

Please solve the exam on the sheets provided. You may use the backs of the sheets as well. Feel free to use the blue books if you need more room!

Problem 1). Root Finding: In this problem we wish to determine the roots of the function:

$$f(x) = x^3 - x + \frac{1}{\sqrt{3}}$$

A. Derive the formula for Newton's method for finding the root of a single equation.

B. Starting with the initial guess for the root of  $x_0 = -1$ , use Newton's method to get the root. Do two iterations.

C. Repeat this for the initial guess of  $x_0 = 0$ , again doing two iterations. Why is the behavior of Newton's method different for this starting point?

Problem 2). Quadrature and Error:

A. A Junior in undergraduate lab wishes to integrate his experimental data over the interval  $[0,1]$ . Unfortunately, because of his experimental approach he can only make measurements at the points  $x_1 = 0.4$  and  $x_2 = 0.8$  rather than at lots of points in the interior. Determine the optimum quadrature rule (e.g., the optimum weights) for integrating his data. **What is the polynomial degree of this quadrature rule?**

B. Another lab group has approached you for advice in error propagation (better you than me, anyway...) for their quadrature method. They are integrating their data using the quadrature rule:

$$I = \sum_{i=1}^n w_i f(x_i)$$

where the  $x_i$  are the locations where they measured the data and the  $f(x_i)$  are their measured values. The quadrature rule itself is specified by the vector of weighting elements  $w_i$ . The problem is that their data is noisy, such that each of the  $f(x_i)$  is characterized by the constant standard deviation  $\sigma_f$ . Determine the resulting random error in the integral  $\sigma_I$ .

Problem 3). Generalized Regression:

In undergraduate laboratory there is an experiment examining the reaction kinetics of a NaOH - phenolphthalein reaction. The extent of reaction is measured using a colorimeter, where the absorbance is proportional to the concentration of the phenolphthalein. The purpose is to measure the reaction rate constant  $K$  at different temperatures and NaOH concentrations to learn something about the reaction mechanism. In the experiment you measure absorbances  $A_i$  at times  $t_i$ . The absorbances should fit an exponential rate law:

$$A = C_1 + C_2 e^{-Kt}$$

where  $C_1$ ,  $C_2$ , and  $K$  are unknown constants. The only one you really want to know is  $K$ .

A. Describe in a concise and complete fashion how you would go about obtaining  $K$  from a set of absorbance data ( $t_i$ ,  $A_i$ ). Use equations in addition to words where possible or appropriate: I am trying to see if you know how to solve the problem!

B. Briefly discuss how you could obtain an error estimate for your fitted value of  $K$ .