

Error (Approximating x with \tilde{x})

$$\text{absolute error} = |\tilde{x} - x|$$

$$\text{relative error} = \frac{|\tilde{x} - x|}{|x|}.$$

Floating Point Number Systems

$\mathbb{F}(\beta, k, m, M)$ is a *finite subset* of the real number system. For $f \in \mathbb{F}$:

$$f = \pm (d_1.d_2d_3 \dots d_k)_{\beta} \times \beta^e$$

- $\beta \in \mathbb{N}$: the base
- $d_1.d_2d_3 \dots d_k$: the significand
- $k \in \mathbb{N}$: #digits in the significand
- $e \in \mathbb{Z}$: the exponent, $m \leq e \leq M$

d_i are base- β digits with $d_1 \neq 0$ unless $f = 0$. For $x \in \mathbb{R}$ and $f > 0$:

$$f_{\min} = \min_{f \in \mathbb{F}} |f| = \beta^m$$

$$f_{\max} = \max_{f \in \mathbb{F}} |f| = (1 - \beta^{-k}) \beta^{M+1}.$$

Underflow: $x < f_{\min}$ (replaced by 0).

Overflow: $x > f_{\max}$ (replaced by ∞).

For $\mathbb{F}^+ = \{f \in \mathbb{F} : f > 0\}$:

$$|\mathbb{F}^+| = (M - m + 1)(\beta - 1)\beta^{k-1}.$$

Representing Real Numbers

If $x \notin \mathbb{F}$, x is rounded to the nearest representable number with $fl : \mathbb{R} \rightarrow \mathbb{F}$. To determine $fl(x)$:

- Express x in base- β .
- Express x in scientific form.
- Verify that $m \leq e \leq M$:

- if $e > M$, then $x = \infty$.
- if $e < m$, then $x = 0$.
- else, round to k digits.

$$\frac{|fl(x) - x|}{|x|} \leq u = \frac{1}{2}\beta^{1-k}.$$

where u is the **unit roundoff** of \mathbb{F} .

Catastrophic Cancellation

The error when subtracting similar floating point numbers, where at least one is not exactly representable.

Taylor Polynomials

The n th degree **Taylor polynomial** of f approximates f for x near x_0 :

$$P_n(x) = \sum_{k=0}^n \frac{f^{(k)}(x_0)}{k!} (x - x_0)^k.$$

If f is $n+1$ times differentiable on $[a, b]$ containing x_0 , then for all $x \in [a, b]$, there exists a value $x_0 < c < x$ such that

$$f(x) = P_n(x) + R_n(x)$$

where

$$R_n(x) = \frac{f^{(n+1)}(c)}{(n+1)!} (x - x_0)^{n+1}$$

is the **remainder (error) term** for P_n . The maximum value of $|R_n(x)|$ on $[a, b]$ bounds the maximum absolute error of the approximation:

$$|f(x) - P_n(x)| = |R_n(x)|.$$

Ordinary Differential Equations

$\frac{dy}{dt} = f(t, y)$ with $y(a) = \alpha$ on $a \leq t \leq b$. Divide $[a, b]$ into n subintervals of width $h = (b - a)/n$. Let $t_i = a + ih$ for $i =$

$0, 1, \dots, n$. Then $y_i = y(t_i)$ approximates y at $t = t_i$, with $y_0 = \alpha$.

Euler's Method (First Order Taylor)

$$y(t_i + h) = y(t_i) + hf'(t_i) + \mathcal{O}(h^2).$$

where the error is proportional to h^2 .

$$y_{i+1} = y_i + hf(t_i, y_i).$$

Local and Global Error

Assuming the solution was correct at the previous step:

Local: error after 1 step — $\mathcal{O}(h^{p+1})$.

Global: error after i steps — $\mathcal{O}(h^p)$.

The **order** of a method is its global error.

Second Order Taylor Method

$$y_{i+1} = y_i + hf(t_i, y_i) + \frac{h^2}{2} f''(t_i, y_i).$$

Modified Euler Method

To avoid computing $f'(t, y)$ use,

$$\frac{f(t_{i+1}, y_{i+1}) - f(t_i, y_i)}{h} + \mathcal{O}(h).$$

$$y_{i+1} = y_i + \frac{1}{2}(k_1 + k_2)$$

$$k_1 = hf(t_i, y_i)$$

$$k_2 = hf(t_i + h, y_i + k_1)$$

Runge-Kutta Method (Fourth Order)

$$y_{i+1} = y_i + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)$$

$$k_1 = hf(t_i, y_i)$$

$$k_2 = hf\left(t_i + \frac{h}{2}, y_i + \frac{k_1}{2}\right)$$

$$k_3 = hf\left(t_i + \frac{h}{2}, y_i + \frac{k_2}{2}\right)$$

$$k_4 = hf(t_i + h, y_i + k_3)$$

$i = 0, 1, \dots, n-1$ for all four methods.

Interpolation

$$P_n(x) = a_0 + a_1x + \dots + a_nx^n.$$

Lagrange Form

Solve for a_i then factor $P_n(x_i)$ for y_i :

$$P_n(x) = \sum_{i=0}^n L_{n,i}(x) y_i$$

$$L_{n,i}(x) = \prod_{\substack{j=0 \\ j \neq i}}^n \frac{x - x_j}{x_i - x_j}, L_{n,i}(x_j) = \delta_{ij}$$

For distinct increasing x_i on $[a, b]$ there exists $c \in [a, b]$ such that

$$f(x) = P_n(x) + \frac{f^{(n+1)}(c)}{(n+1)!} \prod_{i=0}^n (x - x_i).$$

Newton's Divided Difference Form

$$P_n(x) = a_0 + a_1(x - x_0) + a_2(x - x_0)(x - x_1) + \dots + a_n(x - x_0) \dots (x - x_{n-1})$$

$$= \sum_{k=0}^n f[x_0, x_1, \dots, x_k] \prod_{i=0}^{k-1} (x - x_i)$$

Solve $P_n(x_i) = y_i$ for a_0, a_1, \dots, a_n :

$$a_0 = y_0, \quad a_1 = \frac{y_1 - y_0}{x_1 - x_0}$$

$$a_2 = \frac{\frac{y_2 - y_1}{x_2 - x_1} - \frac{y_1 - y_0}{x_1 - x_0}}{x_2 - x_0}$$

Divided Differences (Simplify a_i)

$$f[x_i] = y_i \quad (\text{Zeroth divided difference})$$

$$f[x_i, x_{i+1}, \dots, x_{i+k}] =$$

$$\frac{f[x_{i+1}, \dots, x_{i+k}] - f[x_i, \dots, x_{i+k-1}]}{x_{i+k} - x_i}$$

$$f[x_0, x_1] = \frac{f[x_1] - f[x_0]}{x_1 - x_0} = \frac{y_1 - y_0}{x_1 - x_0}$$

$$f[x_1, x_2] = \frac{f[x_2] - f[x_1]}{x_2 - x_1} = \frac{y_2 - y_1}{x_2 - x_1}$$

$$f[x_0, x_1, x_2] = \frac{f[x_1, x_2] - f[x_0, x_1]}{x_2 - x_0}$$

Newton's Forward Difference Form

Equally spaced abscissas: $h = x_{i+1} - x_i$.

Forward Difference Operator

$$\Delta y_i = y_{i+1} - y_i, \quad \Delta^{k+1} y_i = \Delta(\Delta^k y_i)$$

$$\Delta^2 y_i = y_{i+2} - 2y_{i+1} + y_i$$

$$\Delta^3 y_i = y_{i+3} - 3y_{i+2} + 3y_{i+1} - y_i$$

$$f[x_0, x_1, \dots, x_k] = \frac{\Delta^k y_0}{k! h^k}$$

Substitute $x = x_0 + sh$ ($x_i = x_0 + ih$), with $s = \frac{x - x_0}{h}$ into the divided difference form:

$$P_n(x) = \sum_{k=0}^n \frac{\Delta^k y_0}{k!} \prod_{i=0}^{k-1} (s - i)$$

Root Finding ($f(x) = 0$)

Intermediate Value Theorem

For continuous f on $[a, b]$ with $f(a) \leq k \leq f(b)$, $\exists c_1 \in [a, b] : f(c_1) = k$. If $f(a)f(b) < 0$ ($f(a)$ and $f(b)$ have opposite signs), $\exists c_2 \in [a, b] : f(c_2) = 0$.

Bisection Method

- Find $[a, b]$ such that $f(a)f(b) < 0$.
- For $p = \frac{a+b}{2}$, evaluate $f(p)$.

- If $f(p) = 0$, then p is a root of f .
- If $f(a)f(p) < 0$, then p becomes the new b and the root lies in $[a, p]$.
- If $f(p)f(b) < 0$, then p becomes the new a and the root lies in $[p, b]$.

- Go to step 2.

Fixed-Point Iteration

Rewrite $f(x) = 0$ as $x = g(x)$. Solve by finding a fixed-point p s.t. $g(p) = p$.

$$x_{n+1} = g(x_n) \quad (n \geq 0).$$

Newton's Method

Find the root of the tangent line at each iterate x_n using the first degree Taylor polynomial and solving for x :

$$f(x) \approx f(x_n) + f'(x_n)(x - x_n) \stackrel{\text{set}}{=} 0$$

$$x = x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} \quad (n \geq 0)$$

Secant Method

Approximate $f'(x_n)$ with the secant between x_{n-1} and x_n :

$$f'(x_n) \approx \frac{f(x_n) - f(x_{n-1})}{x_n - x_{n-1}}$$

with two initial values for $n \geq 1$.

Convergence of Rootfinding Methods Numerical Integration (Quadrature)

A convergent $\{x_n\}$ satisfies (for large n)

$$|x_{n+1} - p| \approx \lambda |x_n - p|^r$$

Fixed-point iteration ($r = 1$)

p is a fixed-point and $0 < \lambda < 1$.

Newton's method ($r = 2$)

p is a root and $\lambda > 0$.

Secant method ($r = \frac{1+\sqrt{5}}{2} \approx 1.618$)

p is a root and $\lambda > 0$.

Numerical Differentiation

Forward ($h = x - x_0$, $c \in [x_0, x_0 + h]$)

$$f'(x_0) = \frac{f(x_0 + h) - f(x_0)}{h} - \frac{h}{2} f''(c)$$

Backward ($-h = x - x_0$, $c \in [x_0 - h, x_0]$)

$$f'(x_0) = \frac{f(x_0) - f(x_0 - h)}{h} + \frac{h}{2} f''(c)$$

Central Difference (Second Order)

Derive using $f(x_0 + h) - f(x_0 - h)$:

$$f'(x_0) = \frac{f(x_0 + h) - f(x_0 - h)}{2h} - \frac{h^2}{6} f^{(3)}(c)$$

$f^{(3)}(c) = \frac{f^{(3)}(c_1) + f^{(3)}(c_2)}{2}$ and $c \in [c_1, c_2]$,

with $c_1 \in [x_0 - h, x_0]$ and $c_2 \in [x_0, x_0 + h]$.

Second Derivative (Third Order)

Derive using $f(x_0 + h) + f(x_0 - h)$:

$$f''(x_0) = -\frac{h^2}{12} f^{(4)}(c) + \frac{f(x_0 + h) - 2f(x_0) + f(x_0 - h)}{h^2}$$

$f^{(4)}(c) = \frac{f^{(4)}(c_1) + f^{(4)}(c_2)}{2}$ and $c \in [c_1, c_2]$,

with $c_1 \in [x_0 - h, x_0]$ and $c_2 \in [x_0, x_0 + h]$.

Linear Systems ($\mathbf{Ax} = \mathbf{b}$)

LU Decomposition ($\mathbf{A} = \mathbf{LU} \Rightarrow \mathbf{Lz} = \mathbf{b}$, $\mathbf{Ux} = \mathbf{z}$)

$$\mathbf{LU} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ \frac{a_{21}}{u_{11}} & 1 & 0 & 0 \\ \frac{a_{31}}{u_{11}} & \frac{a_{32} - \ell_{31}u_{12}}{u_{22}} & 1 & 0 \\ \frac{a_{41}}{u_{11}} & \frac{a_{42} - \ell_{41}u_{12}}{u_{22}} & \frac{a_{43} - \ell_{41}u_{13} - \ell_{42}u_{23}}{u_{33}} & 1 \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ 0 & a_{22} - \ell_{21}u_{12} & a_{23} - \ell_{21}u_{13} & a_{24} - \ell_{21}u_{14} \\ 0 & 0 & a_{33} - \ell_{31}u_{13} - \ell_{32}u_{23} & a_{34} - \ell_{31}u_{14} - \ell_{32}u_{24} \\ 0 & 0 & 0 & a_{44} - \ell_{41}u_{14} - \ell_{42}u_{24} - \ell_{43}u_{34} \end{bmatrix}$$
$$= \begin{bmatrix} u_{11} & u_{12} & u_{13} & u_{14} \\ \ell_{21}u_{11} & \ell_{21}u_{12} + u_{22} & \ell_{21}u_{13} + u_{23} & \ell_{21}u_{14} + u_{24} \\ \ell_{31}u_{11} & \ell_{31}u_{12} + \ell_{32}u_{22} & \ell_{31}u_{13} + \ell_{32}u_{23} + u_{33} & \ell_{31}u_{14} + \ell_{32}u_{24} + u_{34} \\ \ell_{41}u_{11} & \ell_{41}u_{12} + \ell_{42}u_{22} & \ell_{41}u_{13} + \ell_{42}u_{23} + \ell_{43}u_{33} & \ell_{41}u_{14} + \ell_{42}u_{24} + \ell_{43}u_{34} + u_{44} \end{bmatrix}$$

Symmetric Positive Definite: $\mathbf{x}^\top \mathbf{Ax} > 0 : \forall \mathbf{x} \in \mathbb{R}^n$.

Cholesky Decomposition ($\mathbf{A} = \mathbf{LL}^\top \Rightarrow \mathbf{Lz} = \mathbf{b}$, $\mathbf{L}^\top \mathbf{x} = \mathbf{z}$)

$$\mathbf{L} = \begin{bmatrix} \sqrt{a_{11}} & 0 & 0 & 0 \\ \frac{a_{21}}{\ell_{11}} & \sqrt{a_{22} - \ell_{21}^2} & 0 & 0 \\ \frac{a_{31}}{\ell_{11}} & \frac{a_{32} - \ell_{21}\ell_{31}}{\ell_{22}} & \sqrt{a_{33} - \ell_{31}^2 - \ell_{32}^2} & 0 \\ \frac{a_{41}}{\ell_{11}} & \frac{a_{42} - \ell_{21}\ell_{41}}{\ell_{22}} & \frac{a_{43} - \ell_{31}\ell_{41} - \ell_{32}\ell_{42}}{\ell_{33}} & \sqrt{a_{44} - \ell_{41}^2 - \ell_{42}^2 - \ell_{43}^2} \end{bmatrix}$$
$$\mathbf{LL}^\top = \begin{bmatrix} \ell_{11}^2 & \ell_{11}\ell_{21} & \ell_{11}\ell_{31} & \ell_{11}\ell_{41} \\ \ell_{11}\ell_{21} & \ell_{21}^2 + \ell_{22}^2 & \ell_{21}\ell_{31} + \ell_{22}\ell_{32} & \ell_{21}\ell_{41} + \ell_{22}\ell_{42} \\ \ell_{11}\ell_{31} & \ell_{21}\ell_{31} + \ell_{22}\ell_{32} & \ell_{31}^2 + \ell_{32}^2 + \ell_{33}^2 & \ell_{31}\ell_{41} + \ell_{32}\ell_{42} + \ell_{33}\ell_{43} \\ \ell_{11}\ell_{41} & \ell_{21}\ell_{41} + \ell_{22}\ell_{42} & \ell_{31}\ell_{41} + \ell_{32}\ell_{42} + \ell_{33}\ell_{43} & \ell_{41}^2 + \ell_{42}^2 + \ell_{43}^2 + \ell_{44}^2 \end{bmatrix}$$

Brouwer's Fixed-Point Theorem

For g continuous on $[a, b]$, and differentiable on (a, b) , with $g(x) \in [a, b] : \forall x \in [a, b]$, let a positive constant $k < 1$ exist such that $|g'(x)| \leq k \forall x \in (a, b)$. Then, g has a unique fixed-point p in $[a, b]$, and $x_{n+1} = g(x_n)$ will converge to p for all x_0 in $[a, b]$.

$$I = \int_a^b f(x) dx \approx \sum_{i=0}^n w_i f(x_i)$$

for weights w_i and abscissas x_i .

Divide $[a, b]$ into n subintervals of width $h = (b - a)/n$. Let $x_i = a + ih$ for $i = 0, 1, \dots, n$, so that $x_0 = a$ and $x_n = b$.

Trapezoidal Rule (Second Order)

Approximate $f(x)$ over each subinterval $[x_{i-1}, x_i]$ with a degree 1 interpolant:

$$P_{1,i}(x) = y_{i-1} + s\Delta y_{i-1} = y_{i-1} + s(y_i - y_{i-1})$$

and integrate w.r.t. s : $x = x_{i-1} + sh$, $dx = h ds$, with limits $s \in [0, 1]$:

$$\int_{x_{i-1}}^{x_i} f(x) dx \approx \int_0^1 P_{1,i}(x) h ds = \frac{h}{2} (y_{i-1} + y_i) \quad (i = 1, 2, \dots, n).$$

$$I = \sum_{i=1}^n \int_{x_{i-1}}^{x_i} f(x) dx \approx \sum_{i=1}^n \frac{h}{2} [f(x_{i-1}) + f(x_i)]$$

$$= \frac{h}{2} \left[f(x_0) + 2 \sum_{i=1}^{n-1} f(x_i) + f(x_n) \right] - \frac{(b-a)h^2}{12} f''(c)$$

Simpson's Rule (Fourth Order)

Approximate $f(x)$ over each subinterval $[x_{2i-2}, x_{2i}]$ with a degree 2 interpolant:

$$P_{2,i}(x) = y_{2i-2} + s\Delta y_{2i-2} + \frac{s(s-1)}{2} \Delta^2 y_{2i-2}$$

$$= y_{2i-2} + s(y_{2i} - y_{2i-1}) + \frac{s(s-1)}{2} (y_{2i} - 2y_{2i-1} + y_{2i-2})$$

and integrate w.r.t. s : $x = x_{2i-2} + sh$, $dx = h ds$, with limits $s \in [0, 2]$:

$$\int_{x_{2i-2}}^{x_{2i}} f(x) dx \approx \int_0^2 P_{2,i}(x) h ds = \frac{h}{3} (y_{2i-2} + 4y_{2i-1} + y_{2i}) \quad (i = 1, 2, \dots, n/2).$$

$$I = \sum_{i=2}^{n/2} \int_{x_{2i-2}}^{x_{2i}} f(x) dx \approx \sum_{i=2}^{n/2} \frac{h}{3} [f(x_{2i-2}) + 4f(x_{2i-1}) + f(x_{2i})]$$

$$= \frac{h}{3} \left[f(x_0) + 4 \sum_{i=1}^{n/2} f(x_{2i-1}) + 2 \sum_{i=1}^{n/2-1} f(x_{2i}) + f(x_n) \right] - \frac{(b-a)h^4}{180} f^{(4)}(c)$$