CH2013
Computational Programming and Simulations Lab
July-Nov 2023
Problem Sheet #5

1. Structure arrays offer a compact notation for sharing data across various parts of the MATLAB code. Look up the syntax, how to set up the values, and how to access each element of the array, carefully.

a) Define a structure array called "reactiondata" to set up values of the pre-exponentials and activation energies for two reactions – in the script file. The pre-exponentials should be in a (vector) field called 'k0' and the activation energies in a (vector) field called 'Eact'. The values are 0.001 and 0.34 for the pre-exponentials, and 12000 and 5600 for the activation energies, respectively.

b) The reaction rates can be calculated as

$$r_i = k_{0i} \exp\left(-\frac{E_{act,i}}{RT}\right) C_1 C_2$$

(same expression for both the reactions, only the values of k0 and Eact are different; R = 8.314 in consistent units)
C_1 and C_2 are two concentrations; T is the temperature.

c) Write a function 'reactionrate1' which has C_1, C_2, T, and the structure array 'reactiondata' as inputs and the outputs are r1 and r2.

d) Call the function 'reactionrate1' to get the values of reaction rate 1 & 2 (call it rate1 and rate2), for the given data - C_1 and C_2 can be assumed be to 0.1 and 0.01, respectively. T varies between 300 & 1000 (consistent units; 100 units intervals). Plot rate1 and rate2 vs. T (use semi log y).

2. Solve the following system of equations using the MATLAB function '**fsolve**'.

$$2e^x + y = 0$$
$$3x^2 + 4y^2 = 8$$

Set the following options –
Maximum number of iterations: 10
Tolerance value (on function): 1.e-6
Display: all the iterations

Use an initial guess of (-1,-2) and put the final solution you obtain in a structure array "**Solution1**" with fields as below.

x1 -> converged solution for x
x2 -> converged solution for y
f1 -> value of the first function at convergence
f2 -> value of the second function at convergence
jacobian -> value of the jacobian at convergence
exitflag -> the exitflag
iterations-> number of iterations

Now use an initial guess of (-2,100) and put the final solution you obtain in a structure array **Solution2**, with the same fields x1, x2, etc. Figure out why this initial guess fails, and try to play around to see how to fix the problem.

3. Use 0^{th} to 5^{th} order approximations of the Taylor series to predict exp(2) starting from exp(0)=1. Use MATLAB to calculate exp(2) and consider it the true value. Now, calculate the truncation error in the form of percent relative error for the different approximations of the Taylor series that you have used.

4. Evaluate the function f(x,y) and the associated round-off error in terms of percent relative error.

$$f(x,y) = (x+y)/(x-y)$$

Given: x=1.5001 and y=1.4999. Use 5-digit, 4-digit, 3-digit, and 2-digit arithmetic with chopping. For example, for doing 3-digit arithmetic, use x=1.50 and y=1.49.

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