Tarefa 1 - Métodos Numéricos 2

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1 Fórmulas da derivada segunda

1.1 Fórmula de Taylor de funções analíticas

$F(x_{k+1}) = f(x_k) + f'(x_k)(\Delta x) + \frac{1}{2!}f''(x_k)(\Delta x)^2 + \frac{1}{3!}f'''(x_k)(\Delta x)^3 + \frac{1}{4!}f^{IV}(x_k)(\Delta x)^4 + \frac{1}{5!}f^V(x_k)(\Delta x)^5 + \frac{1}{6!}f^{VI}(x_k)(\Delta x)^6 + \ldots + \frac{1}{n!}f^n(x_k)(\Delta x)^n$

Isolando a parcela da derivada segunda

$-\frac{1}{2!}f''(x_k)(\Delta x)^2 =$

$-F(x_{k+1}) + f(x_k) + f'(x_k)\Delta x + \frac{1}{3!}f'''(x_k)(\Delta x)^3 + \frac{1}{4!}f^{IV}(x_k)(\Delta x)^4 + \frac{1}{5!}f^V(x_k)(\Delta x)^5 + \frac{1}{6!}f^{VI}(x_k)(\Delta x)^6$

Isolando a derivada segunda

$f''(x_k) =$

$-\frac{2!}{(\Delta x)^2} \cdot [F(x_{k+1}) + f(x_k) + f'(x_k)(\Delta x) + \frac{1}{3!}f'''(x_k)(\Delta x)^3 + \frac{1}{4!}f^{IV}(x_k)(\Delta x)^4 + \frac{1}{5!}f^V(x_k)(\Delta x)^5 + \frac{1}{6!}f^{VI}(x_k)(\Delta x)^6]$

Simplificando:

$f''(x_k) = \frac{2 \cdot F(x_{k+1})}{(\Delta x)^2} - \frac{2 \cdot f(x_k)}{(\Delta x)^2} - \frac{2 \cdot f'(x_k)}{(\Delta x)} - \frac{f'''(x_k)(\Delta x)^1}{3} - \frac{f^{IV}(x_k)(\Delta x)^2}{12} - \frac{f^V(x_k)(\Delta x)^3}{60} - \frac{f^{VI}(x_k)(\Delta x)^4}{360}$ (1)

Para cancelar as derivadas "vilãs" (primeira, terceira, quarta e quinta) vamos ter então 4 equações a mais.

- Para $-2 \cdot (\Delta x)$

  $F(x - 2\Delta x) = f(x_k) + f'(x_k)(-2\Delta x) + \frac{1}{2!}f''(x_k)(-2\Delta x)^2 + \frac{1}{3!}f'''(x_k)(-2\Delta x)^3 + \frac{1}{4!}f^{IV}(x_k)(-2\Delta x)^4 + \frac{1}{5!}f^V(x_k)(-2\Delta x)^5 + \frac{1}{6!}f^{VI}(x_k)(-2\Delta x)^6$ (1)

- Para $-1 \cdot (\Delta x)$

  $F(x - \Delta x) = f(x_k) + f'(x_k)(-\Delta x) + \frac{1}{2!}f''(x_k)(-\Delta x)^2 + \frac{1}{3!}f'''(x_k)(-\Delta x)^3 + \frac{1}{4!}f^{IV}(x_k)(-\Delta x)^4 + \frac{1}{5!}f^V(x_k)(-\Delta x)^5 + \frac{1}{6!}f^{VI}(x_k)(-\Delta x)^6$ (2)

- Para $2 \cdot (\Delta x)$

  $F(x+2\Delta x) = f(x_k) + f'(x_k)(2\Delta x) + \frac{1}{2!}f''(x_k)(2\Delta x)^2 + \frac{1}{3!}f'''(x_k)(2\Delta x)^3 + \frac{1}{4!}f^{IV}(x_k)(2\Delta x)^4 + \frac{1}{5!}f^{V}(x_k)(2\Delta x)^5 + \frac{1}{6!}f^{VI}(x_k)(2\Delta x)^6$ (3)

- Para $3 \cdot (\Delta x)$

  $F(x+3\Delta x) = f(x_k) + 3f'(x_k)(3\Delta x) + \frac{1}{2!}f''(x_k)(3\Delta x)^2 + \frac{1}{3!}f'''(x_k)(3\Delta x)^3 + \frac{1}{4!}f^{IV}(x_k)(3\Delta x)^4 + \frac{1}{5!}f^{V}(x_k)(3\Delta x)^5 + \frac{1}{6!}f^{VI}(x_k)(3\Delta x)^6$ (4)

Temos as seguintes equações:

$\alpha(1) + \beta(2) + \gamma(3) + \Theta(4) + \psi(5) = 0$

$\alpha + (-2)\beta + (-1)\gamma + 2\Theta + 3\psi = 0$

$\alpha + (-8)\beta + (-1)\gamma + 8\Theta + 27\psi = 0$

$\alpha + 16\beta + \gamma + 16\Theta + 81\psi = 0$

$\alpha + (-32)\beta + (-1)\gamma + 32\Theta + 243\psi = 0$

Considerando $\alpha = -1$, temos que:

$$\begin{bmatrix} -2 & -1 & 2 & 3 \\ -8 & -1 & 8 & 27 \\ 16 & 1 & 16 & 81 \\ -32 & -1 & 32 & 243 \end{bmatrix} \begin{bmatrix} \beta \\ \gamma \\ \theta \\ \psi \end{bmatrix} = \alpha \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

Pela resolução da matriz por sistemas lineares temos que, para $\alpha = -1$:

$\beta = \frac{-1}{16}$

$\gamma = 1$

$\Theta = \frac{-1}{16}$

$\psi = 0$

$\alpha(1) + \beta(2) + \gamma(3) + \Theta(4) + \psi(5) = 0$

Os termos das derivadas primeira, terceira, quarta e quinta serão cancelados. Dessa forma, irão restar apenas os termos de $f(x_k), f''(x_k) e f^{VI}(x_k)$. Temos o seguinte:

$-f_k + \frac{-1}{16} \cdot f_{k-2} + f_{k-1} + \frac{-1}{16} \cdot f_{k+2} + 0 \cdot f_{k+3} =$

$f_k(-1 + \frac{-1}{16} + 1 + \frac{-1}{16} + 0) + f_k'' \cdot \frac{1}{2!} \cdot (\Delta x)^2 \cdot (-1 + \frac{-1}{16} + 1 + \frac{-1}{16} + 0) + \frac{1}{6!} \cdot f^{VI} \cdot (\Delta x)^6 (-1 + \frac{-1}{16} + 1 + \frac{-1}{16} + 0)$

Simplificando

$-f_k - \frac{1}{16} \cdot (f_{k-2} + f_{k+2}) + f_{k-1} = \frac{-1}{8} \cdot [f_k + f_k'' \cdot \frac{1}{2!} \cdot (\Delta x)^2] + \frac{-1}{8} \cdot \frac{1}{6!} \cdot f^{VI} \cdot (\Delta x)^6$

Isolando a derivada segunda

$f_k'' = \frac{2}{(\Delta x)^2} \cdot [-8 \cdot (-f_k - \frac{f_{k-2}}{16} - \frac{f_{k+2}}{16} + f_{k-1}) - f_k]$

Cálculo do erro

$\epsilon = \frac{1}{(\Delta x)^2} \cdot -18 \cdot \frac{1}{6!} \cdot f^{VI} \cdot (\Delta x)^6 = \frac{-1}{8} \cdot \frac{1}{6!} \cdot f^{VI} \cdot (\Delta x)^4$

Ou seja, o erro é $o((\Delta x)^4)$ como esperado

1.2 Interpolação de Newton

n = número de pontos = 5

$x(s) = x_k + s \cdot \Delta x$

$g(s) = \sum_{k=0}^{n} \binom{s}{k} \cdot \Delta^k f_0$

Resolvendo o somatório

- Para k = 0

  $\binom{s}{0} = \frac{s!}{0!(s-0)!} = \frac{s!}{s!} = 1$

  $\Delta^0 f_0 = f_0$

  Então,

  $K_0 = f_0$

  $\frac{d^2 K_0}{ds^2} = 0$

- Para k = 1

  $\binom{s}{1} = \frac{s!}{1!(s-1)!} = \frac{s \cdot (s-1)!}{1!(s-1)!} = s$

  $\Delta^1 f_0 = (f_1 - f_0)$

  Então,

  $K_1 = s \cdot (f_1 - f_0)$

  $\frac{d^2 K_1}{ds^2} = 0$

- Para k = 2

  $\binom{s}{2} = \frac{s!}{2!(s-2)!} = \frac{s \cdot (s-1) \cdot (s-2)!}{2!(s-2)!} = \frac{s \cdot (s-1)}{2} = \frac{1}{2} \cdot (s^2 - s)$

  $\Delta^2 f_0 = \Delta^1 f_1 - \Delta^1 f_0 = f_2 - f_1 - f_1 + f_0 = f_2 - 2 \cdot f_1 + f_0$

  Então,

  $K_2 = \frac{1}{2} \cdot (s^2 - s) \cdot (f_2 - 2 \cdot f_1 + f_0)$

  $\frac{d^2 K_2}{ds^2} = 1 \cdot (f_2 - 2 \cdot f_1 + f_0) = f_2 - 2 \cdot f_1 + f_0$

- Para k = 3

  $\binom{s}{3} = \frac{s!}{3!(s-3)!} = \frac{s\cdot(s-1)\cdot(s-2)\cdot(s-3)!}{3!(s-3)!} = \frac{s\cdot(s-1)\cdot(s-2)}{6} = \frac{1}{6}\cdot[s\cdot(s-1)\cdot(s-2)]$

  $\Delta^3 f_0 = \Delta^2 f_1 - \Delta^2 f_0 = f_3 - 3\cdot f_2 + 3\cdot f_1 - f_0$

  Então,

  $K_3 = \frac{1}{6}\cdot[s\cdot(s-1)\cdot(s-2)]\cdot[f_3 - 3\cdot f_2 + 3\cdot f_1 - f_0]$

  $\frac{d^2K_3}{ds^2} = (s-1)\cdot(f_3 - 3\cdot f_2 + 3\cdot f_1 - f_0)$

- Para k = 4

  $\binom{s}{4} = \frac{s!}{4!(s-4)!} = \frac{s\cdot(s-1)\cdot(s-2)\cdot(s-3)\cdot(s-4)!}{4!(s-4)!} = \frac{s\cdot(s-1)\cdot(s-2)\cdot(s-3)}{24}$

  $\Delta^4 f_0 = \Delta^3 f_1 - \Delta^3 f_0 = (\Delta^2 f_2 - \Delta^2 f_1) - (\Delta^2 f_1 - \Delta^2 f_0) = [(\Delta f_3 - \Delta f_2) - (\Delta f_2 - \Delta f_1)] - [(\Delta f_2 - \Delta f_1) - (\Delta f_1 - \Delta f_0)] = [((f_4 - f_3) - (f_3 - f_2)) - ((f_3 - f_2) - (f_2 - f_1))] - [((f_3 - f_2) - (f_2 - f_1)) - ((f_2 - f_1) - (f_1 - f_0))] = f_4 - 4f_3 + 6f_2 - 4f_1 + f_0$

  Então,

  $K_4 = \frac{1}{24}\cdot[s\cdot(s-1)\cdot(s-2)\cdot(s-3))\cdot(f_4 - 4f_3 + 6f_2 - 4f_1 + f_0)]$

  $\frac{d^2K_4}{ds^2} = \frac{1}{24}\cdot(12s^2 - 36s + 22)\cdot(f_4 - 4f_3 + 6f_2 - 4f_1 + f_0)$

- Para k = 5

  $\binom{s}{5} = \frac{s!}{5!(s-5)!} = \frac{s\cdot(s-1)\cdot(s-2)\cdot(s-3)\cdot(s-4)\cdot(s-5)!}{5!(s-5)!} = \frac{s\cdot(s-1)\cdot(s-2)\cdot(s-3)\cdot(s-4)}{5!} = \frac{1}{120}\cdot[(s-1)\cdot(s-2)\cdot(s-3)\cdot(s-4)]$

  $\Delta^5 f_0 = f_5 - 5f_4 + 10f_3 - 10f_2 + 5f_1 - f_0$

  Então,

  $K_5 = \frac{1}{120}\cdot[(s-1)\cdot(s-2)\cdot(s-3)\cdot(s-4)]\cdot[f_5 - 5f_4 + 10f_3 - 10f_2 + 5f_1 - f_0]$

  $\frac{d^2K_5}{ds^2} = \frac{1}{12}\cdot(2s^3 - 12s^2 + 21s - 10)\cdot[f_5 - 5f_4 + 10f_3 - 10f_2 + 5f_1 - f_0]$

Logo, temos que

$g(s) = K_0 + K_1 + K_2 + K_3 + K_4 + K_5$

Agora, podemos calcular sua derivada

$\frac{d^2g(s)}{dx^2} = \frac{1}{(\Delta x)^2}\sum_{k=0}^{n}\frac{d^2}{ds^2}\cdot\binom{k}{s}\cdot\Delta^k f_0$

$\frac{d^2g(s)}{dx^2} = \frac{1}{(\Delta x)^2}\cdot[\frac{d^2}{ds^2}K_1 + \frac{d^2}{ds^2}K_2 + \frac{d^2}{ds^2}K_3 + \frac{d^2}{ds^2}K_4 + \frac{d^2}{ds^2}K_5]$

Substituindo os valores encontrados

$\frac{d^2g(s)}{dx^2} = \frac{1}{(\Delta x)^2}[0 + 0 + (f_2 - 2\cdot f_1 + f_0) + (s-1)\cdot(f_3 - 3\cdot f_2 + 3\cdot f_1 - f_0) + [\frac{1}{24}\cdot(12s^2 - 36s + 22)]\cdot(f_4 - 4f_3 + 6f_2 - 4f_1 + f_0) + [\frac{1}{12}\cdot(2s^3 - 12s^2 + 21s - 10)]\cdot(f_5 - 5f_4 + 10f_3 - 10f_2 + 4f_1 - f_0)]$

Como devemos utilizar a metologia central, consideramos $s = 2$

$F''(x(2)) = \frac{1}{(\Delta x)^2}[(f_2 - 2 \cdot f_1 + f_0) + (2-1) \cdot (f_3 - 3 \cdot f_2 + 3 \cdot f_1 - f_0) + [\frac{1}{24} \cdot (12 \cdot 2^2 - 36s + 22)] \cdot (f_4 - 4f_3 + 6f_2 - 4f_1 + f_0) + [\frac{1}{12} \cdot (2 \cdot 2^3 - 12^2 + 21 \cdot 2 - 10)] \cdot (f_5 - 5f_4 + 10f_3 - 10f_2 + 4f_1 - f_0)]$

Desenvolvendo temos o seguinte:

$F''(x(2)) = \frac{1}{(\Delta x)^2}[(f_2 - 2 \cdot f_1 + f_0) + (f_3 - 3 \cdot f_2 + 3 \cdot f_1 - f_0) + \frac{-1}{12} \cdot (f_4 - 4f_3 + 6f_2 - 4f_1 + f_0)$

Pela metodologia central, consideremos agora $f_0 = f_{-2}$, ou seja f_{-2} será o primeiro ponto que teremos.

$F''(x(2)) = \frac{1}{(\Delta x)^2}[(f_0 - 2 \cdot f_{-1} + f_{-2}) + (f_1 - 3 \cdot f_0 + 3 \cdot f\_1 - f_{-2}) + \frac{-1}{12} \cdot (f_2 - 4f_1 + 6f_0 - 4f_{-1} + f_{-2})$

Desenvolvendo:

$F''(x(2)) = \frac{1}{(\Delta x)^2}[-2 \cdot f_{-1} + f_1 - 2 \cdot f_0 + 3 \cdot f_{-1} + \frac{-f_2}{12} - \frac{-f_1}{3} + \frac{-f_0}{2} - \frac{-f_{-1}}{3} + \frac{-f_{-2}}{12}]$

$F''(x(2)) = \frac{1}{(\Delta x)^2}[\frac{-1f_{-2}}{12} + \frac{4f_{-1}}{3} - \frac{5f_0}{2} + \frac{4f_1}{3} - \frac{f_2}{12}]$

2 Encontrar a derivada segunda

Calculando a derivada da função abaixo para o ponto $x = 2$ utilizando as fórmulas encontradas anteriormente

$f(x) = \sqrt{e^{3x} + 4x^2}$

Primeiro, devemos calcular a função nos pontos necessários. Consideremos $\Delta x = 0.0001$

$f_{k-2} = f(x - 2\Delta x) = f(1.9998) = \sqrt{e^{3 \cdot 1.9998} + 4 \cdot 1.9998^2} \approx 20.4740\ldots$

$f_{k-1} = f(x - \Delta x) = f(1.9999) = \sqrt{e^{3 \cdot 1.9999} + 4 \cdot 1.9999^2} \approx 20.4770\ldots$

$f_k = f(x) = f(2) = \sqrt{e^{3 \cdot 2} + 4 \cdot 2^2} = \sqrt{e^6 + 16} \approx 20.4799\ldots$

$f_{k+1} = f(x + (\Delta x)) = f(2.0001) = \sqrt{e^{3 \cdot 2.0001} + 4 \cdot 2.0001^2} \approx 20.4830\ldots$

$f_{k+2} = f(x + 2 \cdot (\Delta x)) = f(2.0002) = \sqrt{e^{3 \cdot 2.0002} + 4 \cdot 2.0002^2} \approx 20.4859\ldots$

$f_{k+3} = f(x + 3 \cdot (\Delta x)) = f(2.0003) = \sqrt{e^{3 \cdot 2.0003} + 4 \cdot 2.0003^2} \approx 20.4889\ldots$

2.1 Por Taylor

Substituindo os valores calculados na fórmula de Taylor encontrada previamente

$f''_k = \frac{2}{(0.0001)^2} \cdot [-8 \cdot (-20.4799 - \frac{20.4740}{16} - \frac{20.4859}{16} + 20.4770) - 20.4799] = 4650000$

2.2 Por interpolação de Newton

Substituindo os valores calculados na fórmula de interpolação de Newton previamente encontrados.

Sabemos que $F_k = F_0, F_{k+1} = F_1$ e assim sucessivamente.

$F''(x(2)) = \frac{1}{(\Delta x)^2}[\frac{-20.4740}{12} + \frac{4 \cdot 20.4770}{3} - \frac{5 \cdot 20.4799}{2} + \frac{4 \cdot 20.4830}{3} - \frac{20.4859}{12}]$

$F''(x(2)) = \frac{1}{(0.0001)^2} \cdot \frac{31}{120000}$

3 Tabela

$f(x) = \sqrt{e^{3x} + 4x^2}$ Para todas as linhas da tabela, F(x) ≈ 20.47

3.1 Para $\Delta^k = 0.5$

$F''(x) = \frac{1}{(0.5)^2}[\frac{-1 \cdot f(1)}{12} + \frac{4 \cdot f(1.5)}{3} - \frac{5 \cdot f(2)}{2} + \frac{4 \cdot f(2.5)}{3} - \frac{f(3)}{12}] = \frac{1}{(0.5)^2}[\frac{-1 \cdot 4.90}{12} + \frac{4 \cdot 9.95}{3} - \frac{5 \cdot 20.47}{2} + \frac{4 \cdot 42.81}{3} - \frac{90.21}{12}] \approx 44.9833\ldots$

3.2 Para $\Delta^k = 0.25$

$F''(x) = \frac{1}{0.25^2}[\frac{-1 \cdot f(1.5)}{12} + \frac{4 \cdot f(1.75)}{3} - \frac{5 \cdot f(2)}{2} + \frac{4 \cdot f(2.25)}{3} - \frac{f(2.50)}{12}] = [\frac{-1 \cdot 9.95}{12} + \frac{4 \cdot 14.24}{3} - \frac{5 \cdot 20.47}{2} + \frac{4 \cdot 29.56}{3} - \frac{42.81}{12}] \approx 2.8283\ldots$

$e(x) = |\frac{2.8283 - 44.9833}{2.8283}| \approx 14.90\ldots$

3.3 Para $\Delta^k = 0.125$

$F(x) \approx 24.5977\ldots$

$F''(x) = \frac{1}{0.125^2}[\frac{-1 \cdot f(1.75)}{12} + \frac{4 \cdot f(1.875)}{3} - \frac{5 \cdot f(2)}{2} + \frac{4 \cdot f(2.125)}{3} - \frac{f(2.25)}{12}] = \frac{1}{0.125^2} \cdot [\frac{-1 \cdot 14.24}{12} + \frac{4 \cdot 17.06}{3} - \frac{5 \cdot 20.4)}{2} + \frac{4 \cdot 24.59}{3} - \frac{29.56}{12}] \approx 56.5333\ldots$

$e(x) = \frac{56.53 - 2.83}{56.53} \approx 0.9499\ldots$

3.4 Para $\Delta^k = 0.0625$

$F''(x) = \frac{1}{0.0625^2}[\frac{-1 \cdot f(1.875)}{12} + \frac{4 \cdot f(1.9375)}{3} - \frac{5 \cdot f(2)}{2} + \frac{4 \cdot f(2.0625)}{3} - \frac{f(2.125)}{12}] = \frac{1}{0.0625^2} \cdot [\frac{-1 \cdot 17.06}{12} + \frac{4 \cdot 18.69}{3} - \frac{5 \cdot 20.47}{2} + \frac{4 \cdot 22.44}{3} - \frac{24.59}{12}] =\approx 49.7066\ldots$

$e(x) = |\frac{(49.7066 - 56.5333)}{49.7066}| \approx 0.13\ldots$

3.5 Para $\Delta^k = 0.031125$

$F''(x) = \frac{1}{0.0311255^2}[\frac{-1 \cdot f(1.93775)}{12} + \frac{4 \cdot f(1.968875)}{3} - \frac{5 \cdot f(2)}{2} + \frac{4 \cdot f(2.031125)}{3} - \frac{f(2.06225)}{12}] = \frac{1}{0.0311255^2} \cdot [\frac{-1 \cdot 18.70}{12} + \frac{4 \cdot 19.56}{3} - \frac{5 \cdot 20.47}{2} + \frac{4 \cdot 21.43}{3} - \frac{22.43}{12}] =\approx 52.4705\ldots$

$e(x) = |\frac{(52.4705 - 49.7066)}{52.4705}| \approx 0.0526\ldots$

3.6 Para $\Delta^k = 0.0155625$

$F''(x) = \frac{1}{0.0155625^2}[\frac{-1\cdot f(1.968875)}{12} + \frac{4\cdot f(1.9844375)}{3} - \frac{5\cdot f(2)}{2} + \frac{4\cdot f(2.0155625)}{3} - \frac{f(2.031125)}{12}] = \frac{1}{0.0155625^2} \cdot [\frac{-1\cdot 19.56}{12} + \frac{4\cdot 20.01}{3} - \frac{5\cdot 20.47}{2} + \frac{4\cdot 20.95}{3} - \frac{21.43}{12}] \approx 92.90172\ldots$

$e(x) = |\frac{(92.90172-52.4705)}{92.90172}| \approx 0.43\ldots$

Após chegarmos à 6ª iteração, concluímos que isso iria nos demandar muito tempo. Portanto, resolvemos implementar um programa na linguagem Python para facilitar o trabalho. Ao terminar, verificamos no output do programa que o processo contou com mais de 40 iterações. Na página seguinte está o código em questão.

```python
import math

def func(x):
  return math.sqrt( math.exp(3*x) + 4*x*x)

def newton(num,deltax):
 return (1/deltax*deltax) * (-1*(func(num-2*deltax)/12) +(4*func(num - deltax)/3) - (5*func(num)/2)
      + (4*func(num+deltax)/3) - (func(num+2*deltax)/12))

numero = 2
delta_x = 0.5
iteracao = 1
ultima_derivada = None

print("F(x) = ", (func(numero)))
while True:
  print("\n--%d  iterao  " %(iteracao))
  print("Delta X = ", delta_x)
  derivada = newton(numero, delta_x)
  print("Derivada = ", derivada)

  if ultima_derivada:
    erro = (derivada - ultima_derivada) / derivada
    print("Erro = ", erro)
    if abs(erro) < 0.00001:
      print("Erro desejado encontrado")
      break

  ultima_derivada = derivada
  delta_x /= 2
  iteracao += 1
```