CN A – Numerical Integration

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Conteúdo

1 Trapezoidal Rule

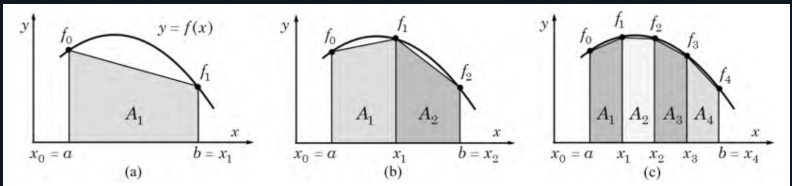

FIGURE 8.2: Graphical depiction of the effect of approximations by (a) one, (b) two, (c) four panels.

$$\boldsymbol{I = \int_{x_0}^{x_n} f(x)\ \mathrm{d}x \approx}$$

$$\boldsymbol{\approx T_n = h\left(\frac{f_n + f_0}{2} + \sum_{i=1}^{n-1} f_i\right); h = \Delta x = \frac{x_n - x_0}{n}} \tag{1}$$

$$I = \int_{x_0}^{x_n} f(x)\ \mathrm{d}x = \begin{pmatrix} +\int_{x_0}^{x_1} f(x)\ \mathrm{d}x \\ +\int_{x_1}^{x_2} f(x)\ \mathrm{d}x \\ \vdots \\ +\int_{x_{n-1}}^{x_n} f(x)\ \mathrm{d}x \end{pmatrix} \approx \begin{pmatrix} +(x_1 - x_0)\frac{f(x_1)+f(x_0)}{2} \\ +(x_2 - x_1)\frac{f(x_2)+f(x_1)}{2} \\ \vdots \\ +(x_n - x_{n-1})\frac{f(x_n)+f(x_(n-1))}{2} \end{pmatrix} =$$

$$= \sum_{i=0}^{n-1}\left((x_{i+1} - x_i)\frac{f_{i+1} + f_i}{2}\right) =$$

$$h = x_{i+1} - x_i = (x_n - x_0)/n$$

$$= \sum_{i=0}^{n-1}\left(h\,\frac{f_{i+1} + f_i}{2}\right) = h\left(\frac{f_0 + f_1}{2} + \frac{f_1 + f_2}{2} + \cdots + \frac{f_{n-1} + f_n}{2}\right) =$$

$$= h\left(\frac{f_0 + f_n}{2} + f_1 + f_2 + \cdots + f_{n-1}\right)$$

1.1 Trapezoidal rule with end correction

$$\boldsymbol{I \approx CT_n = T_n + R_n =}$$

$$\boldsymbol{= h\left(\frac{f(x_n) + f(x_0)}{2} + \sum_{i=1}^{n-1} f_i\right) - \frac{h^2}{2}\left(f'(x_n) - f'(x_0)\right)}$$

$$R_n \equiv \frac{-h^3}{12}\sum_{i=0}^{n} f_i'' = \frac{-h^2}{12}(x_n - x_0)\, f''(\xi) = \frac{-h^2}{12}(f'(x_n) - f'(x_0))$$

Exemplo 1

The tendency of a gas to escape or expand is explained by the fugacity property of the gas. For ideal gases, fugacity f is equal to its pressure, but in real gases, it is computed by the following integral:

$$\ln\left(\frac{f}{P}\right) = \int_0^P \frac{Z(x)-1}{x}\,\mathrm{d}x$$

where P is the pressure, Z is the *compressibility factor*, and f/P is referred to as the *fugacity coefficient*. The data on the compressibility factor of a real gas at a constant temperature are fitted to the curve given below:

$$Z(p) = 1 - 5\,\mathrm{E}^{-4}\, p\, e^{-p/50}, \quad 0 < p < 400\,\mathrm{atm}$$

Estimate $\ln(f/P)$ for $p = 400\,\mathrm{atm}$ using the 8-panel Trapezoiadl rule *with* and *without* end correction. Calculate the true error and global error bounds for both cases

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Resposta

Preparing equation to use trapezoidal rule

$$\ln\left(\frac{f}{P}\right) = \int_0^P \frac{Z(x)-1}{x}\,\mathrm{d}x = \int_0^P \frac{\left(1-5\,\mathrm{E}^{-4}\,x\,e^{-x/50}\right)-1}{x}\,\mathrm{d}x = \cdots =$$
$$= -5\,\mathrm{E}^{-4}\int_0^P x\,e^{-x/50}\,\mathrm{d}x \tag{2}$$

Calculating the value of (2)

$$\ln\left(\frac{f}{P}\right) = -5\,\mathrm{E}^{-4}\int_0^P x\,e^{-x/50}\,\mathrm{d}x =$$

$$\mathrm{P}\,u\,v' = u\,v - \mathrm{P}\,u'\,v \begin{cases} u = p \\ v = e^{-p/50} \end{cases}$$

$$= 1\,\mathrm{E}^{-3}\left(\left(x\,e^{-x/50}\right)\Big|_0^P - \mathrm{P}_x\left(e^{-x/50}\right)\right) =$$
$$= 1\,\mathrm{E}^{-3}\left(P\,e^{-P/50} - 0\,e^{-0/50} - \left(-50\,e^{-x/50}\right)\Big|_0^P\right) =$$
$$= 1\,\mathrm{E}^{-3}\left(P\,e^{-P/50} + 50\,e^{-P/50} - 50\,e^{-0/50}\right) = 1\,\mathrm{E}^{-3}\left((P+50)\,e^{-P/50} - 50\right) \cong$$
$$\cong 2492.4521$$

Calculating f_i for all points

$$T_n = \sum_{i=0}^{n} w_i\,F(i);$$
$$F(i) = e^{-x/50};$$
$$w = \begin{cases} h/2 = 25 & i = \{1,8\} \\ h = 50 & i = \{2,3,4,5,6,7\} \end{cases}$$

i	x_i	F_i	$w_i\,F_i$
0	0	0.0000	0.0000
1	50	18.3940	919.6986
2	100	13.5335	676.6764
3	150	7.4681	373.4030
4	200	3.6631	183.1564
5	250	1.6845	84.2243
6	300	0.7436	37.1813
7	350	0.3192	15.9579
8	400	0.1342	3.3546
		sum:	2293.6526

Calculating interval h

$$h/\mathrm{atm} = \frac{P-0}{8} = 400/8 = 50$$