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PC3236: Assignment 2 Report

Problem 1

In Problem 1, a triple definite integral is to be solved numerically. The triple integral is first broken down into three single integrals as defined below:

$$F(y,z) = \int_0^{\sqrt{1-y}} \sqrt{x^3 + yx^2 + z^3}\,(e^{-x+y^2-z^3})\,dx$$

$$G(z) = \int_0^{z^2} F(z,y)\,dy$$

$$I = \int_0^1 G(z)\,dz$$

Each integral is evaluated using Gaussian integration, specifically the Gauss-Legendre quadrature rule. By using Gram Schmidt's orthogonalization then finding the roots of the orthogonal polynomials, the weights and abscissas can be obtained. For simplicity, these values are directly retrieved from Table 4.1 in the Textbook. For three-point (N = 3) Gauss-Legendre quadrature rule, the abscissas and weights are:

$$x = 0.7745967, -0.7745967, 0.0$$

$$W = 0.55555, 0.55555, 0.88888$$

The integrals can then be calculated using the following summation:

$$\frac{b-a}{2}\sum_{m=1}^{3} W_m f(x_m)$$

The numerical integration method is applied to *F(y, z)*, *G(z)*, and *I* respectively, which yielded a converged answer of **0.0960307**.

Problem 2

In Problem 2, a set of data points are provided along with a proposed function *I(w)* to fit the data in the least-square sense. By doing a simple plot of the data points, it can be verified that the curve is indeed nonlinear which requires the consideration of the least-square error equation:

$$S(a_1, a_2, \ldots, a_m) = \sum_{k=1}^{N} (y_k - Y(x_k; a_1, a_2, \ldots, a_m))^2 \,,$$

In this case, the theoretical function *Y* is the given proposed function *I(w)*, which is parameterized by *a* and *b*. The objective is to determine the values of *a* and *b*.

The function *I(w)* is given as an improper definite integral with respect to *x*. To proceed further, the integration must first be evaluated. Given the complexity of the integrand, it is most easily done using numerical integration. Leveraging the exiting code from Problem 1, the Gauss-Legendre quadrature rule is used once again. However, since it is an improper integral with infinity as one of the limits, a change of variable is required. By setting *x = y / (1 – y)*, the integration bounds are mapped from *[0, inf]* to *[0, 1]*. The remaining singularities at *y = 1* (one of the bounds) can be ignored as Gaussian integration does not require the removal of singularities.

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To minimize S, the following equation must be solved:

$$\frac{\partial S(a_1, a_2, \ldots, a_m)}{\partial a_i} = 0,$$

The system of equations is solved using Newton-Raphson's scheme, which requires the Hessian matrix of S as well as the set of first derivatives. To compute all the first and second partial derivatives, numerical differentiation is used. In both cases, the central finite difference formulas are used for better accuracy.

As part of Newton-Raphson's method, initial guess of the parameters (*a* and *b*) must be provided. Based on trying different combinations of *a* and *b* with the corresponding curve, they are initially estimated to be close to 4 and 2 respectively. By using two cycles of "CRUDE" procedure adopted from the Textbook (using quadratic interpolating polynomial), better initial values were calculated. Plugging these values in, the NR calculation converged to ***a* = 5.50725** and ***b* = 1.49639**.

Below is the fitted curve *I(w)*, in red, superposed on top of the original data points.