on $\partial\Omega$

$N=2$



LAPLACIAN

$$-\Delta u := -\frac{\partial^2 u}{\partial x_0^2} - \frac{\partial^2 u}{\partial x_1^2} = \sum_{d=0}^{N-1} -\frac{\partial^2 u}{\partial x_d^2}$$

$u : \Omega \to \mathbb{R}$

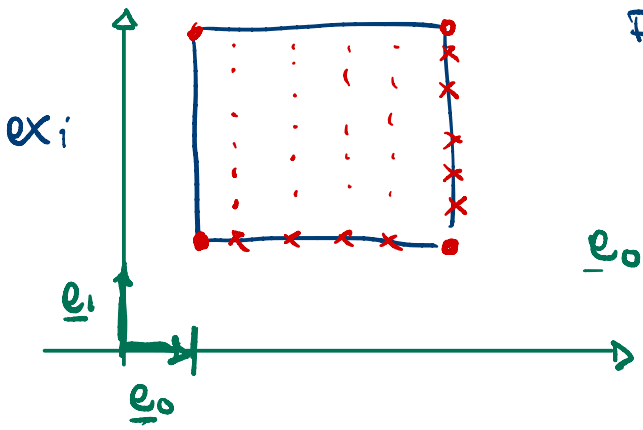
sometimes:

Alternatively, another problem that can appear is

$-\Delta u + u = f$

2) $\frac{\partial u}{\partial n} = 0$ on $\partial\Omega$

For FD Ω has to be "simple" and "regular"



Fix a grid of points $X_{ij} \in \Omega \subset \mathbb{R}^2$

$\Omega = [a,b] \times [c,d]$

$e_0 := (1,0)$ $e_1 = (0,1)$

$$\underline{x} = \underline{e}_0 x^0 + \underline{e}_1 x^1 = \underline{e}_i x^i$$

FD: along e_0: choose n points as $\{\varphi_i\}_{i=0}^{n-1} := [a, a+\dots, \dots, b]$

along e_1: choose m points as $\{\psi_\alpha\}_{\alpha=0}^{m-1} := [c, \dots, \dots, d]$

construct $X_{\alpha i} \in \mathbb{R}^2$ ($n \times m$ points) $\alpha \in [0,\dots,m-1]$, $i \in [0,\dots,n-1]$

$(X_{\alpha i})_d \to d$ comp. of $X_{\alpha i}$

$$X_{\alpha i} := (\varphi_i, \psi_\alpha) \qquad \{X_{\alpha i d}\}_{\substack{\alpha=0,\dots,m-1 \\ i=0,\dots,n-1 \\ d=0,1}}$$

You want same N of pts on both x and y direction, for 2 reasons: 1) simplicity 2) if I flatten the things I get $m \cdot n \cdot 2$ or $n \times m$ points in dimension 2

$$\text{flat}(X) \in \mathbb{R}$$

The X object has elements

$$X_{\alpha i d} = \begin{cases} \varphi_i & \text{if } d = 0 \leftarrow \text{first direction} \\ \psi_\alpha & \text{if } d = 1 \leftarrow \text{second direction} \end{cases}$$

$X \in \mathbb{R}^m \times \mathbb{R}^n \times \mathbb{R}^N$ $\quad shape(X) = (m,n,N)$

$X_{ij} \in \mathbb{R}^N$ $\quad \underline{x}$

$X_{ijd} \in \mathbb{R}$ $\quad x_i$

$X_d \in \mathbb{R}^{n \times N}$

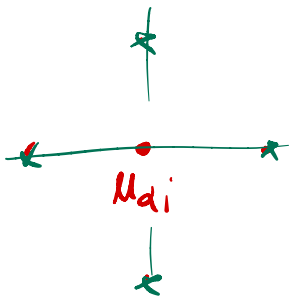
Now we assume we know u on X (that is only on the grid) only (on all $n \cdot m$ points $X_{di} \in \Omega$ such that)

$u_{di} := u(X_{di})$ ← u is a function that if you pass it a "matrix" (matrix element) you get a matrix (matrix element)

We apply CFD to u_{di} on both directions:

CFD^2-1D: $-v_i'' \sim \frac{-v_{i-1} + 2v_i - v_{i+1}}{h^2}$ (along $i \rightsquigarrow e_0$)

CFD^2-1D along $d \rightsquigarrow e_1$ $\quad -w_d'' \sim \frac{-w_{d-1} + 2w_d - w_{d+1}}{h^2}$



you assume that the approximation at u_{di} depends only on the value at these 5 points

$v_i := u_{di}$
$w_d := u_{di}$

$-\Delta u_{di} \simeq \frac{1}{h^2}\left[4u_{di} - u_{d-1\,i} - u_{d+1\,i} - u_{d\,i-1} - u_{d\,i+1}\right]$

$-\tilde{\Delta} u_{di} = f_{di} = f(X_{di})$

$Au = f$

$A \in \mathbb{R}^m \times \mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}^n$

because I have 2 directions $d = 0$ and 1

Construct

$$A_{\alpha i\ \beta J} \quad \text{s.t.} \quad \sum_{\beta,J} A_{\alpha i\ \beta J}\, u_{\beta J} = -\tilde{\Delta}\, u_{\alpha i}$$

$$A_{\alpha i\ \beta J} = \begin{cases} 4 & \beta=\alpha \quad J=i \\ -1 & \beta=\alpha-1 \quad J=i \\ -1 & \beta=\alpha+1 \quad J=i \\ -1 & \beta=\alpha \quad J=i-1 \\ -1 & \beta=\alpha \quad J=i+1 \\ 0 & \text{all other cases} \end{cases}$$

$$A_{\alpha i\ \beta J}\, u_{\beta J} = f_{\alpha i}$$

$$\Downarrow \text{ reshape}$$

$$\sum_J \tilde{A}_{IJ}\, \tilde{u}_J = \tilde{f}_J$$

$$I, J \in [0, \dots, m \cdot n - 1]$$

$$\tilde{u}_J = \sum_I \left(\tilde{A}^{-1}\right)_{JI} \tilde{f}_I$$