

INSTITUTO SUPERIOR TÉCNICO
Licenciatura em Engenharia Química
Licenciatura em Engenharia Biológica
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ANÁLISE E SIMULAÇÃO NUMÉRICA

Formulário

1. Representação de Números e Teoria de Erros

Erro, erro absoluto, erro relativo ($\tilde{x} \approx x$):

$$\begin{aligned} \text{(i)} \quad x \in \mathbb{R}: \quad e_{\tilde{x}} &= x - \tilde{x}, & |e_{\tilde{x}}|, & \quad \delta_{\tilde{x}} = \frac{e_{\tilde{x}}}{x}, & \quad |\delta_{\tilde{x}}| \quad (x \neq 0) \\ \text{(ii)} \quad x \in \mathbb{R}^n: \quad e_{\tilde{x}} &= x - \tilde{x}, & \|e_{\tilde{x}}\|, & \quad \delta_{\tilde{x}} = \frac{e_{\tilde{x}}}{\|x\|}, & \quad \|\delta_{\tilde{x}}\| \quad (x \neq 0) \end{aligned}$$

Representação de números reais (notação científica):

$$\begin{aligned} x &= \sigma m \beta^t \in \mathbb{R} \setminus \{0\} \\ \text{(base)} \quad \beta &\in \mathbb{N} \setminus \{1\}, & \text{(sinal)} \quad \sigma &\in \{+, -\}, & \text{(expoente)} \quad t \in \mathbb{Z} \\ \text{(mantissa)} \quad m &= (0.a_1 a_2 \dots)_\beta \in [\beta^{-1}, 1[, & a_i &\in \{0, 1, \dots, \beta - 1\}, & a_1 \neq 0 \end{aligned}$$

Sistema de ponto flutuante:

$$\begin{aligned} \text{FP}(\beta, n, t_1, t_2) &= \{x \in \mathbb{Q} : x = \sigma m \beta^t\} \cup \{0\} \\ \beta &\in \mathbb{N} \setminus \{1\}, & \sigma &\in \{+, -\}, & t_1 \leq t \leq t_2, & t, t_1, t_2 \in \mathbb{Z} \\ m &= (0.a_1 a_2 \dots a_n)_\beta \in [\beta^{-1}, 1 - \beta^{-n}], & a_i &\in \{0, 1, \dots, \beta - 1\}, & a_1 \neq 0 \end{aligned}$$

Arredondamentos:

$$x = \sigma(0.a_1 a_2 \dots a_n a_{n+1} \dots)_\beta \times \beta^t \in \mathbb{R}, \quad \text{fl}(x) \in \text{FP}(\beta, n, t_1, t_2)$$

(i) arredondamento por corte:

$$\text{fl}(x) = \sigma(0.a_1 a_2 \dots a_n)_\beta \times \beta^t$$

(ii) arredondamento simétrico (β par):

$$\text{fl}(x) = \begin{cases} \sigma(0.a_1 a_2 \dots a_n)_\beta \times \beta^t, & 0 \leq a_{n+1} < \frac{\beta}{2} \\ \sigma[(0.a_1 a_2 \dots a_n)_\beta + \beta^{-n}] \times \beta^t, & \frac{\beta}{2} \leq a_{n+1} < \beta \end{cases}$$

Erros de arredondamento ($x = \sigma m \beta^t \in \mathbb{R}$, $\tilde{x} = \text{fl}(x) \in \text{FP}(\beta, n, t_1, t_2)$):

(i) arredondamento por corte:

$$|e_{\tilde{x}}| \leq \beta^{t-n}, \quad |\delta_{\tilde{x}}| \leq \beta^{1-n} =: U$$

(ii) arredondamento simétrico:

$$|e_{\tilde{x}}| \leq \frac{1}{2} \beta^{t-n}, \quad |\delta_{\tilde{x}}| \leq \frac{1}{2} \beta^{1-n} =: U$$

(U : unidade de arredondamento do sistema $\text{FP}(\beta, n, t_1, t_2)$)

Algarismo significativo:

$$x = \sigma m 10^t \in \mathbb{R}, \quad \tilde{x} = \sigma(0.a_1 a_2 \dots a_n)_{10} \times 10^t \in \text{FP}(10, n, t_1, t_2),$$

$$a_i \text{ é algarismo significativo de } \tilde{x} \text{ se } |e_{\tilde{x}}| \leq \frac{1}{2} \beta^{t-i}$$

Propagação de erros ($x = (x_1, \dots, x_n) \in \mathbb{R}^n$, $\phi : \mathbb{R}^n \rightarrow \mathbb{R}$, $\tilde{x} \approx x$, $\tilde{\phi} = \text{fl} \circ \phi$):

$$\begin{aligned} e_{\phi(\tilde{x})} &= \phi(x) - \phi(\tilde{x}) \approx \tilde{e}_{\phi}(x) = \sum_{k=1}^n \frac{\partial \phi}{\partial x_k}(x) e_{\tilde{x}_k} \\ \delta_{\phi(\tilde{x})} &= \frac{e_{\phi(\tilde{x})}}{\phi(x)} \approx \tilde{\delta}_{\phi}(x) = \sum_{k=1}^n p_{\phi, x_k}(x) \delta_{\tilde{x}_k}, \quad p_{\phi, x_k}(x) = \frac{x_k \frac{\partial \phi}{\partial x_k}(x)}{\phi(x)} \\ \delta_{\tilde{\phi}(\tilde{x})} &= \frac{\phi(x) - \tilde{\phi}(\tilde{x})}{\phi(x)} \approx \tilde{\delta}_{\phi} + \delta_{\text{arr}}, \quad \tilde{\delta}_{\phi} = \sum_{k=1}^n p_{\phi, x_k} \delta_{\tilde{x}_k}, \quad \delta_{\text{arr}} = \sum_{k=1}^m q_k \delta_{\text{arr}_k} \end{aligned}$$

2. Resolução de Equações Não-lineares ($f : \mathbb{R} \rightarrow \mathbb{R}$)

- Método da bissecção ($f(z) = 0$, $f \in C([a, b])$, $f(a)f(b) < 0$):

$$\begin{aligned} x_{m+1} &= x_m + \frac{b-a}{2^{m+1}} \text{sgn}[f(a)f(x_m)], \quad m = 0, 1, \dots \\ |z - x_m| &\leq \frac{b-a}{2^m}, \quad |z - x_{m+1}| \leq |x_{m+1} - x_m| \end{aligned}$$

- Método do ponto fixo ($f(z) = 0 \Leftrightarrow z = g(z)$):

$$(|g(x) - g(y)| \leq L|x - y|, \quad \forall x, y \in I \subset \mathbb{R}, \quad L < 1; \quad g(I) \subset I)$$

$$x_{m+1} = g(x_m), \quad m = 0, 1, \dots$$

$$|z - x_{m+1}| \leq L|z - x_m|, \quad |z - x_m| \leq L^m |z - x_0|$$

$$|z - x_m| \leq \frac{1}{1-L} |x_{m+1} - x_m|, \quad |z - x_{m+1}| \leq \frac{L}{1-L} |x_{m+1} - x_m|$$

$$|z - x_m| \leq \frac{L^m}{1 - L} |x_1 - x_0|$$

- $g'(z) \neq 0$, $g \in C^1(I)$, $L = \max_{x \in I} |g'(x)| < 1$:

$$z - x_{m+1} = g'(\xi_m)(z - x_m), \quad \xi_m \in \text{int}(z, x_m)$$

$$|z - x_{m+1}| \leq L|z - x_m|, \quad |z - x_m| \leq L^m|z - x_0|$$

$$\lim_{m \rightarrow \infty} \frac{|z - x_{m+1}|}{|z - x_m|} = |g'(z)| =: K_\infty^{[1]}$$

- $g^{(r)}(z) = 0$, $r = 1, \dots, p-1$, $g^{(p)}(z) \neq 0$, $p = 2, 3, \dots$, $g \in C^p(I)$

$$z - x_{m+1} = \frac{1}{p!} (-1)^{p+1} g^{(p)}(\xi_m)(z - x_m)^p, \quad \xi_m \in \text{int}(z, x_m)$$

$$|z - x_{m+1}| \leq K_p |z - x_m|^p, \quad |z - x_m| \leq K_p^{\frac{1}{1-p}} \left(K_p^{\frac{1}{p-1}} |z - x_0| \right)^{p^m}$$

$$K_p = \frac{1}{p!} \max_{x \in I} |g^{(p)}(x)|$$

$$\lim_{m \rightarrow \infty} \frac{|z - x_{m+1}|}{|z - x_m|^p} = \frac{1}{p!} |g^{(p)}(z)| =: K_\infty^{[p]}$$

- Método de Newton ($f(z) = 0$, $f'(z) \neq 0$, $f \in C^2(I)$):

$$x_{m+1} = x_m - \frac{f(x_m)}{f'(x_m)}, \quad m = 0, 1, \dots$$

$$z - x_{m+1} = -\frac{f''(\xi_m)}{2f'(x_m)} (z - x_m)^2, \quad \xi_m \in \text{int}(z, x_m)$$

$$|z - x_{m+1}| \leq K |z - x_m|^2, \quad |z - x_m| \leq \frac{1}{K} (K |z - x_0|)^{2^m}$$

$$K = \frac{\max_{x \in I} |f''(x)|}{2 \min_{x \in I} |f'(x)|}$$

$$\lim_{m \rightarrow \infty} \frac{|z - x_{m+1}|}{|z - x_m|^2} = \left| \frac{f''(z)}{2f'(z)} \right| =: K_\infty^{[2]}$$

$$|z - x_{m+1}| \leq \frac{c}{1-c} |x_{m+1} - x_m|, \quad \text{se } K |z - x_m| \leq c < 1$$

- Método de Newton modificado:

$$(f^{(r)}(z) = 0, \quad r = 0, \dots, p-1, \quad f^{(p)}(z) \neq 0, \quad p = 2, 3, \dots, \quad f \in C^p(I))$$

$$x_{m+1} = x_m - p \frac{f(x_m)}{f'(x_m)}, \quad m = 0, 1, \dots$$

$$z - x_{m+1} = -\frac{1}{2} g''(\xi_m)(z - x_m)^2, \quad g(x) = x - p \frac{f(x)}{f'(x)}, \quad \xi_m \in \text{int}(z, x_m)$$

$$|z - x_{m+1}| \leq K_2 |z - x_m|^2, \quad |z - x_m| \leq \frac{1}{K_2} (K_2 |z - x_0|)^{2^m}$$

$$K_2 = \frac{1}{2} \max_{x \in I} |g''(x)|$$

$$\lim_{m \rightarrow \infty} \frac{|z - x_{m+1}|}{|z - x_m|^2} = \frac{1}{2} |g''(z)| = \frac{1}{p} \left| \frac{h'(z)}{h(z)} \right| =: K_\infty^{[2]}$$

onde h é tal que $f(x) = (x - z)^p h(x)$, $h(z) \neq 0$

- Método da secante ($f(z) = 0$, $f \in C^2(I)$):

$$x_{m+1} = x_m - f(x_m) \frac{x_m - x_{m-1}}{f(x_m) - f(x_{m-1})}, \quad m = 1, 2, \dots$$

$$z - x_{m+1} = -\frac{f''(\eta_m)}{2f'(\xi_m)} (z - x_m)(z - x_{m-1}), \quad \xi_m, \eta_m \in \text{int}(x_{m-1}, z, x_m)$$

$$|z - x_{m+1}| \leq K |z - x_m| |z - x_{m-1}|, \quad K = \frac{\max_{x \in I} |f''(x)|}{2 \min_{x \in I} |f'(x)|}$$

$$\lim_{m \rightarrow \infty} \frac{|z - x_{m+1}|}{|z - x_m|^r} = \left| \frac{f''(z)}{2f'(z)} \right|^{r-1} =: K_\infty^{[r]}, \quad r = \frac{\sqrt{5} + 1}{2}$$

$$|z - x_{m+1}| \leq \frac{c}{1-c} |x_{m+1} - x_m|, \quad \text{se } K |z - x_{m-1}| \leq c < 1$$

3. Resolução de Sistemas Lineares ($Ax = b$, $A \in L^n$, $b, x \in \mathbb{R}^n$)

Normas matriciais induzidas por normas vectoriais ($x \in \mathbb{R}^n$, $A \in L^n(\mathbb{R})$):

$$\|x\|_1 = \sum_{i=1}^n |x_i| \quad \|x\|_2 = \sqrt{\sum_{i=1}^n |x_i|^2} \quad \|x\|_\infty = \max_{1 \leq i \leq n} |x_i|$$

$$\|A\|_1 = \max_{1 \leq j \leq n} \sum_{i=1}^n |a_{ij}| \quad \|A\|_2 = \sqrt{r_\sigma(A^*A)} \quad \|A\|_\infty = \max_{1 \leq i \leq n} \sum_{j=1}^n |a_{ij}|$$

(norma por coluna)

(norma por linha)

$$r_\sigma(A) = \max_{1 \leq i \leq n} |\lambda_i|, \quad \lambda_1, \dots, \lambda_n : \text{valores próprios de } A$$

Número de condição de uma matriz:

$$\text{cond}_p(A) = \|A\|_p \|A^{-1}\|_p, \quad p = 1, 2, \infty, \quad \text{cond}_*(A) = r_\sigma(A) r_\sigma(A^{-1})$$

Condicionamento de sistemas lineares ($Ax = b$, $\tilde{A}\tilde{x} = \tilde{b}$):

$$\frac{\|\tilde{x} - x\|_p}{\|x\|_p} \leq \frac{\text{cond}_p(A)}{1 - \frac{\|\tilde{A} - A\|_p}{\|A\|_p} \text{cond}_p(A)} \left(\frac{\|\tilde{A} - A\|_p}{\|A\|_p} + \frac{\|\tilde{b} - b\|_p}{\|b\|_p} \right)$$

$$\|\tilde{A} - A\|_p \|A^{-1}\|_p < 1, \quad p = 1, 2, \infty$$

Métodos iterativos:

$$x^{(k+1)} = Cx^{(k)} + w, \quad k = 0, 1, \dots$$

$$C = -M^{-1}N, \quad w = M^{-1}b, \quad M + N = A = L + D + U$$

$$\|x - x^{(k+1)}\| \leq c\|x - x^{(k)}\|, \quad \|x - x^{(k)}\| \leq c^k\|x - x^{(0)}\|$$

$$\|x - x^{(k)}\| \leq \frac{1}{1-c} \|x^{(k+1)} - x^{(k)}\|, \quad \|x - x^{(k+1)}\| \leq \frac{c}{1-c} \|x^{(k+1)} - x^{(k)}\|$$

$$\|x - x^{(k)}\| \leq \frac{c^k}{1-c} \|x^{(1)} - x^{(0)}\|, \quad (c = \|C\| < 1)$$

- Método de Jacobi ($M = D$):

$$x^{(k+1)} = D^{-1} [b - (L + U)x^{(k)}], \quad k = 0, 1, \dots$$

$$\|x - x^{(k)}\|_{\infty} \leq \mu^k \|x - x^{(0)}\|_{\infty}$$

$$\mu = \max_{1 \leq i \leq n} (\alpha_i + \beta_i), \quad \alpha_i = \sum_{j=1}^{i-1} \left| \frac{a_{ij}}{a_{ii}} \right|, \quad \beta_i = \sum_{j=i+1}^n \left| \frac{a_{ij}}{a_{ii}} \right|$$

- Método de Gauss-Seidel ($M = D + L$):

$$x^{(k+1)} = D^{-1} (b - Lx^{(k+1)} - Ux^{(k)}), \quad k = 0, 1, \dots$$

$$\|x - x^{(k)}\|_{\infty} \leq \eta^k \|x - x^{(0)}\|_{\infty}$$

$$\eta = \max_{1 \leq i \leq n} \frac{\beta_i}{1 - \alpha_i}, \quad \alpha_i = \sum_{j=1}^{i-1} \left| \frac{a_{ij}}{a_{ii}} \right|, \quad \beta_i = \sum_{j=i+1}^n \left| \frac{a_{ij}}{a_{ii}} \right|$$

- Método da iteração simples ou da relaxação linear $\left(M = \frac{I}{\omega}, \omega \in \mathbb{R} \setminus \{0\} \right)$:

$$x^{(k+1)} = x^{(k)} + \omega (b - Ax^{(k)}), \quad k = 0, 1, \dots$$

- Método de Jacobi modificado $\left(M = \frac{D}{\omega}, \omega \in \mathbb{R} \setminus \{0\} \right)$:

$$x^{(k+1)} = (1 - \omega)x^{(k)} + \omega D^{-1} [b - (L + U)x^{(k)}], \quad k = 0, 1, \dots$$

- Método de Gauss-Seidel modificado ou SOR $\left(M = \frac{D}{\omega} + L, \omega \in \mathbb{R} \setminus \{0\} \right)$:

$$x^{(k+1)} = (1 - \omega)x^{(k)} + \omega D^{-1} (b - Lx^{(k+1)} - Ux^{(k)}), \quad k = 0, 1, \dots$$

4. Resolução de Sistemas Não-lineares ($f : \mathbb{R}^n \rightarrow \mathbb{R}^n$)

- Método do ponto fixo ($f(z) = 0 \Leftrightarrow z = g(z)$):

$$(|g(x) - g(y)| \leq L|x - y|, \quad \forall x, y \in D \subset \mathbb{R}^n, \quad L < 1; \quad g(D) \subset D)$$

$$\left(g \in C^1(D), \quad L = \sup_{x \in D} \|J_g(x)\| \right)$$

$$x^{(m+1)} = g(x^{(m)}), \quad m = 0, 1, \dots$$

$$\|z - x^{(m+1)}\| \leq L\|z - x^{(m)}\|, \quad \|z - x^{(m)}\| \leq L^m\|z - x^{(0)}\|$$

$$\|z - x^{(m)}\| \leq \frac{1}{1-L}\|x^{(m+1)} - x^{(m)}\|, \quad \|z - x^{(m+1)}\| \leq \frac{L}{1-L}\|x^{(m+1)} - x^{(m)}\|$$

$$\|z - x^{(m)}\| \leq \frac{L^m}{1-L}\|x^{(1)} - x^{(0)}\|$$

- Método de Newton generalizado ($f(z) = 0$, $f \in C^2(D)$, $\det[J_f(z)] \neq 0$):

$$\begin{cases} x^{(m+1)} = x^{(m)} + \Delta x^{(m)}, \\ J_f(x^{(m)})\Delta x^{(m)} = -f(x^{(m)}), \end{cases} \quad m = 0, 1, \dots$$

$$\|z - x^{(m+1)}\| \leq K\|z - x^{(m)}\|^2, \quad \|z - x^{(m)}\| \leq \frac{1}{K} (K\|z - x^{(0)}\|)^{2^m}$$

$$K = \frac{M_2}{2M_1} \begin{cases} \frac{1}{M_1} = \sup_{x \in D} \|[J_f(x)]^{-1}\|, \\ M_2 = \max_{1 \leq i \leq n} \sup_{x \in D} \|H_{f_i}(x)\|, \quad H_{f_i} \in L^n, \quad (H_{f_i})_{jk} = \frac{\partial^2 f_i}{\partial x_j \partial x_k} \end{cases}$$

5. Interpolação Polinomial

Fórmula interpoladora de Lagrange:

$$p_n(x) = \sum_{j=0}^n f_j l_j(x), \quad l_j(x) = \prod_{i=0, i \neq j}^n \frac{x - x_i}{x_j - x_i}$$

Fórmula interpoladora de Newton:

$$p_n(x) = f[x_0] + \sum_{j=1}^n f[x_0, \dots, x_j] \prod_{i=0}^{j-1} (x - x_i), \quad f[x_0, \dots, x_j] = \sum_{l=0}^j \frac{f(x_l)}{\prod_{i=0, i \neq l}^j (x_l - x_i)}$$

$$\begin{cases} f[x_0, x_1, \dots, x_j] = \frac{f[x_1, x_2, \dots, x_j] - f[x_0, x_1, \dots, x_{j-1}]}{x_j - x_0}, & j = 2, 3, \dots, \\ f[x_0, x_1] = \frac{f[x_1] - f[x_0]}{x_1 - x_0} \end{cases}$$

Fórmula do erro:

$$e_n(x) = f(x) - p_n(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!} W_{n+1}(x) = f[x_0, \dots, x_n, x] W_{n+1}(x)$$

$$W_{n+1}(x) = \prod_{i=0}^n (x - x_i), \quad \xi \in \text{int}(x_0, \dots, x_n, x)$$

6. Teoria da Aproximação

Melhor aproximação ϕ^* mínimos quadrados de $f \in E$ em $F \subset E$, F subespaço de dimensão n gerado por $\{\varphi_0, \dots, \varphi_n\}$, E espaço pré-Hilbertiano:

$$\|f - \phi^*\|_2 = \inf_{\phi \in F} \|f - \phi\|_2 \Leftrightarrow \langle f - \phi^*, \phi \rangle = 0, \quad \forall \phi \in F$$

$$\phi^* = \sum_{k=0}^n a_k^* \varphi_k, \quad a_k^* = \sum_{j=0}^n (M^{-1})_{kj} \langle f, \varphi_j \rangle, \quad M \in L^n, \quad M_{jk} = \langle \varphi_j, \varphi_k \rangle$$

$$\phi^* = \sum_{k=0}^n a_k^* \varphi_k, \quad a_k^* = \frac{\langle f, \varphi_k \rangle}{\langle \varphi_k, \varphi_k \rangle}, \quad \text{se } \{\varphi_0, \dots, \varphi_n\} \text{ é um sistema ortogonal}$$

Polinómios ortogonais com respeito ao produto interno

$$\langle f, g \rangle = \int_a^b w(x) f(x) g(x) dx, \quad (f, g \in C([a, b]), \quad w \in C([a, b]), \quad w(x) \geq 0)$$

- Fórmula de recorrência:

$$\begin{cases} \varphi_{n+1}(x) = (x - B_{n+1})\varphi_n(x) - C_{n+1}\varphi_{n-1}(x), & n = 1, 2, \dots \\ \varphi_0(x) = 1, & \varphi_1(x) = x - B_1 \end{cases}$$

$$B_{n+1} = \frac{\langle x\varphi_n, \varphi_n \rangle}{\langle \varphi_n, \varphi_n \rangle}, \quad n = 0, 1, \dots, \quad C_{n+1} = \frac{\langle x\varphi_n, \varphi_{n-1} \rangle}{\langle \varphi_{n-1}, \varphi_{n-1} \rangle}, \quad n = 1, 2, \dots$$

- Polinómios de Legendre, P_n ($x \in [a, b] = [-1, 1], \quad w(x) = 1$):

$$\begin{cases} P_{n+1}(x) = \frac{2n+1}{n+1} x P_n(x) - \frac{n}{n+1} P_{n-1}(x), & n = 1, 2, \dots \\ P_0(x) = 1, & P_1(x) = x \end{cases}$$

$$P_n(x) = \frac{(-1)^n}{2^n n!} \frac{d^n}{dx^n} [(1-x^2)^n], \quad n = 1, \dots$$

$$\langle P_n, P_m \rangle = 0, \quad \forall n \neq m, \quad \langle P_n, P_n \rangle = \frac{2}{2n+1}, \quad n = 0, 1, \dots$$

- Polinómios de Chebyshev, T_n ($x \in [a, b] = [-1, 1]$, $w(x) = 1/\sqrt{1-x^2}$):

$$\begin{cases} T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x), & n = 1, 2, \dots \\ T_0(x) = 1, & T_1(x) = x \end{cases}$$

$$T_n(x) = \cos(n \arccos x), \quad n = 0, 1, \dots$$

$$\langle T_n, T_m \rangle = 0, \quad \forall n \neq m, \quad \langle T_0, T_0 \rangle = \pi, \quad \langle T_n, T_n \rangle = \frac{\pi}{2}, \quad n = 1, 2, \dots$$

$$T_n(x_i) = 0, \quad x_i = \cos \frac{(2i+1)\pi}{2n}, \quad i = 0, \dots, n-1, \quad n = 1, 2, \dots$$

7. Integração

Fórmulas de Newton-Cotes fechadas de ordem n ($f \in C([a, b])$):

$$I(f) = \int_a^b f(x) dx \approx I_n(f) = \sum_{j=0}^n w_{j,n} f(x_{j,n})$$

$$I_n(x^k) = I(x^k), \quad k = 0, 1, \dots, n$$

$$x_{j,n} = a + jh, \quad j = 0, 1, \dots, n, \quad h = \frac{b-a}{n}$$

$$w_{j,n} = I(l_{j,n}) = \frac{h(-1)^{n-j}}{j!(n-j)!} \int_0^n \prod_{i=0, i \neq j}^n (t-i) dt, \quad w_{j,n} = w_{n-j,n}$$

$$E_n(f) = I(f) - I_n(f) = C_{n,\nu} h^{n+1+\nu} f^{(n+\nu)}(\xi), \quad \begin{cases} \nu = 1, & n \text{ ímpar} \\ \nu = 2, & n \text{ par} \end{cases}$$

$$C_{n,\nu} = \frac{1}{(n+\nu)!} \int_0^n t^{\nu-1} \prod_{i=0}^n (t-i) dt, \quad \xi \in (a, b)$$

- Regra dos trapézios (Newton-Cotes fechada com $n = 1$, $h = b - a$):

$$I_1(f) = \frac{b-a}{2} [f(a) + f(b)], \quad E_1(f) = -\frac{h^3}{12} f''(\xi), \quad \xi \in (a, b)$$

- Regra de Simpson (Newton-Cotes fechada com $n = 2$, $h = \frac{b-a}{2}$):

$$I_2(f) = \frac{b-a}{6} \left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right], \quad E_2(f) = -\frac{h^5}{90} f^{(4)}(\xi)$$

- Regra dos três oitavos (Newton-Cotes fechada com $n = 3$, $h = \frac{b-a}{3}$):

$$I_3(f) = \frac{b-a}{8} [f(a) + 3f(a+h) + 3f(b-h) + f(b)], \quad E_3(f) = -\frac{3h^5}{80} f^{(4)}(\xi)$$

- Regra de Milne $\left(\text{Newton-Cotes fechada com } n = 4, h = \frac{b-a}{4} \right)$:

$$I_4(f) = \frac{b-a}{90} \left[7f(a) + 32f(a+h) + 12f\left(\frac{a+b}{2}\right) + 32f(b-h) + 7f(b) \right]$$

$$E_4(f) = -\frac{8h^7}{945} f^{(6)}(\xi), \quad \xi \in (a, b)$$

Fórmulas de Newton-Cotes abertas de ordem n :

$$I(f) = \int_a^b f(x) dx \approx I_n(f) = \sum_{j=0}^n w_{j,n} f(x_{j,n})$$

$$I_n(x^k) = I(x^k), \quad k = 0, 1, \dots, n$$

$$x_{j,n} = a + (j+1)h, \quad j = 0, 1, \dots, n, \quad h = \frac{b-a}{n+2}$$

$$w_{j,n} = I(l_{j,n}) = \frac{h(-1)^{n-j}}{j!(n-j)!} \int_{-1}^{n+1} \prod_{i=0, i \neq j}^n (t-i) dt, \quad w_{j,n} = w_{n-j,n}$$

- Regra do ponto médio $\left(\text{Newton-Cotes aberta com } n = 0, h = \frac{b-a}{2} \right)$:

$$I_0(f) = (b-a) f\left(\frac{a+b}{2}\right), \quad E_0(f) = \frac{h^3}{3} f''(\xi), \quad \xi \in (a, b)$$

Fórmulas de Newton-Cotes compostas:

$$x_j = a + jh_M, \quad j = 0, 1, \dots, M, \quad h_M = \frac{b-a}{M}, \quad f_j := f(x_j)$$

- Regra dos trapézios composta :

$$I_1^{(M)}(f) = \frac{h_M}{2} \left[f_0 + f_M + 2 \sum_{j=1}^{M-1} f_j \right]$$

$$E_1^{(M)}(f) = -\frac{(b-a)h_M^2}{12} f''(\xi), \quad \xi \in (a, b)$$

- Regra de Simpson composta (M par):

$$I_2^{(M)}(f) = \frac{h_M}{3} \left[f_0 + f_M + 4 \sum_{j=1}^{M/2} f_{2j-1} + 2 \sum_{j=1}^{M/2-1} f_{2j} \right]$$

$$E_2^{(M)}(f) = -\frac{(b-a)h_M^4}{180} f^{(4)}(\xi), \quad \xi \in (a, b)$$

- Regra dos três oitavos composta (M múltiplo de 3):

$$I_3^{(M)}(f) = \frac{3h_M}{8} \left[f_0 + f_M + 2 \sum_{j=1}^{M/3-1} f_{3j} + 3 \sum_{j=1}^{M/3} f_{3j-1} + 3 \sum_{j=1}^{M/3} f_{3j-2} \right]$$

$$E_3^{(M)}(f) = -\frac{(b-a)h_M^4}{80} f^{(4)}(\xi), \quad \xi \in (a, b)$$

- Regra de Milne composta (M múltiplo de 4):

$$I_4^{(M)}(f) = \frac{4h_M}{90} \left[7f_0 + 7f_M + 14 \sum_{j=1}^{M/4-1} f_{4j} + 32 \sum_{j=1}^{M/4} f_{4j-1} + 12 \sum_{j=1}^{M/4} f_{4j-2} + 32 \sum_{j=1}^{M/4} f_{4j-3} \right]$$

$$E_4^{(M)}(f) = -\frac{2(b-a)h_M^6}{945} f^{(6)}(\xi), \quad \xi \in (a, b)$$

- Regra do ponto médio composta (M par):

$$I_0^{(M)}(f) = 2h_M \sum_{j=1}^{M/2} f_{2j-1}, \quad E_0^{(M)}(f) = \frac{(b-a)h_M^2}{6} f''(\xi), \quad \xi \in (a, b)$$

Fórmulas de Gauss:

$$I(f) = \int_a^b w(x)f(x) dx \approx I_n(f) = \sum_{j=0}^n w_{j,n} f(x_{j,n})$$

$$I_n(x^k) = I(x^k), \quad k = 0, 1, \dots, 2n+1$$

$x_{j,n}$, $j = 0, 1, \dots, n$: zeros do polinómio Φ_{n+1} de grau $n+1$ pertencente ao sistema $\{\Phi_0, \Phi_1, \dots\}$ de polinómios mónicos ortogonais com respeito ao produto interno $\langle f, g \rangle = I(fg)$.

$$w_{j,n} = I(l_{j,n}) = I(l_{j,n}^2) = -\frac{\langle \Phi_{n+1}, \Phi_{n+1} \rangle}{\Phi'_{n+1}(x_{j,n})\Phi_{n+2}(x_{j,n})}, \quad j = 0, 1, \dots, n$$

$$E_n(f) = \frac{\langle \Phi_{n+1}, \Phi_{n+1} \rangle}{(2n+2)!} f^{(2n+2)}(\xi), \quad \xi \in (a, b)$$

- Fórmulas de Gauss-Legendre ($[a, b] = [-1, 1]$, $w(x) \equiv 1$):

$x_{j,n}$, $j = 0, 1, \dots, n$: zeros do polinómio de Legendre P_{n+1}

$$w_{j,n} = -\frac{2}{(n+2)P'_{n+1}(x_{j,n})P_{n+2}(x_{j,n})}, \quad j = 0, 1, \dots, n$$

$$E_n(f) = \frac{2^{2n+3}[(n+1)!]^4}{(2n+3)[(2n+2)!]^3} f^{(2n+2)}(\xi), \quad \xi \in (a, b)$$

- $I_0(f) = 2f(0)$

- $I_1(f) = f\left(-\frac{\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right)$

- $I_2(f) = \frac{5}{9}f\left(-\sqrt{\frac{3}{5}}\right) + \frac{8}{9}f(0) + \frac{5}{9}f\left(\sqrt{\frac{3}{5}}\right)$

$$\bullet I_3(f) = w_{0,3}f(x_{0,3}) + w_{1,3}f(x_{1,3}) + w_{2,3}f(x_{2,3}) + w_{3,3}f(x_{3,3})$$

$$x_{0,3} = -\sqrt{\frac{1}{7} \left(3 + 2\sqrt{\frac{6}{5}} \right)} = -x_{3,3}, \quad x_{1,3} = -\sqrt{\frac{1}{7} \left(3 - 2\sqrt{\frac{6}{5}} \right)} = -x_{2,3}$$

$$w_{0,3} = \frac{1}{6} \left(3 - \sqrt{\frac{5}{6}} \right) = w_{3,3}, \quad w_{1,3} = \frac{1}{6} \left(3 + \sqrt{\frac{5}{6}} \right) = w_{2,3}$$

- Fórmulas de Gauss-Chebyshev ($[a, b] = [-1, 1]$, $w(x) = 1/\sqrt{1-x^2}$):

$$x_{j,n} = \cos \left(\frac{2j+1}{2n+2} \pi \right), \quad w_{j,n} = \frac{\pi}{n+1}, \quad j = 0, 1, \dots, n$$

$$E_n(f) = \frac{\pi}{2^{2n+1}(2n+2)!} f^{(2n+2)}(\xi), \quad \xi \in (a, b)$$

- Fórmulas de Gauss-Legendre compostas:

$$I(f) = \int_a^b f(x) dx \approx I_n^{(M)}(f) = \frac{h_M}{2} \sum_{j=0}^n w_{j,n} \sum_{m=1}^M f(x_{j,n}^{(m)})$$

$$x_{j,n}^{(m)} = a + h_M(m-1) + \frac{h_M}{2}(x_{j,n} + 1), \quad h_M = \frac{b-a}{M}$$

9. Resolução de Equações Diferenciais Ordinárias: Problemas de Valor Inicial

$$\begin{cases} Y'(x) = f(x, Y(x)), & x_0 \leq x \leq b \\ Y(x_0) = Y_0 \end{cases}$$

Métodos de passo simples:

$$y_{n+1} = y_n + h \varphi(x_n, y_n; h), \quad n \geq 0$$

$$x_n = x_0 + nh, \quad n = 0, 1, \dots, N, \quad h = \frac{b-x_0}{N}$$

- Erro de discretização local:

$$\tau(x, y; h) = \frac{1}{h} [Y(x+h) - Y(x)] - \varphi(x, y; h), \quad Y(x) = y$$

- Erro de discretização global:

$$|Y(x_n) - y_n(h)| \leq e^{M(x_n-x_0)} |Y(x_0) - y_0(h)| + \frac{\tau(h)}{M} [e^{M(x_n-x_0)} - 1]$$

$$0 \leq n \leq N$$

$$\tau(h) = \max_{0 \leq n \leq N} \tau(x_n, Y(x_n); h), \quad M : \text{constante de Lipschitz de } \varphi$$

- Método de Euler:

$$y_{n+1} = y_n + hf(x_n, y_n)$$

$$\tau(x, y; h) = \frac{h}{2}(Df)(x, y) + \mathcal{O}(h^2)$$

$$(Df)(x, y) = \frac{\partial f}{\partial x}(x, y) + f(x, y)\frac{\partial f}{\partial y}(x, y) = (f_x + ff_y)(x, y)$$

- Métodos de Taylor de ordem p :

$$y_{n+1} = y_n + h \sum_{j=0}^{p-1} \frac{h^j}{(j+1)!} (D^j f)(x_n, y_n)$$

$$\tau(x, y; h) = \frac{h^p}{(p+1)!} (D^p f)(x, y) + \mathcal{O}(h^{p+1})$$

- Métodos de Runge-Kutta de ordem 2:

$$\varphi(x, y; h) = (1 - \gamma)f(x, y) + \gamma f\left(x + \frac{h}{2\gamma}, y + \frac{h}{2\gamma}f(x, y)\right)$$

$$\tau(x, y; h) = \frac{h^2}{2} \left[\left(1 - \frac{3}{4\gamma}\right) (Df_x + fDf_y) + (Df)f_y \right] (x, y) + \mathcal{O}(h^3)$$

- Método de Euler modificado ou do ponto médio ($\gamma = 1$):

$$y_{n+1} = y_n + hf\left(x_n + \frac{h}{2}, y_n + \frac{h}{2}f(x_n, y_n)\right)$$

- Método de Heun ($\gamma = \frac{1}{2}$):

$$y_{n+1} = y_n + \frac{h}{2} [f(x_n, y_n) + f(x_n + h, y_n + hf(x_n, y_n))]$$

- Método de Runge-Kutta de ordem 2 (propriamente dito) ($\gamma = \frac{3}{4}$):

$$y_{n+1} = y_n + \frac{h}{4} \left[f(x_n, y_n) + 3f\left(x_n + \frac{2h}{3}, y_n + \frac{2h}{3}f(x_n, y_n)\right) \right]$$

- Método de Runge-Kutta clássico de ordem 4:

$$y_{n+1} = y_n + \frac{h}{6} [\varphi_1 + 2\varphi_2 + 2\varphi_3 + \varphi_4],$$

$$\varphi_1 = f(x_n, y_n), \quad \varphi_2 = f\left(x_n + \frac{h}{2}, y_n + \frac{h}{2}\varphi_1\right)$$

$$\varphi_3 = f\left(x_n + \frac{h}{2}, y_n + \frac{h}{2}\varphi_2\right), \quad \varphi_4 = f(x_n + h, y_n + h\varphi_3)$$

$$\tau(x, y; h) = \mathcal{O}(h^4)$$

Métodos multipasso lineares com $p + 1$ passos, $p > 0$:

$$y_{n+1} = \sum_{k=0}^p a_k y_{n-k} + h \sum_{k=-1}^p b_k f(x_{n-k}, y_{n-k}), \quad n \geq p$$

$$|a_p| + |b_p| \neq 0$$

$$x_n = x_0 + nh, \quad n = 0, 1, \dots, N, \quad h = \frac{b - x_0}{N}$$

- Erro de discretização local:

$$\begin{aligned} \tau(x, y; h) = \frac{1}{h} & \left[Y(x+h) - \sum_{k=0}^p a_k Y(x-kh) \right] \\ & - \sum_{k=-1}^p b_k f(x-kh, Y(x-kh)), \quad Y(x) = y \end{aligned}$$

- Condições de consistência ($q \geq 1$):

$$\begin{cases} \sum_{k=0}^p a_k = 1, & -\sum_{k=0}^p k a_k + \sum_{k=-1}^p b_k = 1, \\ \sum_{k=0}^p (-k)^j a_k + j \sum_{k=-1}^p (-k)^{j-1} b_k = 1, & j = 2, \dots, q \end{cases}$$

$$\tau(x, y; h) = \frac{h^q}{(q+1)!} C_{p,q}(D^q f)(x, y) + \mathcal{O}(h^{q+1})$$

$$C_{p,q} = 1 - \sum_{k=0}^p (-k)^{q+1} a_k - (q+1) \sum_{k=-1}^p (-k)^q b_k$$

- Condição da raiz:

$$\rho(r) = r^{p+1} - \sum_{k=0}^p a_k r^{p-k} = \prod_{j=0}^p (r - r_j)$$

$$(i) \quad |r_j| \leq 1, \quad j = 0, 1, \dots, p; \quad (ii) \quad |r_j| = 1 \Rightarrow \rho'(r_j) \neq 0$$

- Métodos de Adams-Bashforth ($f_m := f(x_m, y_m)$):

$$y_{n+1} = y_n + h \sum_{k=0}^p b_k f_{n-k}, \quad n \geq p$$

$$\circ \bullet \quad p = 1, \quad q = 2: \begin{cases} y_{n+1} = y_n + \frac{h}{2} [3f_n - f_{n-1}] \\ \tau(x, y; h) = \frac{5h^2}{12} (D^2 f)(x, y) + \mathcal{O}(h^3) \end{cases}$$

$$\begin{aligned}
\circ \bullet \quad p = 2, \quad q = 3: & \begin{cases} y_{n+1} = y_n + \frac{h}{12} [23f_n - 16f_{n-1} + 5f_{n-2}] \\ \tau(x, y; h) = \frac{3h^3}{8} (D^3 f)(x, y) + \mathcal{O}(h^4) \end{cases} \\
\circ \bullet \quad p = 3, \quad q = 4: & \begin{cases} y_{n+1} = y_n + \frac{h}{24} [55f_n - 59f_{n-1} + 37f_{n-2} - 9f_{n-3}], \\ \tau(x, y; h) = \frac{251h^4}{720} (D^4 f)(x, y) + \mathcal{O}(h^5) \end{cases}
\end{aligned}$$

- Méthodes de Adams-Moulton ($f_m := f(x_m, y_m)$):

$$y_{n+1} = y_n + h \sum_{k=-1}^p b_k f_{n-k}, \quad n \geq p$$

$$\begin{aligned}
\circ \bullet \quad p = 0, \quad q = 2: & \begin{cases} y_{n+1} = y_n + \frac{h}{2} [f_{n+1} + f_n] \\ \tau(x, y; h) = -\frac{h^2}{12} (D^2 f)(x, y) + \mathcal{O}(h^3) \end{cases} \\
\circ \bullet \quad p = 1, \quad q = 3: & \begin{cases} y_{n+1} = y_n + \frac{h}{12} [5f_{n+1} + 8f_n - f_{n-1}] \\ \tau(x, y; h) = -\frac{h^3}{24} (D^3 f)(x, y) + \mathcal{O}(h^4) \end{cases} \\
\circ \bullet \quad p = 2, \quad q = 4: & \begin{cases} y_{n+1} = y_n + \frac{h}{24} [9f_{n+1} + 19f_n - 5f_{n-1} + f_{n-2}] \\ \tau(x, y; h) = -\frac{19h^4}{720} (D^4 f)(x, y) + \mathcal{O}(h^5) \end{cases}
\end{aligned}$$