Statistical and Numerical Methods for Chemical Engineers
Solutions : Exercise 1

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1 Programming for fun: Conway's Game of Life

Refer to the separately attached solution mfile `SNM_Ex1_Q1.m`.

2 Linear Interpolation

1. Estimate by linear interpolation the velocity of the particle at time t = 2.5.
   The linear polynomial interpolating the data in the interval [2,3] is

$$v(t) = 18 + \frac{27-18}{3-2}(t-2) = 18 + 9(t-2) = 9t \tag{1}$$

   So we obtain

$$v(t=2.5) = 22.5[m/s] \tag{2}$$

2. Estimate by linear interpolation the distance travelled by the particle between times t = 2 and t = 3.
   The travelled distance can be computed by integrating the velocity in the given time interval

$$d = \int_{t_0}^{t_1} v(t)dt \tag{3}$$

   So we simply integrate the linearly inrerpolated velocity $v(t)$ over the interval $[2,3]$ to get

$$d = \int_{2}^{3} v(t)dt = \int_{2}^{3} 9tdt = 22.5[m] \tag{4}$$

3. Estimate by linear interpolation the instant acceleration of the particle a time t = 2.5.
   The instant acceleration is obtained by differentiating the velocity

$$a(t) = \frac{dv}{dt} = 9 \tag{5}$$

   We differentiate the linearly interpolated velocity profile $v(t)$ and evaluate it at $t = 2.5$

$$a(2.5) = \frac{dv}{dt}|_{t=2.5} = 9 \tag{6}$$

3 The method of finite differences

The solutions to the coding part of the assignment are given in separately attached mfile `SNM_Ex1_Q3.m`.
In the following paragraphs, the order of accuracy of the forward and centered finite difference methods are derived :

3.1 Forward Finite Differences

The explicit expression of the forward finite difference method u^{FD} for the approximation of the first derivative of a function $f(x)$ at the point x_0 can be written as

$$f'(x_0) = \frac{df(x)}{dx}\Big|_{x=x_0} \approx u^{FD} = \frac{f(x_0+h) - f(x_0)}{h} \tag{7}$$

To estimate the order of accuracy is then sufficient to expand f using Taylor's theorem obtaining

$$f(x_0+h) = f(x_0) + hf'(x_0) + O(h^2) \tag{8}$$

as $h \to 0$. From (8) it follows that

$$\frac{f(x_0+h) - f(x_0)}{h} = f'(x_0) + O(h) \tag{9}$$

where we use the fact that $h^{-1}O(h^2) = O(h^{-1}h^2) = O(h)$.
Note that the first term on the right hand side is exactly the first derivative of f, we can conclude that the forward finite difference method is a first-order approximation to the first derivative of f (**order of accuracy 1**).

3.2 Centered Finite Differences

The centered finite difference method is based on the following approximation formula

$$f'(x_0) \approx u^{CD} = \frac{f(x_0+h) - f(x_0-h)}{2h} \tag{10}$$

Given both the forward and backwards Taylor expansions

$$\begin{aligned} f(x_0+h) &= f(x_0) + f'(x_0)h + \frac{1}{2}f''(x_0)h + O(h^3) \\ f(x_0-h) &= f(x_0) + f'(x_0)(-h) + \frac{1}{2}f''(x_0)(-h)^2 + O(h^3) \end{aligned} \tag{11}$$

we can subtract the second from the first to obtain

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

which proves that the centered finite difference is a second-order approximation to the first derivative of f (**order of accuracy 2**).