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SCUOLA DI INGEGNERIA INDUSTRIALE
E DELL'INFORMAZIONE

Numerical Integration

Calcoli di Processo dell' Ingegneria Chimica

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Numerical Integration

We will discuss several methods to compute (numerically) the integral of a given function!

- **Classical Analysis**:

$$I = \int_a^b f(x)dx \quad = \quad F(a) - F(b).$$

  If and only if $F(x)$ is the antiderivative of $f(x)$

- **Numerical Analysis**: Let's build an approximation of $f(x) = \tilde{f}(x)$ by means of a suitable polynomial.

$$I = \int_a^b f(x)dx \quad \approx \int_a^b \tilde{f}(x)dx.$$

$\tilde{f}(x)$ as a Linear approximation

$$\tilde{f}(x) = P(x) = \frac{(b-x)f(a) + (x-a)f(b)}{b-a}$$

$$I = \int_a^b f(x)dx \approx \int_a^b P(x)dx = \frac{1}{2}(b-a)\left[f(a) + f(b)\right]$$

Trapezoidal interpolation method or Bézout interpolation formula. Generalizing the formula can be written as follow:

$$I \approx h\left[0.5f(x_0) + f(x_1) + f(x_2) + \ldots + f(x_{n-1}) + 0.5f(x_n)\right]$$

$$h = \frac{b-a}{n} \quad x_i = a + i \times h \quad i = 0, 1, \ldots, n \quad n \geq 1$$

$\tilde{f}(x)$ as a Quadratic approximation

$$\tilde{f}(x) = P(x) = \frac{(x-c)(x-b)}{2h^2} f(a) + \frac{(x-a)(x-b)}{-h^2} f(c) + \frac{(x-a)(x-c)}{2h^2} f(b)$$

$$I = \int_a^b f(x)dx \approx \int_a^b P(x)dx = \frac{h}{3}\left[f(a) + 4f(c) + f(b)\right]$$

With:

$$h = \frac{b-a}{2}$$

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

This is the formula of Simpson or Simpson-Cavalieri.

Generalizing:

$$I \approx \frac{h}{3}\left[f(x_0) + 4f(x_1) + 2f(x_2) + \ldots + 2f(x_{n-2}) + 4f(x_{n-1} + f(x_n))\right]$$

$$h = \frac{b-a}{n} \quad x_i = a + i \times h \quad i = 0, 1, \ldots, n \quad n \in \mathbb{N}$$

Aitken formula

It should be noted that, when employing both methods, increasing the number of intervals over which the integral is calculated in order to enhance the precision of the evaluation does not preclude the utilisation of the preceding iteration's evaluations of the function in question (this necessitates the storage of the function's value in an array). The ratio between the errors of two successive iterations is constant (provided the function is differentiable), indicating a linear convergence. Consequently, if the estimate of the integral is evaluated for a number of sub-intervals equal to n, $2n$, or $4n$, the value of the integral can be extrapolated using the following formula:

$$I \approx I_{4n} - \frac{(I_{4n} - I_{2n})^2}{(I_{4n} - I_{2n}) - (I_{2n} - I_n)}$$

Exercises

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- Write a MATLAB function to perform the numerical integration with the bezout formula and aitken formula.
- **Exercise 1**: A collection tank receive polluted water from a variable source. The istantaneous flow rate of the inlet dpends on the time of the day according to the following relationship:

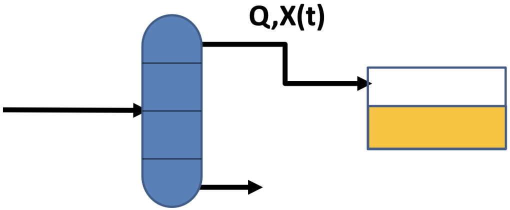
$$Q(t) = 2sin^2\left(\frac{t}{24}\pi\right) \quad [l/min]$$

At the end of the 24 hours period tank is emptied and the water is moved to a treatment facility. Determine the appropriate size of the tank (i.e., the volume of the tank).

- **Exercise 2**: The DIPPR database reports the following expression for the cp of SO_2 (T in K, Cp in $[J/kmolK]$). For SULFUR DIOXIDE The Ideal Gas Heat Capacity can be calculated as follows:

$$Cp = A + B \times \left(\frac{C}{T \times sinh\left(\frac{C}{T}\right)} \right)^2 + D \times \left(\frac{E}{T \times cosh\left(\frac{E}{T}\right)} \right)^2$$

$A = 3.3375e^{04}$, $B = 2.5864e^{04}$, $C = 9.3280e^{02}$, $D = 1.0880e^{04}$, $E = 4.2370e^{02}$ In the range: 100.00 K to 1500.00 K. Using the trapezoidal rule, calculate the power necessary to heat 300 $kmol/h$ of SO_2 from 230 to 480 $°C$. Calculate the error if we assume the Cp constant at the initial temperature, at the average temperature or the final temperature.



- **Exercise 3**: A distillation process enables the recovery of the product, designated as X, in a stream that is subsequently collected in a tank. The current entering the tank has a constant volumetric flow rate, and the concentration of the product X in time is given by the following law: $X(t)$ is expressed in mol/L, t in hours.

$$X(t) = sin(\sqrt{t})exp(-2t^2)$$

The objective is to determine the requisite time for maximizing the recovery of component X, which has a concentration of 0.3 mol/L. The problem should be solved using a variety of approaches, including the trapezoidal rule, Simpson's rule, and the trapezoidal rule with Aitken extrapolation.

Total volume recovered in the collection tank

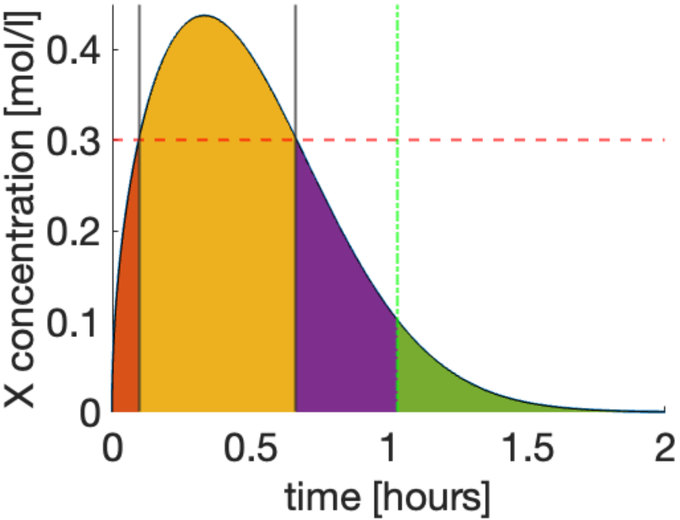
$$V_{tot}(t) = Qt$$

Total moles of X recovered in the collection tank

$$mol_{X_{tot}}(t) = Q \int_0^t f(x)dx$$

Equation solving the problem: a function containing an integral that need to be zeroed

$$C_X(t) = \frac{\int_0^t f(x)dx}{t} = 0.3$$


X concentration [mol/l]
0.4
0.3
0.2
0.1
0
0
0.5
1
1.5
2
time [hours]

Thank you for the attention!