Numerical Methods - Lab. 1

Errors

1. The derivative of $f(x) = 1/(1-3x^2)$ is given by
$$\frac{6x}{(1-3x^2)^2}.$$
   i. Implement f in Mathematica and recompute its derivative.
   ii. Do you expect to have difficulties to evaluate f' at $x = 0.577$? Try it using a $3-$ and a $4-$digit arithmetic precision with chopping.

2. Use the Taylor series to estimate $f(x) = \mathrm{e}^{-x}$ at $x_{i+1} = 1$ for $x_i = 0.25$. Employ the zero-, first-, second- and third-order versions and compute ε_t for each case.

3. Use the zeroth through forth-order Taylor series expansion to predict $f(2)$ for $f(x) = \ln x$ using a base point at $x = 1$. Compute the true percent relative error for each approximation. Discuss the meaning of the results.

4. Use forward and backward difference approximations of $O(h)$ and centered difference approximations of $O(h^2)$ to estimate the first derivative of
$$f(x) = 25x^3 - 6x^2 + 7x - 88.$$
Evaluate the derivative at $x = 2$ using a step-size of $h = 0.25$. Compare the results with the true value of the derivative.

5. Find the forward, backward and centered finite difference approximations for the second derivative.

6. Consider the function $f(x) = x^3 - 2x + 4$ on the interval $[-2, 2]$ with $h = 0.25$. Use the forward, backward, and centered difference approximations for the first and second derivatives so as to graphically illustrate which approximation is most accurate. Graph all three first-derivative finite difference approximations along with the theoretical, and do the same for the second derivative as well.

Modeling and Euler's method

7. The amount of a uniformly distributed radioactive contaminant contained in a closed reactor is measured by its concentration c (becquerel/liter or Bq/L). The contaminant decreases at a decay rate proportional to its concentration; that is
$$\text{Decay rate} = -kc,$$
where k is a constant with units of day^{-1} (or d^{-1}). Therefore, according to the fact that
$$\text{change} = \text{increases} - \text{decreases},$$
a mass balance for the reactor can be written as
$$\frac{\mathrm{d}c}{\mathrm{d}t} = -kc$$
$$\text{change in mass} = \text{decrease by decay}.$$
   i. Use Euler's method to solve this equation from $t = 0$ to $1d$ with $k = 0.175d^{-1}$. Employ a step size of $h = 0.1d$. The concentration at $t = 0$ is 100 Bq/L.
   ii. Plot the solution on a semilog graph (i.e., $\ln c$ versus t) and determine the slope. Interpret your results.