Homework 20

Ch En 263 – Numerical Tools

Due date: 9 Jun. 2020

Instructions

- Do the following problems in a **Jupyter notebook** named `LastName_FirstName_HW20.ipynb`.
- Please report how long it took you to complete the assignment (in hours) in the "Notes" section on Learning Suite.

Problems

1. Format your homework in the Jupyter notebook by:
   - Giving each problem a markdown cell with a heading named `Problem X` where `X` is the problem number.
   - Separating the problems into different markdown/code cells
2. Do the following using the symbolic module in Python.
   (a) Simplify the expression:
   $$\frac{x^2 - x - 6}{x^2 - 3x}.$$
   (b) Expand the expression:
   $$(x+1)^3(x-2)^2.$$
   (c) Factor the expression:
   $$3x^4 - 36x^3 + 99x^2 - 6x - 144.$$
   (d) Compute the symbolic derivative:
   $$\frac{d}{dx}\sin^2(x)e^{2x}.$$
   Then evaluate the resulting expression for $x = 3.3$.
   (e) Evaluate the integral:
   $$\int_0^5 x^2 \sin(x^2)\, dx.$$
3. Evaluate the integral
   $$I = \int_{-50}^{50} x^2 f(x)\, dx$$
   using the data contained in the file "HW20_Prob3_Data.csv" with an appropriate `Scipy` function. The first column of the data file contains x, the second column contains $f(x)$. Make sure you print the value of I in your notebook.

4. Use the symbolic math engine in Python to find the four possible partial derivatives ($\partial f_0/\partial x_1$, $\partial f_0/\partial T$, $\partial f_1/\partial x_1$, $\partial f_1/\partial T$), of the vector function in residual form

$$\boldsymbol{f}(x_1, T) = \begin{bmatrix} x_1 10^{A_1 - B_1/(T+C_1)} - p_1, \\ (1-x_1)10^{A_2 - B_2/(T+C_2)} - p_2 \end{bmatrix} = \mathbf{0}$$

where A_1, B_1, C_1, A_2, B_2, C_2, p_1 and p_2 are known constants. Be sure to display these expressions in the notebook.

5. Recall that the enthalpy of gaseous CO_2 is given by

$$h(T) = h(298.15) + \int_{298.15}^{T} c_p(T) dT.$$

The units of h are J/mol. The heat capacity (J/mol K) is given by

$$c_p(T) = R_g(a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4),$$

where $R_g = 8.314$ J/(mol K), and $a_1 = 2.275724$, $a_2 = 0.009922$, $a_3 = -1.04091 \times 10^{-5}$, $a_4 = 6.86669 \times 10^{-9}$, $a_5 = -2.11728 \times 10^{-12}$. Also, $h(298.15) = -393549.1$ J/mol.

In problem 1 of HW 15, we solved for the temperature when $h(T) = -362828$ J/mol. We did this by evaluating the integral by hand, and then we used `root` to solve the resulting non-linear equation. This time, use `quad` to do the integral and `root` to solve for T. Be sure to print the value of T in the notebook.

Hint: You will need to set up a function to pass to `root` *that uses* `quad` *inside of it. Also, you my want to compare the answer you get here with the one you found in HW 15.*