Analisi Numerica
Error analysis

Università di **Perugia**, **Italia**

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Rational numbers are infinitely many $\Rightarrow$ we can only deal with finite sets of numbers.

Problem

Select a finite number of representatives to approximate real numbers.

Naive attempt for numbers: **uniform distribution**. Choose $\varepsilon > 0$, N even and

$$\mathcal{E} = \left\{ \varepsilon k \,:\, -\frac{N}{2} < k \leqslant \frac{N}{2},\, k \in \mathbb{Z} \right\}.$$

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Representation function (from real numbers to the chosen set)

$$e : S \to \mathcal{E}, \quad x \to k\varepsilon, \quad (k-1)\varepsilon < x \leqslant k\varepsilon.$$

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Representation absolute error

$$e(x) - x, \qquad \max_{x \in S} |e(x) - x| < \varepsilon$$

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Representation error

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This choice makes the absolute error uniformly small.

Absolute vs. Relative Error

- Absolute error $\widetilde{x} - x$.
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x	$\widetilde{x}$	absolute	relative
1.234	1.235	$1 \cdot 10^{-3}$	$8.1 \cdot 10^{-4}$
1234	1235	1	$8.1 \cdot 10^{-4}$
0.001234	0.001235	$1 \cdot 10^{-6}$	$8.1 \cdot 10^{-4}$

We wish to have a small relative error.

New problem

Select a finite number of representatives to approximate real numbers with a uniformly bounded relative error.

Idea: consider the digit representation of a real number.

Given a numeration basis $\beta \geqslant 2$, there is a correspondence between real numbers in $[0, 1)$ and sequences of digits

$$\mathbb{R} \Longleftrightarrow \{d_i\}_{i=1,2,\ldots}, \ d_i \in \{0, \ldots, \beta - 1\}.$$

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- fixed point (natural): $x \to (\{d_i\}_{i=1,2,\dots}, M)$ (d_i is the ith digit and M says where the point is).
- floating point (scientific): $x \to (0.d_1 d_2 d_3 \cdots)\beta^p$, with $d_1 \neq 0$.

$$12.38 = 0.1238 \cdot 10^2.$$

Theorem (Basis representation theorem)

Let $x \in \mathbb{R} \setminus \{0\}$ and let $\beta \geqslant 2$ be a numeration basis, there exist unique $p \in \mathbb{Z}$ and a sequence $\{d_i\}_{i=1,2,\ldots}$ such that

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(i) $d_i \in \{0, 1, \ldots, \beta - 1\}$;

(ii) $d_1 \neq 0$; *(To avoid ambiguity, e.g.,* $0.03 \cdot 10^2$ *and* $0.3 \cdot 10^1$*)*

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(ii) $d_1 \neq 0$;

(iii) *d_i not definitely equal to $\beta - 1$; (There exists an infinite set of indices K such that $d_k \neq \beta - 1$ for every $k \in K$)*

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such that

$$x = sign(x)\beta^p \sum_{i=1}^{\infty} \beta^{-i} d_i.$$

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Idea: consider numbers with finite mantissa

Given a numeration basis $\beta \geqslant 2$, the number $t > 0$ of digits of the mantissa, and m, M positive integers, we define a set of **floating point numbers**

$$\mathcal{F}(\beta, t, m, M) = \{0\} \cup \Big\{ \pm \beta^p \sum_{i=1}^{t} \beta^{-i} d_i, \\ -m \leqslant p \leqslant M,\ 0 \leqslant d_i < \beta \text{ integer for } i = 1, \ldots, t,\ d_1 \neq 0 \Big\}.$$

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We will use this set to represent real numbers.

As an example

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- $12 \in \mathcal{F}$? yes $\Longleftarrow 12 = 0.12 \cdot 10^2$
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- $\pi \in \mathcal{F}$?

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- $12.345 \in \mathcal{F}$? no $\Longleftarrow 12.345 = 0.12345 \cdot 10^2$ (more than two digits)
- $1000 \in \mathcal{F}$?

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- $1/10000 \in \mathcal{F}$? no $\Longleftarrow 0.001 = 0.10 \cdot 10^{-3}$ (too small in modulus)

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For $x \geqslant \Omega$ we cannot represent numbers, for $0 < x < \omega$ we make a large relative error.

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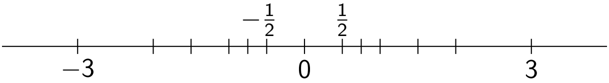
They are **not uniform**: between $1/2$ and $1/4$ and between $1/2$ and 1 there is the same number of elements of $\mathcal{F}$.



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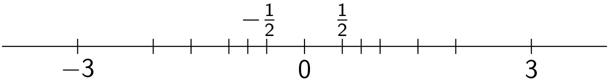
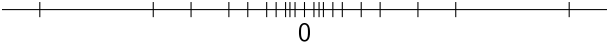


$\mathcal{F}(2,2,2,2)$ has 21 numbers



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Given $S = \{x \in \mathbb{R} \,:\, \omega \leqslant x \leqslant \Omega\}$, we construct a **representation function**

$$\mathrm{fl} : \mathbb{R} \longrightarrow \mathcal{F} \cup \{\pm\infty\}$$

with one of the two rules, where $x = \beta^p \sum_{i=1}^{\infty} \beta^{-i} d_i \in S$,

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If $x > \Omega$ we set $\mathrm{fl}(x) = \infty$ (**overflow**), if $0 \leqslant x < \omega$ we set $\mathrm{fl}(x) = 0$ (**underflow**) and for negative numbers the extension is straightforward.

We define the **machine precision** as $u = \beta^{-t+1}$ in the case of truncation and $u = \beta^{-t+1}/2$ in the case of rounding.

Theorem

Let $x \in S$ then we have the following bound for the relative error

$$\left| \frac{\mathrm{fl}(x) - x}{x} \right| < u.$$

Proof. For the truncation

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Theorem

Let $x \in S$ then we have the following bound for the relative error

$$\left|\frac{\mathrm{fl}(x) - x}{x}\right| < u.$$

Proof. For the truncation

$$\frac{|\,\mathrm{fl}(x) - x|}{|x|} = \frac{x - \mathrm{fl}(x)}{x}$$

Since $x \geqslant \mathrm{fl}(x)$.

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By definition: $\sum_{i=1}^{\infty} \beta^{-i} d_i - \sum_{i=1}^{t} \beta^{-i} d_i = \sum_{i=t+1}^{\infty} \beta^{-i} d_i$.

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$$\sum_{i=1}^{\infty} \beta^{-i} d_i \geqslant \beta^{-1}.$$

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$$\sum_{i=t+1}^{\infty} \beta^{-i} d_i \leqslant (\beta - 1) \sum_{i=t+1}^{\infty} \beta^{-i} = (\beta - 1)\Big(\sum_{i=0}^{\infty} \beta^{-i} - \sum_{i=0}^{t} \beta^{-i}\Big)$$

$$= (\beta - 1)\Big(\frac{1}{1 - 1/\beta} - \frac{1 - \beta^{-t-1}}{1 - 1/\beta}\Big) = \frac{\beta - 1}{\frac{\beta-1}{\beta}} \beta^{-t-1} = \beta^{-t}.$$

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Floating point on a computer

For the single precision floating point (`float` 32 bits)

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Floating point on a computer

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For the double precision floating point (`double` 64 bits)

$$\mathcal{F}(2, 52, 1022, 1023), \qquad u = 2^{-52} \approx 2.2 \cdot 10^{-16}.$$

Bad news: $\mathcal{F}$ has **few algebraic properties**, e.g.,

$$x, y \in \mathcal{F} \not\Rightarrow x + y \in \mathcal{F}$$

We must define floating point operations.

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We may assume that there exists a floating point sum $\oplus$ such that, if $x, y \in \mathcal{F}$, then (if overflow does not occur)

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Similarly we define $\otimes$, $\ominus$, $\oslash$.

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Similarly we define $\otimes$, $\ominus$, $\oslash$.

A simple idea is to define, for instance, $x \otimes y = \mathrm{fl}(x + y)$, but details are more complicate.

Floating point operations verify just some properties

- $x \oplus y = y \oplus x$ (commutativity of the sum);
- $x \otimes y = y \otimes x$ (commutativity of the product);
- $x \oslash x = 1$.

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- $x \oslash x = 1$.

They do not verify others

- associativity of the sum and product;
- distributive law;
- simplification (it may happen $x \otimes (y \oslash x) \neq y$);
- no null factor law (it may happen $x \otimes y = z \otimes y$ with $y \neq 0$ and $x \neq z$)

Well-posed problems

Which problems are we interested in?

Well-posed problems

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But first. . .

Well-posed problems

What is a problem?

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What is a problem?

A problem is made of three parts

- Data
- Unknowns
- Conditions

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Given a matrix A (coefficient) and a vector b (right hand side), find all vectors x (unknown) such that $Ax = b$.

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Example 2: the **polynomial equation** problem.

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Example 2: the **polynomial equation** problem.

Given a polynomial $p(x)$, find all complex numbers x (unknowns) such that $p(x) = 0$.

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Example 3: the **integration**.

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Given a continuous function $f(x)$ (integrand) and two real numbers $a \leqslant b$ (extremes),

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Example 3: the **integration**.

Given a continuous function $f(x)$ (integrand) and two real numbers $a \leqslant b$ (extremes), find a real number I (unknown) such that $I = \int_a^b f(x)dx$.

Well-posed problems

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A problem is made of three parts

- Data
- Unknowns
- Conditions

In all cases the unknowns are functions of the data.

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In all cases the unknowns are functions of the data.

Solutions of problems $\Longleftrightarrow$ Evaluation of a function

In practical cases, only an **approximation** can be provided.

Well-posed problems

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Well-posed problems

-
-
-

Well-posed problems

Which problems are we interested in?

Well-posed problems

- They have a solution
-
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Which problems are we interested in?

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- They have a solution (or else what are we computing?)
-
-

Well-posed problems

Which problems are we interested in?

Well-posed problems

- They have a solution
- The solution is unique
-

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Which problems are we interested in?

Well-posed problems

- They have a solution
- The solution is unique (or else what is the correct answer?)
-

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- They have a solution
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- The solution depends continuously from the data

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- They have a solution
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- The solution depends continuously from the data

Continuous dependence from data is (less obviously) important

- Data in real problems are affected by errors
- Computation is made on finite arithmetic and there are rounding errors

Continuous dependence from data

Consider a problem with data and unknowns in the Banach spaces V and W, respectively.

The problem **strongly** continuously depends from data at $A \in V$ if there exists a neighborhood $\mathcal{U} \subset V$ of A such that the problem has a unique solution $X(B)$ for $B \in \mathcal{U}$ and $\lim_{B \to A} X(B) = X(A)$.

The problem **weakly** continuously depends from data at $A \in V$ if for $B \in V$, there exists $t_0 > 0$ such that the problem with data $A + tB$ has a unique solution $X(t)$ for $t \in [0, t_0)$ and $\lim_{t \to 0^+} X(t) = X(0)$.

Strong dependence implies weak dependence, but not the contrary.

Weak dependence is more frequent and sometimes it is enough in applications.

Implicit functions theorem

A problem is often stated as an implicit equation (e. g. systems of equations, zeros of polynomials, ODEs, PDEs).

Theorem (Implicit functions)

Let $F : \Omega \to \mathbb{R}^n$, *with* $F \in C^1(\Omega)$, $\Omega \in \mathbb{R}^n \times \mathbb{R}^m$ *such that* $F_x(x_0, y_0) : \mathbb{R}^n \to \mathbb{R}^n$ *is invertible for* $(x_0, y_0) \in \Omega$[a]*.*
There exist neighborhoods $\mathcal{U} \ni (x_0, y_0)$ *and* $\mathcal{V} \ni y_0$ *and* $g : \mathcal{V} \to \mathbb{R}^n$, *with* $g \in C^1(\mathcal{V})$ *such that for* $(x, y) \in \mathcal{U}$

$$F(x, y) = F(x_0, y_0) \Longleftrightarrow x = g(y).$$

[a] we use the notation $F(x, y)$ with $x \in \mathbb{R}^n$ and $y \in \mathbb{R}^m$

An analogous results holds for $F : \Omega \to \mathbb{C}^n$ and F analytic in $\Omega \in \mathbb{C}^n \times \mathbb{C}^m$. In this case g is analytic as well.

Example: square linear system

Theorem

Let $A \in \mathbb{C}^{n \times n}$. The linear system $Ax = b$ is **strongly** *well posed for $b \in \mathbb{C}^n$ if and only A is invertible.*

Proof.

$\square$

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Proof.

Since $(A, b) \in \mathbb{C}^{n\times n} \times \mathbb{C}^n \cong \mathbb{C}^{n^2+n}$, we can see data as belonging to a vector space.

Let $F : \mathbb{C}^{n^2+n} \times \mathbb{C}^n \to \mathbb{C}^n$ be such that $F((A, b), x) = Ax - b$.
Writing

$$F((A,b),x) = \begin{bmatrix} F_1 \\ F_2 \\ \vdots \\ F_n \end{bmatrix} = \begin{bmatrix} a_{11}x_1 + \cdots + a_{1n}x_n - b_1 \\ a_{21}x_1 + \cdots + a_{2n}x_n - b_2 \\ \vdots \\ a_{n1}x_1 + \cdots + a_{nn}x_n - b_n \end{bmatrix},$$

we see that F is differentiable, since its components are polynomials.

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Proof.

The derivative with respect to x_i is $\frac{\partial F_i}{\partial F_j} = a_{ij}$ and thus the Jacobian matrix is A and we can say that $F_x((A, b), x)[h] = Ah$, with $h \in \mathbb{C}^n$.

The function F is differetiable with F_x invertible, the implicit functions theorem implies that there exists a neighborhood of $((A, b), x)$ such that $Ax = b$, where

$$\widetilde{A}\widetilde{x} - \widetilde{b} = F((\widetilde{A}, \widetilde{b}), \widetilde{x}) = F((A, b), x) = Ax - b = 0$$

if and only if $\widetilde{x} = g(\widetilde{A}, \widetilde{b})$ with g differentiable. (Note that $g(\widetilde{A}, \widetilde{b}) = \widetilde{A}^{-1}\widetilde{b}$.) $\square$

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Proof.

The converse is left as an exercise. $\square$

The theorem can be proved using only linear algebra.

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The linear system $Ax = b$ with A square and invertible.

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The solution is $x = A^{-1}b$. Let $(A^{-1})_{ij} = \widetilde{a}_{ij}$, for $i, j = 1, \ldots, n$, be the elements of the inverse

$$x_i = \sum_{j=1}^{n} \widetilde{a}_{ij} b_j$$

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$$x_i = \sum_{j=1}^{n} \widetilde{a}_{ij} b_j$$

with (adjoint's formula, **inefficient!**)

$$\widetilde{a}_{ij} = \frac{1}{\det(A)} (-1)^{i+j} \det(M^{(ij)}),$$

where $M^{(ij)}$ is obtained removing the i-th row and the j-th column from A^T.

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Note that

- the first formula is a polynomial;
- $\det(X)$ is a polynomial of the entries of X;
- the second formula is a rational function.

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Note that

- the first formula is a polynomial;
- $\det(X)$ is a polynomial of the entries of X;
- the second formula is a rational function.

Thus, x_i is a rational function (continuous) of the data. We can write

$$x = f(a_{11}, \dots, a_{nn}, b_1, \dots, b_n), \qquad f : \mathbb{K}^{n^2+n} \to \mathbb{K}^n.$$

We have translated a problem to a function.

Example: roots of polynomials

The roots of the polynomial

$$az^2 + bz + c = 0,$$

can be written as

$$z_1 = \frac{-b + \sqrt{b^2 - 4ac}}{2a}, \qquad z_2 = \frac{-b - \sqrt{b^2 - 4ac}}{2a},$$

where the complex square root is the one with positive real part (or positive imaginary part if the real part is 0).

They are analytic functions of the coefficients if $b^2 - 4ac \neq 0$ in a neighborhood of the polynomial, while for $b^2 - 4ac = 0$ they loose analyticy (and continuity in some sense).

Example: roots of polynomials

Theorem

Let $p(z) \in \mathbb{C}[z]$. The polynomial equations $p(z) = 0$ is a **strongly** *well posed problem if p has distinct roots.*

Proof.

$\square$

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Proof.

We prove the theorem by induction on the degree n of p.

If $n = 1$ then $p(z) = a_1 z + a_0$ has one distinct root α. If $\widetilde{p}(z) = \widetilde{a}_1 z + \widetilde{a}_0$ lies in a neighboor of $p(z)$ with $\widetilde{a}_1 \neq 0$ then $\widetilde{p}(z)$ has a unique root $\widetilde{\alpha} = -\widetilde{a}_0/\widetilde{a}_1$. Note that $\widetilde{\alpha}$ is a continuous function of the coefficients of $\widetilde{p}$ and $\lim_{\widetilde{p} \to p} \widetilde{\alpha} = -a_0/a_1 = \alpha$.[a]

$\square$

[a] We have that $\widetilde{p} \to p$, if and only if $\widetilde{a}_0 \to a_0, \ldots, \widetilde{a}_n \to a_n$.

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Let $p(z) \in \mathbb{C}[z]$. The polynomial equations $p(z) = 0$ is a **strongly** *well posed problem if p has distinct roots.*

Proof.

If $p(z) = a_0 + a_1 z + \cdots + a_n z^n$, and α is a root of p, then

$$p(z) = (z - \alpha) \underbrace{\left(b_0 + b_1 z + \cdots + b_{n-1} z^{n-1}\right)}_{q(z)},$$

for a unique $q(z)$, from which we get the system of equations

$$\begin{cases} a_0 + \alpha b_0 = 0, \\ a_1 + \alpha b_1 - b_0 = 0, \\ \quad \vdots \\ a_{n-1} + \alpha b_{n-1} - b_{n-2} = 0, \\ a_n - b_{n-1} = 0. \end{cases}$$

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$$\begin{cases} a_0 + \alpha b_0 = 0, \\ a_1 + \alpha b_1 - b_0 = 0, \\ \quad \vdots \\ a_{n-1} + \alpha b_{n-1} - b_{n-2} = 0, \\ a_n - b_{n-1} = 0. \end{cases}$$

can be written as $F(a_0, \ldots, a_n, \alpha, b_0, \ldots, b_{n-1}) = 0$. We have that $F : \mathbb{C}^{n+1} \times \mathbb{C}^{n+1} \to \mathbb{C}^{n+1}$ is differentiable (it is a polynomial) and

$$\frac{\partial F}{\partial \alpha} = \begin{bmatrix} b_0 \\ \vdots \\ b_{n-1} \\ 0 \end{bmatrix} \in \mathbb{C}^{n+1}, \qquad \frac{\partial F}{\partial b} = \begin{bmatrix} \alpha & 0 & \cdots & 0 \\ -1 & \alpha & \ddots & \vdots \\ 0 & -1 & \ddots & 0 \\ \vdots & \ddots & \ddots & \alpha \\ 0 & \cdots & 0 & -1 \end{bmatrix} \in \mathbb{C}^{(n+1)\times n}.$$

Example: roots of polynomials

Theorem

Let $p(z) \in \mathbb{C}[z]$. The polynomial equations $p(z) = 0$ is a **strongly** *well posed problem if p has distinct roots.*

Proof.

The partial Fréchet derivative is associated with the matrix

$$F_{\alpha, b_0, \dots, b_{n-1}} = \begin{bmatrix} \frac{\partial F}{\partial \alpha} & \frac{\partial F}{\partial b_{n-1}} \end{bmatrix} \in \mathbb{C}^{(n+1)\times(n+1)}.$$

We claim that $F_{\alpha, b_0, \dots, b_{n-1}}$ is invertible if and only if $q(\alpha) \neq 0$, that is α is not a root of q.

Since the last row of $F_{\alpha, b_0, \dots, b_{n-1}}$ contains just a -1 in the last position, it is sufficient to consider

$$M := \begin{bmatrix} b_0 & \alpha & 0 & \cdots & 0 \\ b_1 & -1 & \alpha & \ddots & \vdots \\ \vdots & 0 & \ddots & \ddots & 0 \\ b_{n-1} & \vdots & \ddots & \ddots & \alpha \\ 0 & 0 & \cdots & 0 & -1 \end{bmatrix}$$

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We prove that M is singular if and only if $q(\alpha) = 0$. If $q(\alpha) = 0$, then

$$\begin{aligned} &\begin{bmatrix} 1 & \alpha & \alpha^2 & \cdots & \alpha^{n-1} \end{bmatrix} M \\ &= \begin{bmatrix} b_0 + b_1\alpha + b_2\alpha^2 + \cdots + b_{n-1}\alpha^{n-1} & \alpha - \alpha & \cdots & \alpha^{n-1} - \alpha^{n-1} \end{bmatrix} \\ &= \begin{bmatrix} q(\alpha) & 0 & \cdots & 0 \end{bmatrix} = 0. \end{aligned}$$

We have proved that M^T has a nonzero kernel, this implies that M^T is singular and thus M is singular. □

Example: roots of polynomials

Theorem

Let $p(z) \in \mathbb{C}[z]$. The polynomial equations $p(z) = 0$ is a **strongly** *well posed problem if p has distinct roots.*

Proof.

On the contrary, if M is singular, then there exists a nonzero vector $v = \begin{bmatrix} y_0 & y_1 & \cdots & y_{n-1} \end{bmatrix}$ such that $vM = 0$.
The equation $vM = 0$ is equivalent to

$$\begin{cases} b_0 y_0 + b_1 y_1 + \cdots + b_{n-1} y_{n-1} = 0 \\ \alpha y_0 - y_1 = 0 \\ \alpha y_1 - y_2 = 0 \\ \vdots \\ \alpha y_{n-2} - y_{n-1} = 0, \end{cases}$$

that gives $y_1 = \alpha y_0, \ldots, y_{n-1} = \alpha^{n-1} y_0$ and

$$(b_0 + b_1 \alpha + \cdots + b_{n-1} \alpha^{n-1}) y_0 = q(\alpha) y_0 = 0$$

Since $y_0 \neq 0$ (or else $v = 0$) we obtain $q(\alpha) = 0$. $\square$

Example: roots of polynomials

Theorem

Let $p(z) \in \mathbb{C}[z]$. The polynomial equations $p(z) = 0$ is a **strongly** *well posed problem if p has distinct roots.*

Proof.

The hypotheses of the implicit functions theorem are fulfilled if $q(\alpha) \neq 0$.

For any $\widetilde{p}(z)$ in a neighborhood of $p(z)$ there exists $\widetilde{\alpha}_1$ and $\widetilde{q}(z)$ such that $\widetilde{p}(z) = (z - \widetilde{\alpha})\widetilde{q}(z)$ and $\widetilde{\alpha}_1$ and $\widetilde{b}_0, \ldots, \widetilde{b}_{n-1}$ are analytic functions of the coefficients of $\widetilde{p}(z)$.

The polynomial $q(z)$ has distinct roots. By induction, there exists $\widetilde{\alpha}_2, \ldots, \widetilde{\alpha}_n$ that are solutions of $\widetilde{q}(z)$ (in a smaller neighborhood if necessary) and that are analytic with respect to the coefficients of $\widetilde{p}(z)$. Since the composition of analytic functions is analytic the roots are analytic functions of the coefficients of $\widetilde{p}(z)$. $\square$

Example: roots of polynomials

The roots of the polynomial

$$x^2 - \alpha = 0, \qquad \alpha = \rho e^{i\theta} \in \mathbb{C},$$

are $\varphi_1(\alpha) = \sqrt{\rho} e^{i\theta/2}$ and $\varphi_2(\alpha) = -\sqrt{\rho} e^{i\theta/2}$.

Theorem

There exists no square root function continuous in a neighborhood of $0 \in \mathbb{C}$.

Proof.

$\square$

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The roots of the polynomial

$$x^2 - \alpha = 0, \qquad \alpha = \rho e^{i\theta} \in \mathbb{C},$$

are $\varphi_1(\alpha) = \sqrt{\rho} e^{i\theta/2}$ and $\varphi_2(\alpha) = -\sqrt{\rho} e^{i\theta/2}$.

Theorem

There exists no square root function continuous in a neighborhood of $0 \in \mathbb{C}$.

Proof.

If there exist a continuous function $\lambda : \mathcal{U} \to \mathbb{C}$ such that $\lambda(z)^2 = z$, where $\mathcal{U}$ is a neighborhood of 0.
We have $\lambda(z)^2 = z$ on a circle $S^1 = \{z \in \mathbb{C} \, : \, |z| = \rho\}$, with $\rho > 0$.
Define the two sets

$$\mathcal{U}_1 := \{z \in S^1 \, : \, \lambda(z) = \varphi_1(z)\}, \quad \mathcal{U}_2 := \{z \in S^1 \, : \, \lambda(z) = \varphi_2(z)\}.$$

We claim that $\mathcal{U}_1$ is open in S^1. $\square$

Example: roots of polynomials

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Proof.

For $z \in \mathcal{U}_1$ there exists a neighborhood $\mathcal{V}$ of z such that $|\lambda(w) - \lambda(z)| < \sqrt{\rho}$ because λ is continuous, but $|\varphi_1 - \varphi_2| = 2\sqrt{\rho}$ and thus $\lambda(z) \equiv \varphi_1(z)$ on $\mathcal{V}$.
Analogously $\mathcal{U}_2$ is open.

The two open subset of S^1 are disjoint and their union is S^1, but since S^1 is a connected set, we have that $S^1 = \mathcal{U}_1$ or $S^1 = \mathcal{U}_2$.

In both cases $\lim_{\theta \to 0^+} \lambda(z) \neq \lim_{\theta \to 2\pi^-} \lambda(z)$, while they should coincide if λ is continuous. (For instance if $S^1 = \mathcal{U}_1$ we get $\sqrt{\rho}$ and $-\sqrt{\rho}$ for the two limits.) $\square$

Example: roots of polynomials

Find all solutions of the polynomial equations
$p(x) = a_0 + a_1 x + \cdots + a_n x^n = 0$, where $p \in \mathbb{C}_n[x]$ with $a_n \neq 0$.

Is the problem well posed? The equation has n solutions $\xi_1, \ldots, \xi_n$ counted with multiplicity (fundamental theorem of algebra).

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If the roots are distinct, let $p(x) + tq(x)$, for $t \in [-a, a]$ and $q(x)$ polynomial of the same degree as $p(x)$, with $a > 0$, be a polynomial. We have $p_t \rightarrow_{t \rightarrow 0} p(x)$, then

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for a sufficiently small t the polynomial $p_t(x)$ has distinct roots $\zeta_1(t), \ldots, \zeta_n(t)$ which are analytic (continuous) functions of t and $\zeta_i(0) = \xi_i$ (a theorem in complex analysis).

The problem is well-posed: we have a function $f : \Omega \to \mathbb{C}^n$ ($\Omega \subset \mathbb{C}^n$ open)

Example: integrals

Compute $\int_a^b f(x)dx$, with f continuous on $[a, b]$.

Riemann (Lebesgue) integrability guarantees the existence and uniqueness (fundamental theorem of calculus).

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Riemann (Lebesgue) integrability guarantees the existence and uniqueness (fundamental theorem of calculus).

The problem can be stated as a function evaluation

$$f : C[a, b] \to \mathbb{R}$$

where $C[a, b]$ are continuous functions on $[a, b]$.

Notice that the space $C[a, b]$ as a vector space has infinite dimension!

Problems to be solved

What do we need to solve?

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What can we solve?

By hand or with a computer, we can evaluate only **rational functions**

$$f : \mathbb{R}^n \to \mathbb{R}, \qquad f = \frac{p(x_1, \dots, x_n)}{q(x_1, \dots, x_n)}$$

with p, q polynomials (in n variables).
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Moreover we cannot use all real numbers but just a fistful of them.

This is awkward!

Approximation

We accept an approximated solution.

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- Go from a generic function to a rational function.

We make the following approximation

$$\widehat{f} : V \to W \quad \Longrightarrow \quad \varphi : \mathbb{R}^n \to \mathbb{R} \quad \Longrightarrow \quad f : \mathbb{R}^n \to \mathbb{R}$$

with f rational.

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with f rational. The function f evaluated on finite arithmetic is said to be a **numerical algorithm**.

We can define the relative analytic error, when $\varphi(x) \neq 0$, as

$$\varepsilon_{AN} = \frac{f(x) - \varphi(x)}{\varphi(x)}$$

Analytic error

Let $\operatorname{conv}(a, b) = \operatorname{conv}(\{a, b\})$ be the interval $[a, b]$ if $a < b$; the interval $[b, a]$ if $a > b$; or the point a if $a = b$.

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Theorem (Taylor's formula)

Let $f \in C^{r+1}(\mathbb{R})$ and let $x_0 \in \mathbb{R}$. Then for $x \in \mathbb{R}$, there exists $\xi(x) \in$conv(x_0, x), such that

$$f(x) = p(x) + r(x)$$

where

$$p(x) = f(x_0) + f'(x_0)(x - x_0) + \cdots + \frac{f^{(r)}(x_0)}{r!}(x - x_0)^r$$

and

$$r(x) = \frac{f^{(r+1)}(\xi(x))}{(r+1)!}(x - x_0)^{r+1}$$

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$p(x)$ is the Taylor polynomial of degree r at x_0.

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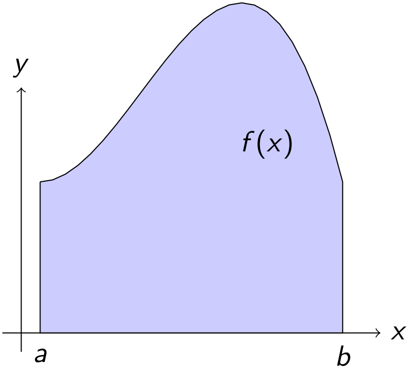
$r(x)$ is the remainder (Lagrange's remainder) and it is an **absolute** analytic error (that is small for x near to x_0).

Analytic error

The integral of $f \in C[a, b]$, with $f > 0$ can be approximated by a trapezoid (trapezoidal rule).



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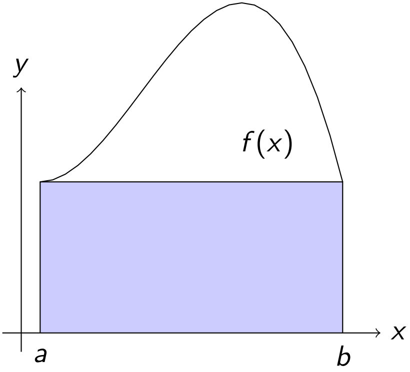

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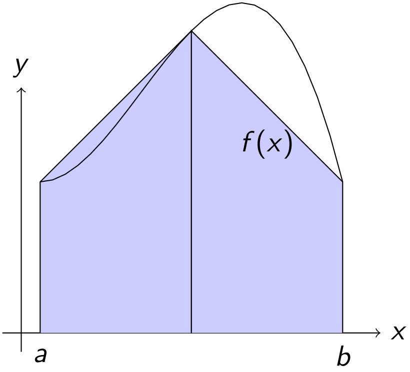

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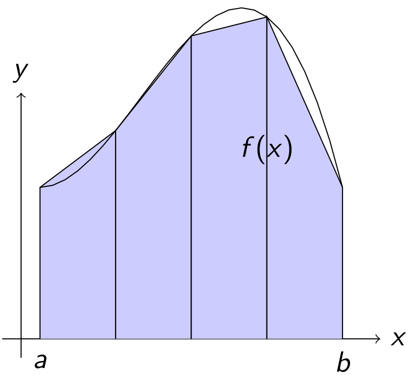

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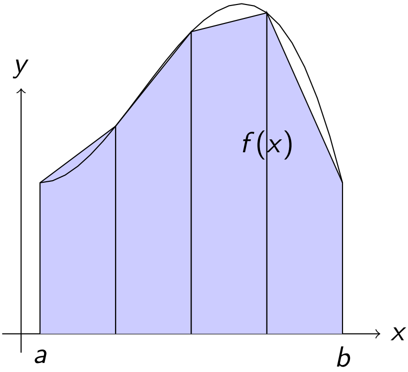

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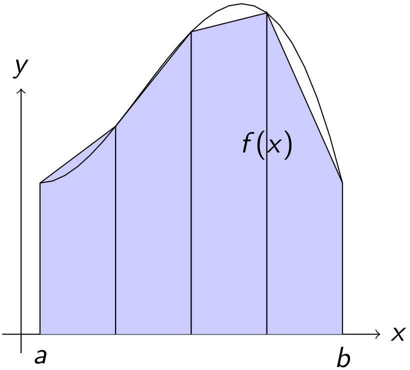

Let $h = (b-a)/n$, and let $x_i = a + \frac{b-a}{n} i$, then

$$\int_a^b f(x)dx = h\Big(\frac{1}{2}f(x_0) + f(x_1) + \cdots + f(x_{n-1}) + \frac{1}{2}f(x_n)\Big) + r(x)$$

It can be proved that, if $f \in C^2[a,b]$, there exists $\xi \in (a,b)$, such that

$$r(x) = \frac{(b-a)^3}{12n^2} f''(\xi).$$

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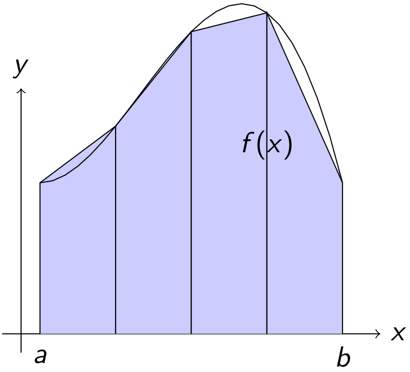

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Disclaimer

We will not discuss anymore of the analytic error, and we will only consider rational functions (or elementary functions).

Error for rational functions

Let $f : \mathbb{R}^n \to \mathbb{R}$ rational, that is $f = p/q$ with p, q polynomials.

From mathematical analysis we know that f is defined and differentiable for $q \neq 0$. (We may assume that p and q are prime).

Examples of rational functions:

$$f(x) = \frac{x^2 + 2x}{x + 1}, \qquad f(x) = \frac{xy + x^2 + 5x^2yz}{z + \pi y^2}$$

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- the Taylor polynomial (one variable);
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There are two types of error in the evaluation of f at x on floating point numbers.

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- **Inherent error**. We do not evaluate $f(x)$ but rather $f(\widetilde{x})$ where $\widetilde{x} = \mathrm{fl}(x)$

$$\varepsilon_{IN} = \frac{f(\widetilde{x}) - f(x)}{f(x)}, \qquad f(x) \neq 0.$$

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Inherent error can be defined also for non-rational functions.

Algorithmic error can be defined also for elementary functions, which are treated as operations.

Error for rational functions

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$$\varepsilon_{IN} = \frac{f(\widetilde{x}) - f(x)}{f(x)}, \qquad f(x) \neq 0.$$

  If the inherent error is relatively small we say that the problem is **well-conditioned** or else **ill-conditioned**.

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$$\varepsilon_{ALG} = \frac{\widetilde{f}(\widetilde{x}) - f(\widetilde{x})}{f(\widetilde{x})}, \qquad f(\widetilde{x}) \neq 0.$$

  If the algorithmic error is relatively small we say that algorithm f is **numerically stable** or else **numerically unstable**.

A bit imprecise. Can be made more precise assuming $u \to 0$ and asking $\lim_{u\to 0} \varepsilon_{IN/ALG} = 0$.

Error for rational functions

Let $f : \mathbb{R}^n \to \mathbb{R}$ rational, that is $f = p/q$ with p, q polynomials.

The total error (or forward error) is

$$\varepsilon_{TOT} = \frac{\widetilde{f}(\widetilde{x}) - f(x)}{f(x)}, \qquad f(x) \neq 0,$$

which gives a genuine measure of the error in the evaluation.

The ideal situation is $|\varepsilon_{TOT}| < u$, where u is the machine precision.
But, in practice, it is sufficient $|\varepsilon_{TOT}| \leqslant Mu$, with M constant.

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What is the relationship between these errors?

Error for rational functions

Theorem

Let $x \in \mathbb{R}^n \setminus \{0\}$, *and* $f : \mathbb{R}^n \to \mathbb{R}$ *rational with* $f(x) \neq 0$ *and* $f(\widetilde{x}) \neq 0$, *where* $\widetilde{x} = \mathrm{fl}(x)$, *then*

$$\varepsilon_{TOT} = \varepsilon_{IN} + \varepsilon_{ALG} + \varepsilon_{IN}\varepsilon_{ALG}.$$

Error for rational functions

Theorem

Let $x \in \mathbb{R}^n \setminus \{0\}$, and $f : \mathbb{R}^n \to \mathbb{R}$ rational with $f(x) \neq 0$ and $f(\widetilde{x}) \neq 0$, where $\widetilde{x} = \mathrm{fl}(x)$, then

$$\varepsilon_{TOT} = \varepsilon_{IN} + \varepsilon_{ALG} + \varepsilon_{IN}\varepsilon_{ALG}.$$

Proof.

$$\begin{aligned}
\varepsilon_{TOT} &= \frac{\widetilde{f}(\widetilde{x}) - f(\widetilde{x}) + f(\widetilde{x}) - f(x)}{f(x)} = \frac{\widetilde{f}(\widetilde{x}) - f(\widetilde{x})}{f(x)} + \frac{f(\widetilde{x}) - f(x)}{f(x)} \\
&= \frac{\widetilde{f}(\widetilde{x}) - f(\widetilde{x})}{f(\widetilde{x})} \frac{f(\widetilde{x})}{f(x)} + \varepsilon_{IN} = \varepsilon_{ALG}\left(\frac{f(\widetilde{x})}{f(x)} - 1 + 1\right) + \varepsilon_{IN} \\
&= \varepsilon_{ALG}\left(\frac{f(\widetilde{x}) - f(x)}{f(x)} + 1\right) + \varepsilon_{IN} = \varepsilon_{ALG}(\varepsilon_{IN} + 1) + \varepsilon_{IN} \\
&= \varepsilon_{IN} + \varepsilon_{ALG} + \varepsilon_{IN}\varepsilon_{ALG}.
\end{aligned}$$

□

Error for rational functions

Theorem

Let $x \in \mathbb{R}^n \setminus \{0\}$, and $f : \mathbb{R}^n \to \mathbb{R}$ rational with $f(x) \neq 0$ and $f(\widetilde{x}) \neq 0$, where $\widetilde{x} = \mathrm{fl}(x)$, then

$$\varepsilon_{TOT} = \varepsilon_{IN} + \varepsilon_{ALG} + \varepsilon_{IN}\varepsilon_{ALG}.$$

If ε_{IN} and ε_{ALG} are small (tends to zero as $u \to 0$, we have)

$$\varepsilon_{TOT} = \varepsilon_{IN} + \varepsilon_{ALG} + o(u) \doteq \varepsilon_{IN} + \varepsilon_{ALG}$$

Error analysis

Error analysis consists in relating the forward error with the error in the representation (and thus on the machine precision)

Formulae cannot be used directly

- Inherent error, we use the derivative (if the function is differentiable).
- Algorithmic error, we use a diagram analysis

Inherent error

Let $f : \mathbb{R}^n \to \mathbb{R}$, rational,

$$\varepsilon_{IN} = \frac{f(\widetilde{x}) - f(x)}{f(x)}, \qquad f(x) \neq 0.$$

where $\widetilde{x} = \mathrm{fl}(x)$.
If $x_i \neq 0$, for $i = 1, \ldots, n$, we want to relate ε_{IN} with the representation errors

$$\varepsilon_i = \frac{\widetilde{x}_i - x_i}{x_i},$$

and we make the usual assumption

$$|\varepsilon_i| < u,$$

where u is the machine precision. Ignoring overflow and underflow for simplicity.

Inherent error

We try to use the definition.

Example 1.

$$f(x) = x^2,$$

Let $\widetilde{x} = \mathrm{fl}(x) = x(1+\varepsilon_1)$, with $|\varepsilon_1| < u$, obtained as

$$\frac{\widetilde{x} - x}{x} = \varepsilon_1 \Longleftrightarrow \widetilde{x} - x = x\varepsilon_1 \Longleftrightarrow \widetilde{x} = x(1+\varepsilon_1).$$

We have, for $x \neq 0$,

$$\varepsilon_{IN} = \frac{\widetilde{x}^2 - x^2}{x^2} = \frac{x^2(1+\varepsilon_1)^2 - x^2}{x^2} = \frac{x^2(1+2\varepsilon+\varepsilon_1^2-1)}{x^2} = 2\varepsilon_1 + \varepsilon_1^2.$$

Since we are mostly interested on what happens as $u \to 0$, we can consider only first order terms

$$\varepsilon_{IN} \doteq 2\varepsilon_1$$

or $\varepsilon_{IN} = 2\varepsilon_1 + o(u)$. **Well-conditioned!**

Inherent error

In general using the definition is complicated. A simpler technique is obtained using the following.

Theorem

Let $x, \widetilde{x} \in \mathbb{R} \setminus \{0\}$ and let $f \in C^1(conv(x, \widetilde{x}))$, with $f(x) \neq 0$. There exists $\xi \in conv(x, \widetilde{x})$, such that

$$\varepsilon_{IN} = \frac{x}{f(x)} f'(\xi) \varepsilon_x,$$

where $\varepsilon_x = \varepsilon_1$ is the representation error on x. If, moreover $f \in C^2(conv(x, \widetilde{x}))$, then

$$\varepsilon_{IN} = \frac{x}{f(x)} f'(x) \varepsilon_x + o(u),$$

that is $\varepsilon_{IN} \doteq \frac{x}{f(x)} f'(x) \varepsilon_x$.

The formula above is very useful.

Inherent error

Proof.

$$\frac{f(\widetilde{x})-f(x)}{f(x)}=\frac{f'(\xi)(\widetilde{x}-x)}{f(x)}\frac{x}{x}=\frac{xf'(\xi)}{f(x)}\frac{\widetilde{x}-x}{x}=\frac{x}{f(x)}f'(\xi)\varepsilon_1.$$

The mean value theorem has been used. $\square$

Inherent error

$$\varepsilon_{IN} = \frac{f(\widetilde{x}) - f(x)}{f(x)} \doteq \frac{x}{f(x)} f'(x)\varepsilon_x.$$

The term $c_x = \frac{x}{f(x)} f'(x)$ is said to be **amplification factor** and measure the amplification of the error.

We use the formula with the function $f(x) = x^2$.

$$\varepsilon_{IN} \doteq \frac{x}{x^2} 2x\varepsilon_1 = 2\varepsilon_1$$

Much easier!

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Much easier!

What happens for more than one variable?

Inherent error

If $x = (x_1, \dots, x_n)$, and consider $f(x)$, we have the formula (with $x_i \neq 0$, $f(x) \neq 0$)

$$\varepsilon_{IN} \doteq \frac{x_1}{f(x)}\frac{\partial f}{\partial x_1}(x)\varepsilon_1 + \frac{x_2}{f(x)}\frac{\partial f}{\partial x_2}(x)\varepsilon_2 + \cdots + \frac{x_n}{f(x)}\frac{\partial f}{\partial x_n}(x)\varepsilon_n$$

where

$$\varepsilon_i = \frac{\widetilde{x}_i - x_i}{x_i}, \qquad c_i = \frac{x_i}{f(x)}\frac{\partial f}{\partial x_i}(x),$$

are the representation error and the amplification coefficients, respectively.

Inherent error on operations

$$\varepsilon_{IN} \doteq c_1\varepsilon_1 + \cdots c_n\varepsilon_n, \qquad c_i = \frac{x}{f(x)}\frac{\partial f}{\partial x_i}(x).$$

Let $f(x, y) = xy$, the multiplication. Then $\varepsilon_{IN} \doteq c_x\varepsilon_x + c_y\varepsilon_y$, where

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Thus we have

$$c_x = 1, \qquad c_y = 1,$$

and the problem is well-conditioned. Obvious, really!

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Thus we have

$$c_x = x/(x+y), \qquad c_y = y/(x+y),$$

and the problem becomes ill-conditioned when $x \approx -y$. Perhaps surprising!

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This phenomenon is said to be **numerical cancellation** and can be understood intuitively.

If we subtract two very near numbers we loose significant digits.

Example. In $\mathbb{R}$, $\pi - 3.1 \approx 0.0415926$. In $\mathcal{F}(10, 3, *, *)$, $\mathrm{fl}(\pi) = 3.14$ and $\mathrm{fl}(3.1) = 3.1$, and thus $\mathrm{fl}(\pi) - \mathrm{fl}(3.1) = 0.04$ (while $\mathrm{fl}(\pi - 3.1) = 0.0416$) and we have lost two significant digits.

Inherent error for some functions

operation	c_x	c_y
$x+y$	$\frac{x}{x+y}$	$\frac{y}{x+y}$

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$x+y$	$\frac{x}{x+y}$	$\frac{y}{x+y}$
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$$c_x = \frac{x}{x-y}\frac{\partial f}{\partial x} = \frac{x}{x-y}, \qquad c_y = \frac{y}{x-y}\frac{\partial f}{\partial y} = \frac{y}{x-y}\cdot(-1)$$

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$x + y$	$\frac{x}{x+y}$	$\frac{y}{x+y}$
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xy	1	1

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$x+y$	$\frac{x}{x+y}$	$\frac{y}{x+y}$
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xy	1	1
x/y	1	-1

$$c_x = \frac{x}{f}\frac{\partial f}{\partial x} = \frac{x}{x/y}\frac{1}{y} = x\frac{y}{x}\frac{1}{y} = 1, \qquad c_y = \frac{y}{x/y}\frac{-x}{y^2} = -1,$$

Inherent error for some functions

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$x+y$	$\frac{x}{x+y}$	$\frac{y}{x+y}$
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$\exp(x)$	x	

$$c_x = \frac{x}{\exp(x)} \exp(x) = x,$$

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$x+y$	$\frac{x}{x+y}$	$\frac{y}{x+y}$
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xy	1	1
x/y	1	-1
$\exp(x)$	x	
$\sqrt{x}$	$\frac{1}{2}$	

$$c_x = \frac{x}{\sqrt{x}} \frac{1}{2\sqrt{x}} = \frac{1}{2},$$

Inherent error for some functions

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$x+y$	$\frac{x}{x+y}$	$\frac{y}{x+y}$
$x-y$	$\frac{x}{x-y}$	$\frac{-y}{x-y}$
xy	1	1
x/y	1	-1
$\exp(x)$	x	
$\sqrt{x}$	$\frac{1}{2}$	
x^α	α	

$$c_x = \frac{x}{x^\alpha} \alpha x^{\alpha-1} = \alpha.$$

Exercise

Study the inherent error (conditioning) of $f(x, y) = x^2 - y^2$.

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$$\varepsilon_{IN} = \frac{2x^2}{x^2 - y^2}\varepsilon_x + \frac{-2y^2}{x^2 - y^2}\varepsilon_y,$$

where ε_x and ε_y are the representation errors for x and y, respectively.

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It is apparent that the inherent error is large for $x^2 \approx y^2$, that is

$$x \approx \pm y.$$

We expect a large error when x is near to y or $-y$.

Algorithmic error

$$\varepsilon_{ALG} = \frac{\widetilde{f}(\widetilde{x}) - f(\widetilde{x})}{f(\widetilde{x})}$$

Algorithmic error is very hard to be computed using the definition.

We drop the tilde for simplicity.

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This is a special case: a single operation.

Algorithmic error

Consider the function $f(x, y) = x^2 - y^2$ and the two algorithms

$$\begin{cases} z^{(1)} = x^2, \\ z^{(2)} = y^2, \\ f = z^{(3)} = z^{(1)} - z^{(2)}. \end{cases}$$

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where $|\varepsilon_i| \leqslant u$, $|\eta_i| \leqslant u$.

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Studying the algorithmic error using the definition is horrible

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$$= \frac{x^2\varepsilon_1 - y^2\varepsilon_2 + x^2\varepsilon_3 - y^2\varepsilon_3 - x^2\varepsilon_1\varepsilon_3 - y^2\varepsilon_2\varepsilon_3}{x^2 - y^2}$$

Algorithmic error

$$\begin{aligned}
\varepsilon_{ALG} &= \frac{(x \otimes x) \ominus (y \otimes y) - (x^2 - y^2)}{x^2 - y^2} \\
&= \frac{\big(x^2(1+\varepsilon_1) - y^2(1+\varepsilon_2)\big)(1+\varepsilon_3) - (x^2 - y^2)}{x^2 - y^2} \\
&= \frac{(x^2 - x^2\varepsilon_1 - y^2 - y^2\varepsilon_2)(1+\varepsilon_3) - (x^2 - y^2)}{x^2 - y^2} \\
&= \frac{x^2 - x^2\varepsilon_1 - y^2 - y^2\varepsilon_2 + x^2\varepsilon_3 - x^2\varepsilon_1\varepsilon_3 - y^2\varepsilon_3 - y^2\varepsilon_2\varepsilon_3 - x^2 + y^2}{x^2 - y^2} \\
&= \frac{x^2\varepsilon_1 - y^2\varepsilon_2 + x^2\varepsilon_3 - y^2\varepsilon_3 - x^2\varepsilon_1\varepsilon_3 - y^2\varepsilon_2\varepsilon_3}{x^2 - y^2} \\
&\doteq \frac{x^2\varepsilon_1 - y^2\varepsilon_2 + (x^2 - y^2)\varepsilon_3}{x^2 - y^2} = \frac{(x^2 - y^2)\varepsilon_3}{x^2 - y^2} + \frac{x^2\varepsilon_1 - y^2\varepsilon_2}{x^2 - y^2}
\end{aligned}$$

Algorithmic error

$$\varepsilon_{ALG} = \frac{(x \otimes x) \ominus (y \otimes y) - (x^2 - y^2)}{x^2 - y^2}$$

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$$= \varepsilon_3 + \frac{x^2\varepsilon_1 - y^2\varepsilon_2}{x^2 - y^2}$$

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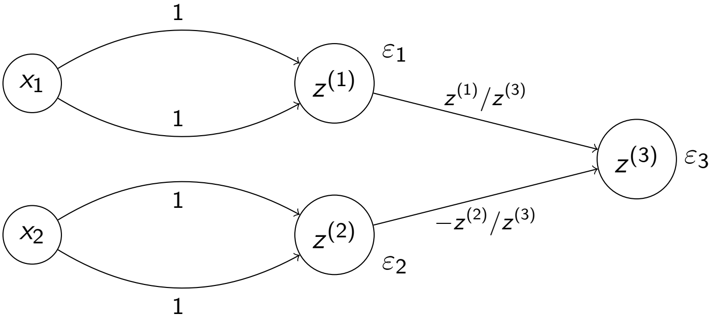
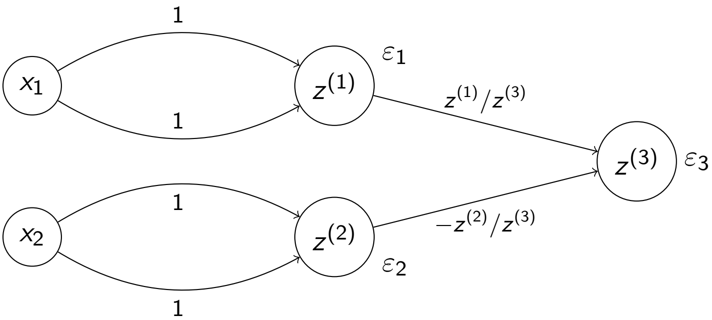


Algorithmic error

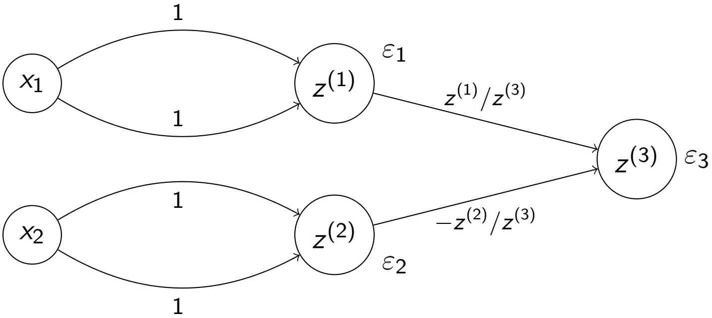
$$\begin{cases} z^{(1)} = x^2, & \varepsilon_1, \\ z^{(2)} = y^2, & \varepsilon_2, \\ f = z^{(3)} = z^{(1)} - z^{(2)}, & \varepsilon_3. \end{cases}$$



$$\varepsilon_{ALG} \doteq \varepsilon_3 + \frac{z^{(1)}}{z^{(3)}}\varepsilon_1 - \frac{z^{(2)}}{z^{(3)}}\varepsilon_2 =$$

Algorithmic error

$$\begin{cases} z^{(1)} = x^2, & \varepsilon_1, \\ z^{(2)} = y^2, & \varepsilon_2, \\ f = z^{(3)} = z^{(1)} - z^{(2)}, & \varepsilon_3. \end{cases}$$



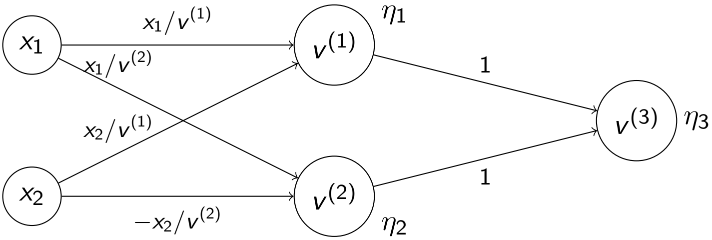
$$\varepsilon_{ALG} \doteq \varepsilon_3 + \frac{z^{(1)}}{z^{(3)}}\varepsilon_1 - \frac{z^{(2)}}{z^{(3)}}\varepsilon_2 = \varepsilon_3 + \frac{x^2\varepsilon_1 - y^2\varepsilon_2}{x^2 - y^2}$$

Algorithmic error

$$\begin{cases} v^{(1)} = x + y, & \eta_1, \\ v^{(2)} = x - y, & \eta_2, \\ f = v^{(3)} = v^{(1)} v^{(2)}, & \eta_3. \end{cases}$$

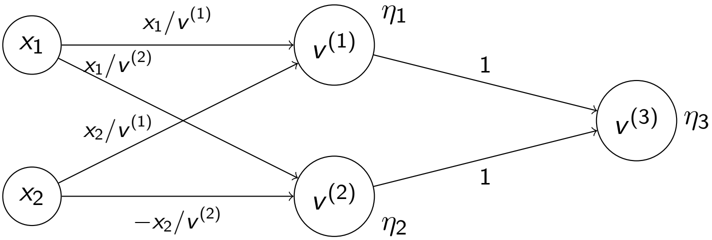
Algorithmic error

$$\begin{cases} v^{(1)} = x + y, & \eta_1, \\ v^{(2)} = x - y, & \eta_2, \\ f = v^{(3)} = v^{(1)} v^{(2)}, & \eta_3. \end{cases}$$



Algorithmic error

$$\begin{cases} v^{(1)} = x + y, & \eta_1, \\ v^{(2)} = x - y, & \eta_2, \\ f = v^{(3)} = v^{(1)} v^{(2)}, & \eta_3. \end{cases}$$



$$\varepsilon_{ALG} \doteq \eta_3 + \eta_1 + \eta_2$$

Algorithmic error

Which is the best?

$$\varepsilon_{ALG}^{(1)} \varepsilon_3 + \frac{x^2\varepsilon_1 - y^2\varepsilon_2}{x^2 - y^2} \qquad \varepsilon_{ALG}^{(2)} \doteq \eta_3 + \eta_1 + \eta_2.$$

Algorithmic error

Which is the best?

$$\varepsilon^{(1)}_{ALG}\varepsilon_3 + \frac{x^2\varepsilon_1 - y^2\varepsilon_2}{x^2 - y^2} \qquad \varepsilon^{(2)}_{ALG} \doteq \eta_3 + \eta_1 + \eta_2.$$

We can bound

$$|\varepsilon^{(1)}_{ALG}| \leqslant \left(1 + \frac{x^2 + y^2}{|x^2 - y^2|}\right)u, \qquad |\varepsilon^{(2)}_{ALG}| \leqslant 3u.$$

The second is the best in most cases.