Master in High Performance Computing

Applied Mathematics: an introduction to Scientific Computing by Numerical Analysis

Lecture 01 - INTRODUCTION

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What is numerical analysis?

1. Approximation
2. Algorithms (formal study of numerical methods)
3. Go from analytical to numerical

Given a "problem", $\underbrace{\text{find a way to solve it approximately}}_{\text{algorithm}}$,

$\underbrace{\text{write a computer code that solves it}}_{\text{implementation}}$, and estimate

$\underbrace{\text{how far you are from reality}}_{\text{error analysis}}$ -

$\boxed{\text{Abstract Problem}}$

x : input data, in a space $\mathcal{X}$, $\|\cdot\|_{\mathcal{X}}$

y : output data, in a space $\mathcal{Y}$, $\|\cdot\|_{\mathcal{Y}}$

$y = f(x) \qquad f : \mathcal{X} \longrightarrow \mathcal{Y}$

When is "$y = f(x)$" ($\equiv$ a problem)

is $\boxed{\text{well posed}}$?

Absolute Well posedness

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

2) $\exists!\, y$ (the sol. is unique!)

3) Absolute Stability: $\exists\, K_{abs}$ s.t.

$\forall x \in \mathcal{X}$, $\forall\, \delta x$ s.t. $x + \delta x \in \mathcal{X}$

$$\boxed{\|\delta y = f(x+\delta x) - f(x)\|_{\mathcal{Y}} \leq K_{abs} \|\delta x\|_{\mathcal{X}}}$$

$$K_{abs} := \sup_{x \in \mathcal{X}} \ \sup_{\delta x \,|\, x+\delta x \in \mathcal{X}} \frac{\| f(x+\delta x) - f(x) \|}{\| \delta x \|}$$

$\boxed{\text{A problem is relatively well conditioned}}$

$\Longleftrightarrow$

1) the pb. is abs. well conditioned and $\exists$ k_{rel} s.t.

2) $\forall x \mid \|x\|_{\mathcal{X}} \neq 0$ and s.t. $\|f(x)\|_{\mathcal{Y}} \neq 0$

$$\boxed{\frac{\|f(x+\delta x) - f(x)\|_{\mathcal{Y}}}{\|f(x)\|} \leq k_{rel} \frac{\|\delta x\|}{\|x\|}}$$

$$\boxed{k_{rel} := \sup_{x \in \mathcal{X}} \sup_{\delta x \mid \delta x + x \in \mathcal{X}} \frac{\|\delta y\|}{\|\delta x\|} \frac{\|x\|}{\|\delta x\|}}$$

Example

$\mathcal{X} := \mathbb{R}^2$ $\qquad x = (x_1, x_2)$ $\qquad \|x\|_{\mathcal{X}} = \|x\|_{e_1} := |x_1| + |x_2|$

$\mathcal{Y} := \mathbb{R}$ $\qquad \|y\|_{\mathcal{Y}} = |y|$

$$f(x) = x_1 + x_2$$

$$f(x+\delta x) = x_1 + \delta x_1 + x_2 + \delta x_2$$

$\|\delta x\| = |\delta x_1| + |\delta x_2|$ $\qquad \|\delta y\| = |\delta x_1 + \delta x_2|$

$$\kappa_{abs} := \sup_{\delta x} \frac{\|\delta y\|}{\|\delta x\|} := \sup_{\delta x} \frac{|\delta x_1 + \delta x_2|}{|\delta x_1| + |\delta x_2|} \leq$$

$$\kappa_{abs} \leq \frac{|\delta x_1| + |\delta x_2|}{|\delta x_1| + |\delta x_2|} := 1$$

$$\kappa_{rel} := \sup_{\delta x, x} \frac{\|\delta y\|}{\|y\|} \frac{\|x\|}{\|\delta x\|}$$

$$\sup_{\delta x, x} \frac{(|\delta x_1 + \delta x_2|)(|x_1| + |x_2|)}{(|x_1 + x_2|)(|\delta x_1| + |\delta x_2|)} \leq$$

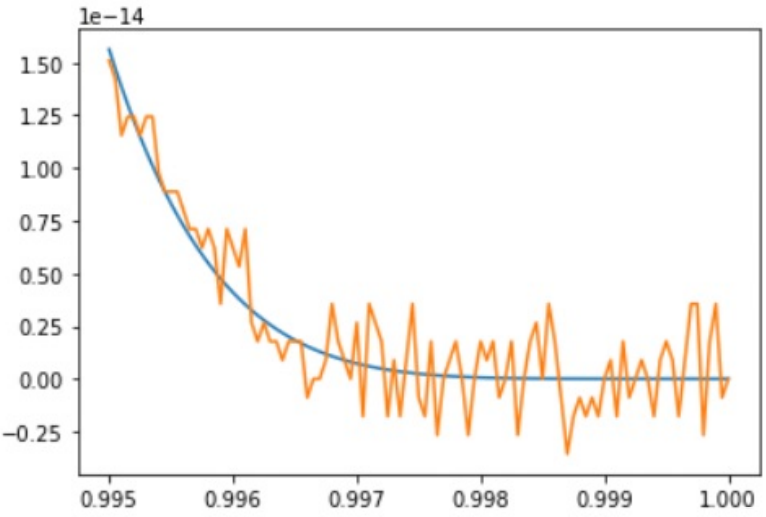
$$\boxed{\kappa_{rel} := \sup_{x} \frac{|x_1| + |x_2|}{|x_1 + x_2|} = \infty}$$

x_1, x_2 $\quad x_1 \cdot x_2 < 0$, $|x_1| \sim |x_2|$

$$\Longrightarrow \quad |x_1 + x_2| \sim 0$$

$$10^5 + (-10^5 + 10^{-1})$$

Think of. $\left(\sum_{i=1}^{10^6} x_i \right)$



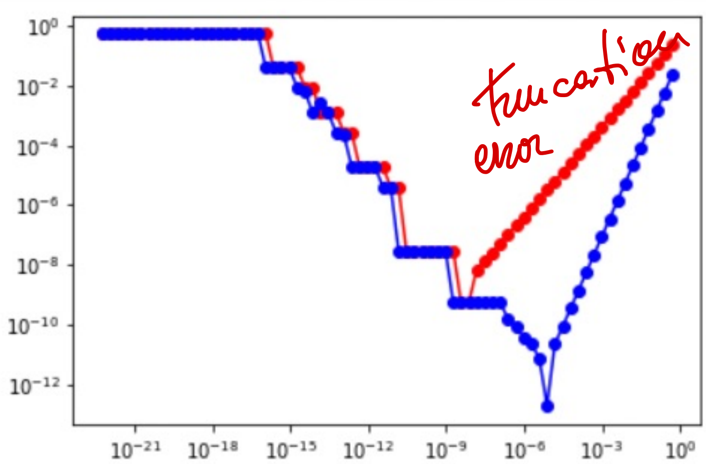
—: $(1-x)^6$

~~~: $x^6 - 6x^5 + \dots + 1$

a) sum of 2 terms

b) sum of 7 terms

a is better conditioned



FD v CFD

Given g, compute $g'(x) = y$

FD: $g' \sim \dfrac{g(x+h) - g(x)}{h}$

CFD: $g' \sim \dfrac{g(x+h) - g(x-h)}{2h}$

Numerical analysis in abstract problems:

Replace x, y, f by $\boxed{x_n, y_n, f_n}$

$\boxed{\text{sequences}}$ of data/output/models which are computable

$x_n \in \mathcal{X}_n, \quad y_n \in \mathcal{Y}_n$
~~~

$\boxed{\text{When do a numerical problem converge?}}$

for $n \to \infty$ you "improve":

$$\boxed{\begin{aligned} x_n &\longrightarrow x \\ y_n &\longrightarrow y \\ f_n &\longrightarrow f \end{aligned}}$$

The abstract pb: $\quad y = f(x)$ forward

defines two other problems: $\quad x = f^{-1}(y)$ inverse

$$f = F\left(\{x_i, y_i\}_{i=1}^{n}\right)$$ model identification

A numerical approximation is well posed if

$$\boxed{f_n(x_n) = y_n \quad \text{is well posed} \quad \forall n}$$

It is <u>consistent</u> if $x \in X_n \ \forall n$ and

$$\lim_{n\to\infty} \| f_n(x) - f(x) \|_{\mathcal{Y}} = 0$$

It is <u>convergent</u> if $x_n \to x$

$$\lim_{n\to\infty} \| f_n(x_n) - f(x) \|_{\mathcal{Y}} = 0$$

Theorem Lax - Richtmeyer :

If approximation is consistent

then

$\boxed{\text{stability}} \iff \boxed{\text{convergence}}$

Example.

$$f(g) = g'(\xi) \rightsquigarrow f_n(g) = \frac{g(\xi + \frac{1}{n}) - g(\xi)}{1/n}$$

$$x \in C^1(I(\xi)) \equiv \mathcal{X} \qquad I(\xi) := [\xi - a, \xi + a]$$

$$f(x) = g'(\xi) \in \mathbb{R} \equiv \mathcal{Y}$$

$$\|u\|_{\mathcal{X}} := \max_{s \in I(\xi)} |u(s)| + \max_{s \in I(\xi)} |u'(s)|$$

$$\|y\|_{\mathcal{X}} := |y|$$

$$f_n : \frac{g(\xi + \frac{1}{n}) - g(\xi)}{1/n}$$

$$\lim_{n \to \infty} f_n(g) - f(x) = 0$$

by construction

$$\lim_{n \to \infty} f_n(x) - f(x) = 0$$

Truncation Error

by Taylor expansion

$$\left| f_n(x) - f(x) \right| = \left|\right.$$

$$f_n(g) = \left(g\left(\xi + \frac{1}{n}\right) - g(\xi) \right) n$$

$$= \left(\left[\cancel{g(\xi)} + g'(\xi)\cancel{\frac{1}{n}} + \frac{1}{2} g''(\xi)\left(\frac{1}{n}\right)^2 + \sum_{k=3}^{\infty} \frac{1}{k!} g^{(k)}(\xi) \left(\frac{1}{n}\right)^k \right] - \cancel{g(\xi)} \right) \cancel{n}$$

$$= g'(\xi) + \underbrace{\left[\sum_{k=2}^{\infty} \frac{g^{(k)}}{k!} \left(\frac{1}{n}\right)^{k-1} \right]}_{\text{Truncation error}}$$

Rounding error :

error mode in $\boxed{x + \delta x}$