Revisão de Cálculo Numérico

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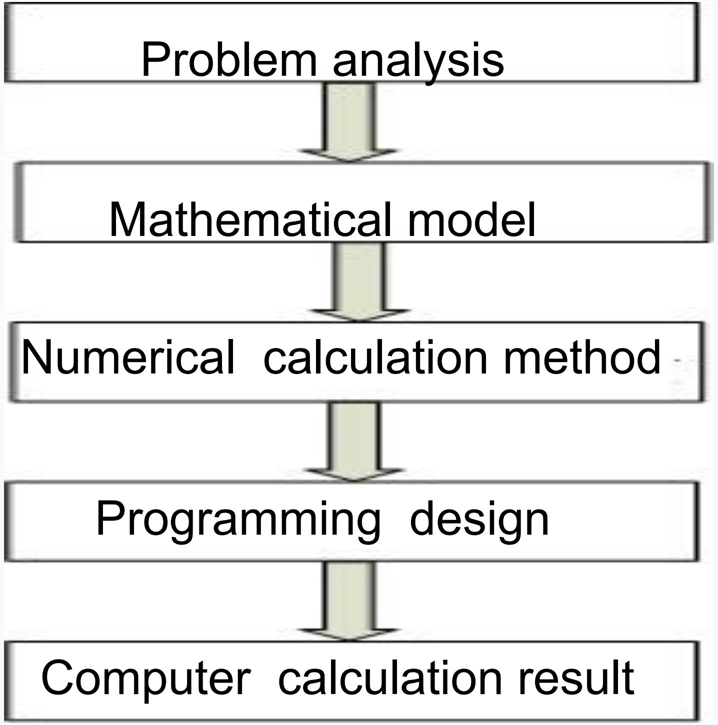
Numerical analysis

Numerical analysis is the study of algorithms that use numerical approximation using a digital computer to solve approximate solutions of mathematical problems

Numerical calculation: Refers to the method and process of effectively using a digital computer to solve approximate solutions of mathematical problems

Numerical Calculation



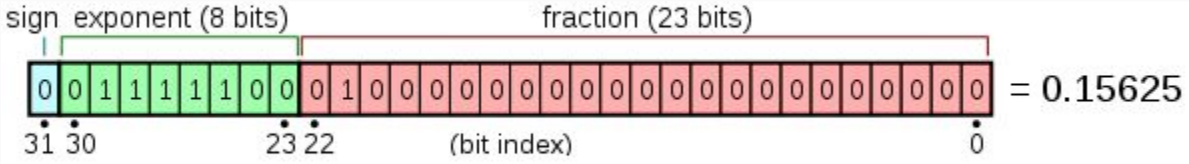
Round-off errors

- Impossible to represent all real numbers exactly on a machine with finite memory.
- Iterative method is terminated or a mathematical procedure is approximated.
- The solution of the discrete problem does not coincide with the solution of the continuous problem.

Number representation

- Limited number of bits
- Integer
- Floating-point

$$1.2345 = \underbrace{12345}_{\text{significand}} \times \underbrace{10}_{\text{base}}{}^{\overbrace{-4}^{\text{exponent}}}$$



Types of errors

- Modeling errors
- Input errors
- Storage errors
- Change of base
- Once an error is generated, it will generally propagate through the calculation.

Overflow and Underflow

Underflow: number is rounded to zero. Big difference in many functions

Overflow: large number is approximated to infinite. Many functions are undefined for infinity

The large number and small number: $a \gg b \Rightarrow a + b = a$

$$softmax(x)_i = \frac{\exp(x_i)}{\sum_{j=1}^{n} \exp(x_j)}.$$

Number of Ill-Conditions

- Ill-condition number: speed of change with small changes of input.

$$f(x) = A^\wedge(-1)\, x \qquad \max_{i,j} \left| \frac{\lambda_i}{\lambda_j} \right|$$

- The modulus ratio of the maximum and minimum eigenvalues.
- Matrix inversion is sensitive to input errors when large.
- Intrinsic characteristics of the matrix itself.
- Not the result of the rounding error.

Linear systems

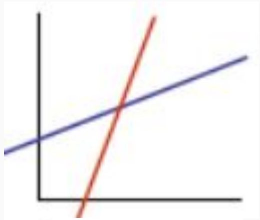
$$
\begin{aligned}
a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n &= b_1, \\
a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n &= b_2, \\
\vdots \qquad\qquad & \quad \vdots \\
a_{n1}x_1 + a_{n2}x_2 + \cdots + a_{nn}x_n &= b_n.
\end{aligned}
$$

$$\mathbf{A}\mathbf{x} = \mathbf{b},$$

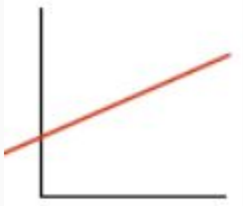
$$
\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix}, \quad \mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}
$$

Solution

- Possible and determined
  - One solution
  - Determinant different from 0



- Possible and undetermined
  - Infinite solutions
  - Determinant equal to 0



- Impossible
  - No solutions
  - Determinant equal to 0

Iterative methods

- Direct methods
  - Gaussian Elimination
  - LU decomposition
- Computationally inefficient
- Unsuitable for large number of variables

Jacobi Method

- Iterative

$$
\begin{array}{ccccccccccc}
a_{11}x_1 & + & a_{12}x_2 & + & a_{13}x_3 & + & \dots & + & a_{1n}x_n & = & b_1 \\
a_{21}x_1 & + & a_{22}x_2 & + & a_{23}x_3 & + & \dots & + & a_{2n}x_n & = & b_2 \\
\vdots & & \vdots & & \vdots & & \vdots & & \vdots & & \vdots \\
a_{n1}x_1 & + & a_{n2}x_2 & + & a_{n3}x_3 & + & \dots & + & a_{nn}x_n & = & b_n
\end{array}
$$

$$
\begin{aligned}
x_1 &= \frac{1}{a_{11}}\left[b_1 - a_{12}x_2 - a_{13}x_3 - \ldots - a_{1n}x_n\right] \\
x_2 &= \frac{1}{a_{22}}\left[b_2 - a_{21}x_1 - a_{23}x_3 - \ldots - a_{2n}x_n\right] \\
\vdots & \quad \vdots \\
x_n &= \frac{1}{a_{nn}}\left[b_n - a_{n1}x_1 - a_{n2}x_2 - \ldots - a_{n,n-1}x_{n-1}\right]
\end{aligned}
$$

Jacobi Method

$$
\begin{aligned}
x_1 &= \frac{1}{a_{11}}\left[b_1 - a_{12}x_2 - a_{13}x_3 - \ldots - a_{1n}x_n\right] \\
x_2 &= \frac{1}{a_{22}}\left[b_2 - a_{21}x_1 - a_{23}x_3 - \ldots - a_{2n}x_n\right] \\
\vdots & \quad \vdots \\
x_n &= \frac{1}{a_{nn}}\left[b_n - a_{n1}x_1 - a_{n2}x_2 - \ldots - a_{n,n-1}x_{n-1}\right]
\end{aligned}
$$

$$
\begin{aligned}
x_1^{(k+1)} &= \frac{1}{a_{11}}\left(b_1 - a_{12}x_2^{(k)} - a_{13}x_3^{(k)} - \ldots - a_{1n}x_n^{(k)}\right) \\
x_2^{(k+1)} &= \frac{1}{a_{22}}\left(b_2 - a_{21}x_1^{(k)} - a_{23}x_3^{(k)} - \ldots - a_{2n}x_n^{(k)}\right) \\
\vdots & \quad \vdots \\
x_n^{(k+1)} &= \frac{1}{a_{nn}}\left(b_n - a_{n1}x_1^{(k)} - a_{n2}x_2^{(k)} - \ldots - a_{n,n-1}x_{n-1}^{(k)}\right)
\end{aligned}
$$

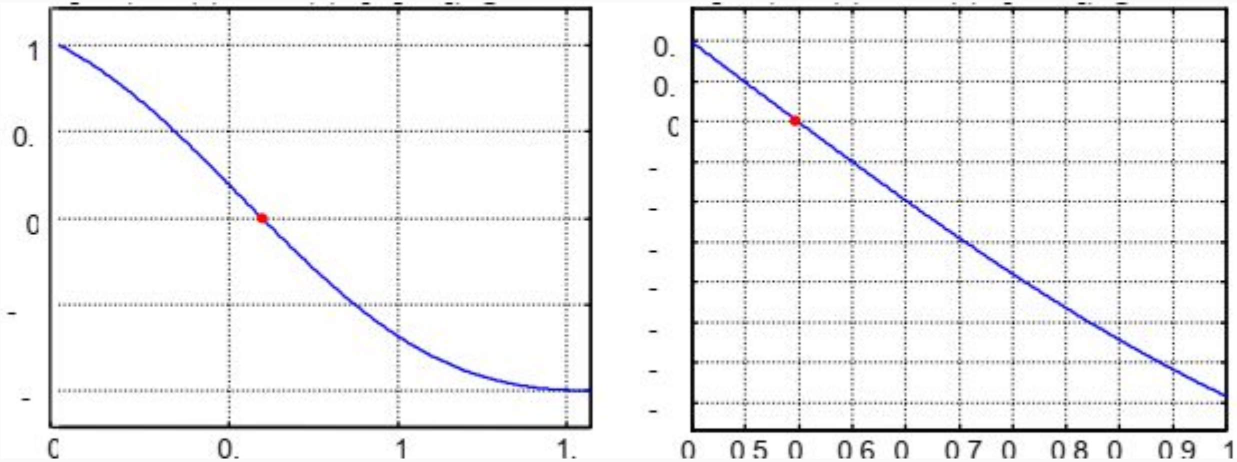
Gauss–Seidel method

- Already calculated variables are used

$$
\begin{aligned}
x_1^{(k+1)} &= \frac{1}{a_{11}}\left(b_1 - a_{12}x_2^{(k)} - a_{13}x_3^{(k)} - \cdots - a_{1n}x_n^{(k)}\right)\\
x_2^{(k+1)} &= \frac{1}{a_{22}}\left(b_2 - a_{21}x_1^{(k+1)} - a_{23}x_3^{(k)} - \cdots - a_{2n}x_n^{(k)}\right)\\
x_3^{(k+1)} &= \frac{1}{a_{33}}\left(b_3 - a_{31}x_1^{(k+1)} - a_{32}x_3^{(k+1)} - \cdots - a_{3n}x_n^{(k)}\right)\\
\vdots \quad &\quad \vdots\\
x_n^{(k+1)} &= \frac{1}{a_{nn}}\left(b_n - a_{n1}x_1^{(k+1)} - a_{n2}x_2^{(k+1)} - \cdots - a_{n,n-1}x_{n-1}^{(k+1)}\right)
\end{aligned}
$$

Function zeros

- Find values where function is 0
- Evaluate the function at various points
- Brute force

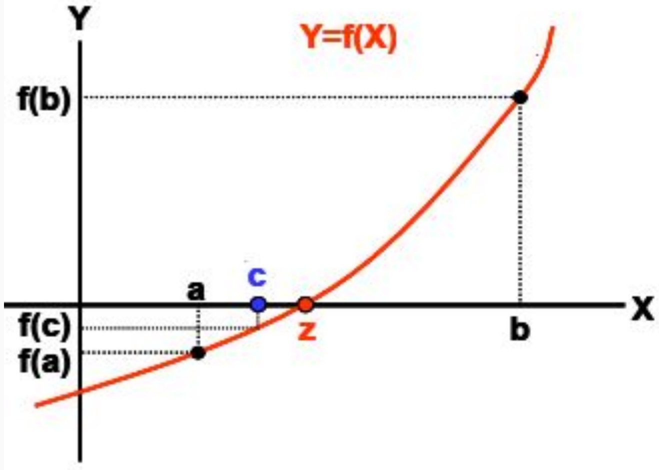


Requirements

- Continuous in the interval
- Change in signal at the extremes, $f(a)\ f(b) < 0$
- Guarantees at least one zero
- Find new suitable smaller interval
- Repeat until suitable tolerance

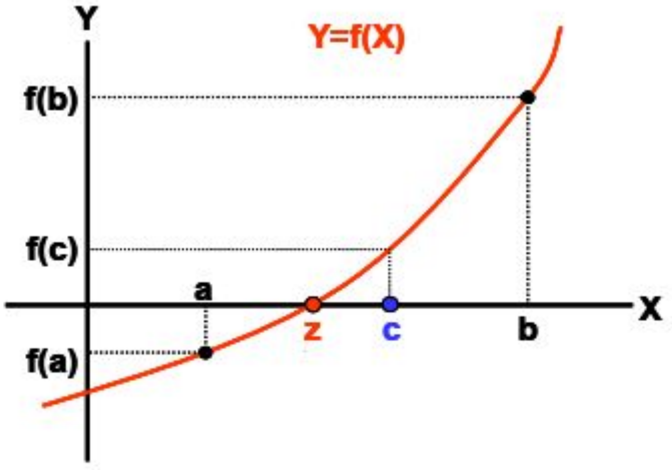
Interval splitting

$f(a)f(c) > 0$



new interval [c,b]

$f(a)f(c) < 0$

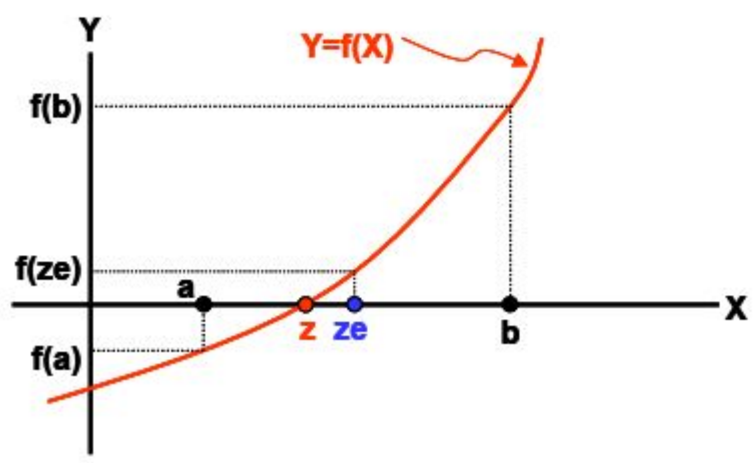


new interval [a,c]

Bisection

- Split interval in the middle

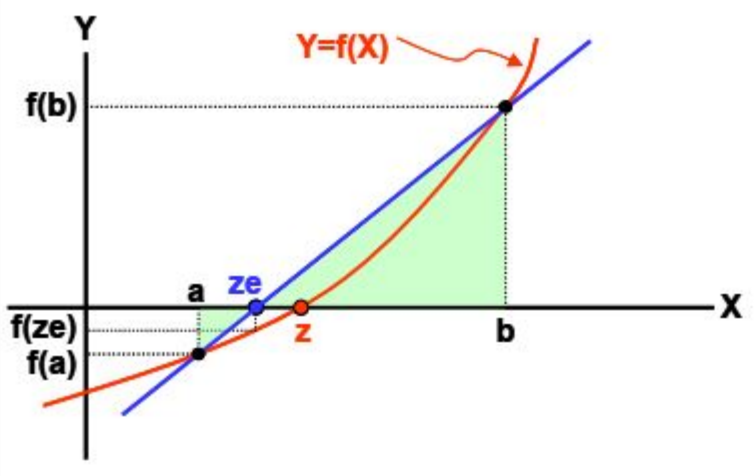
$$ze = \frac{a + b}{2}$$



Secant

- Better for zeros near the extremes
- Scant line between f(a) and f(b)

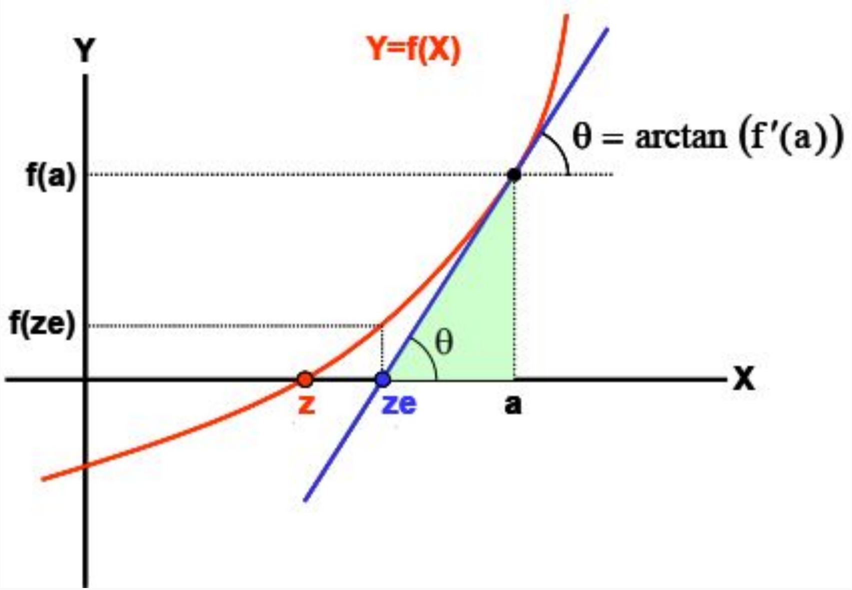
$$ze = \frac{a \cdot f(b) - b \cdot f(a)}{f(b) - f(a)}$$



Newton

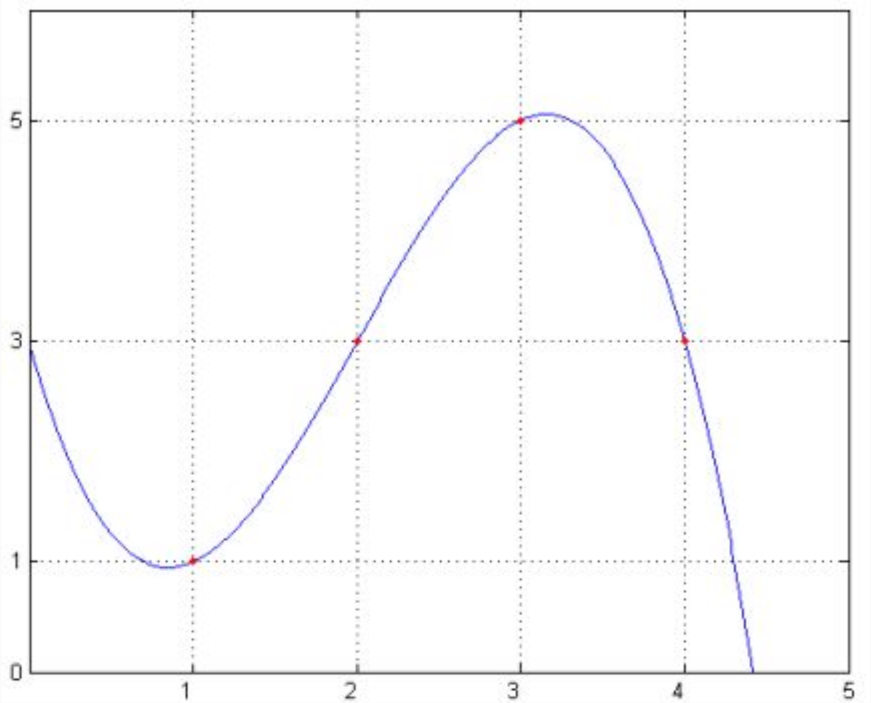
- Tangent line
- Most complex
- Usually faster

$$ze = a - \frac{f(a)}{f'(a)}$$



Interpolation

- Some function values are unknown
- Approximate by other function
- The original funcion is too complex
- Polynomial interpolation
- Vandermonde polynomial
- Lagrange polynomial
- Newton polynomial



Vandermonde polynomial

- Most straightforward construction
- n+1 linear equations
- The n+1 unknown coefficients
- n+1 known points

$$
\begin{aligned}
y_0 &= c_0 x_0^n + c_1 x_0^{n-1} + \cdots + c_{n-1} x_0 + c_n \\
y_2 &= c_0 x_1^n + c_1 x_1^{n-1} + \cdots + c_{n-1} x_1 + c_n \\
\vdots & \qquad\qquad\quad \vdots \qquad\qquad\qquad \vdots \\
y_n &= c_0 x_n^n + c_1 x_n^{n-1} + \cdots + c_{n-1} x_n + c_n .
\end{aligned}
$$

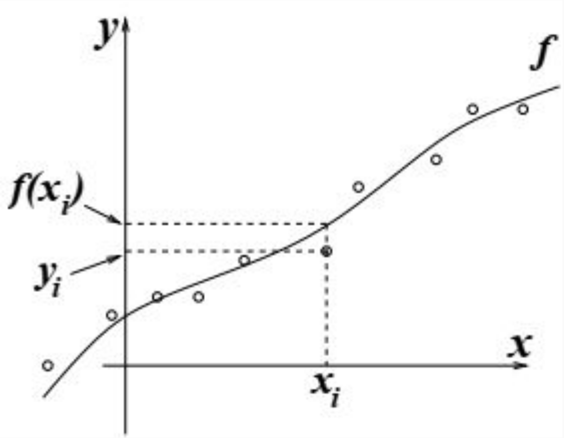
$$P_n(x) = c_0 x^n + c_1 x^{n-1} + \cdots + c_n .$$

$$
\begin{pmatrix}
x_0^n & x_0^{n-1} & \cdots & x_0 & 1 \\
x_1^n & x_1^{n-1} & \cdots & x_1 & 1 \\
\vdots & \vdots & \ddots & \vdots & \\
x_n^n & x_n^{n-1} & \cdots & x_n & 1
\end{pmatrix}
\begin{pmatrix} c_0 \\ c_1 \\ \vdots \\ c_n \end{pmatrix}
=
\begin{pmatrix} y_0 \\ y_1 \\ \vdots \\ y_n \end{pmatrix}
$$

Regression

- Fit a parameterized curve to experimental data
- Similar to interpolation
- Value at know points may not be exact
- Least squares

$$\rho = \sum_{i=1}^{n} r_i^2 \qquad r_i = y_i - y(x_i)$$



Linear Least Squares

- Linear combination of functions
- Functions may be non-linear

$$y(x) = \sum_{j=1}^{m} c_j f_j(x).$$

$$\mathbf{r} = \mathbf{y} - \mathrm{A}\mathbf{c}$$

$$\mathbf{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}, \quad \mathbf{c} = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_m \end{pmatrix},$$

$$\mathrm{A} = \begin{pmatrix} f_1(x_1) & f_2(x_1) & \cdots & f_m(x_1) \\ f_1(x_2) & f_2(x_2) & \cdots & f_m(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ f_1(x_n) & f_2(x_n) & \cdots & f_m(x_n) \end{pmatrix}$$

$$\frac{\partial c_i}{\partial c_j} = \begin{cases} 1, & \text{if } i = j; \\ 0, & \text{otherwise.} \end{cases}$$

$$\mathrm{A}^T\mathrm{A}\mathbf{c} = \mathrm{A}^T\mathbf{y}.$$