Process model formulation and solution, 3E4

Tutorial 7

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Tutorial objectives: Numerical differentiation and plotting.

Question 1 [2]

This question uses the experimental data from the class notes. A batch system was charged with reactant A at time $t = 0$ at a concentration of 1.0 mol/L. As the assumed first-order reaction evolved, the concentrations were recorded:

Time (minutes)	Concentration (mol/L)
0	1.00
5	0.84
10	0.72
20	0.57
30	0.47
45	0.37
60	0.30

The dynamic balance for this system can be shown to be $\dfrac{dC_\mathsf{A}(t)}{dt} = -kC_\mathsf{A}(t)$.

1. Reproduce the above table and add a column that provides an approximation of $\dfrac{dC_\mathsf{A}(t)}{dt}$ at each time step.
2. Add a fourth column that lists the order of your approximation listed in part 1.
3. Use a 2nd order Lagrange polynomial to approximate the $C_\mathsf{A}(t)$ data, and use this polynomial to estimate ${C_\mathsf{A}}'(t)$ at time $t = 15$ minutes.
4. Can you provide an $O(h^2)$ estimate of $\dfrac{dC_\mathsf{A}(t)}{dt}$ at $t = 0$? If so, please calculate it.

Question 2 [1.5]

A second order reaction in a constant-volume batch reactor has the following time-dependent behaviour:

$$C_\mathsf{A}(t) = \frac{C_\mathsf{A}(0)}{C_\mathsf{A}(0)kt + 1} \qquad \text{with} \qquad k = 0.002\frac{\text{m}^3}{\text{mol.s}} \qquad \text{and} \qquad C_\mathsf{A}(0) = 2.5\frac{\text{mol}}{\text{m}^3}$$

Starting with $h = 1.0$ and decreasing in powers of 10, which step size, $h = \Delta t$, provides the lowest error estimate of $\left.\dfrac{dC_\mathsf{A}}{dt}\right|_{t=100}$ at $t = 100$ seconds?

Present your results in tabular form with these 5 columns:

- Step size, $h = \Delta t$
- Forward difference approximation
- Error in the forward difference approximation
- Central difference approximation
- Error in the backwards difference approximation

Bonus question [0.5]

Show the two error columns from question 2 in graphical form, using log-axes for both the x- and y-axis. Search for help over the internet if you don't know how to plot log-plots in MATLAB, or with Python's `matplotlib` library. Add a legend, grid lines and axis labels to the plot.

END