AE/ME 5830 Applied Computational Methods, Test 1, 04/13/2021

Name: **Signature:**

Test 1 is due 5:00 pm CST, Thursday April 15. Please present your results in an organized and clear way with sufficient explanation as you do in homework solutions. Include the program listings at the end as an Appendix. **No consultation with other students is allowed. All submitted solutions and computer programs should be based on your individual work. Failure to obey this will be considered as an act of academic dishonesty and may result in receiving no credit from the test.** By signing above, you acknowledge that all submitted answers are prepared by you and you have not received any unauthorized help from other people or sources. **Good luck!**

Question 1 (25 points)

The following function $f(M)$ describes the total pressure ratio (P_{0_r}) across a normal shock wave for a calorically perfect gas where M is the Mach number upstream of the shock:

$$P_{0_r} = f(M) = \left[1 + \frac{2\gamma}{\gamma+1}(M^2 - 1)\right]^{\frac{-1}{\gamma-1}} \times \left[\frac{2 + (\gamma-1)M^2}{(\gamma+1)M^2}\right]^{\frac{-\gamma}{\gamma-1}} \tag{1}$$

Here γ is the specific heats ratio and constant. Using the Secant Method and for $\gamma = 1.4$, find the upstream Mach number (M) for **(i)** a total pressure ratio of $P_{0_r} = 0.1386$ and **(ii)** a total pressure ratio of $P_{0_r} = 1.0$. For both cases, use $M_0 = 2.8$ and $M_1 = 2.2$ as the initial guesses to start the Secant method and approximate the upstream Mach number with a convergence criterion of $(\epsilon_n)_r = \frac{|M_{n+1} - M_n|}{|M_n|} < 10^{-8}$ where n is the iteration number.

(a) For each pressure ratio, tabulate the values of M_n, $\Delta_n M = M_{n+1} - M_n$, and M_{n+1} at each iteration.

(b) Comment on the converge of the Secant Method for each case. If there is a difference in convergence, what can be the possible reason for this?

(c) Now assume that you use Newton's method instead of Secant method for both pressure ratios. Would you expect to see a similar difference in the convergence between two pressure ratio cases? Why or why not? Explain briefly (in words) how you can improve the convergence for the case which has a slower convergence rate.

Question 2 (25 points)
An objective function of two design variables $\vec{x} = \{x_1, x_2\}$ is defined as:

$$f(x_1, x_2) = Cos(x_1^2 - x_2) + Sin(x_1^2 + x_2^2) \tag{2}$$

By starting with the initial design point, $\vec{x}^0 = \{0.1, -0.1\}$,

(a) Formulate the problem as a one-dimensional minimization problem to calculate the next design point $\vec{x}^1$ along the search direction, $s^1 = -\nabla f(\vec{x}^0)$. (Do not scale the search direction for this question). Show the steps in your formulation clearly and give the expression for the one-dimensional objective function ($f(\alpha)$) you have obtained.

(b) Perform one-dimensional optimization to determine the minimum of the objective function ($f(\alpha)$) obtained in part (a) using the Golden-Section search algorithm. Use $0.0 \leq \alpha \leq 1.2$ as your initial interval. First, calculate the number of iterations required to reduce this interval by 8 orders of magnitude and then perform the Golden-Section search to determine the optimum value of α (i.e., α^*), corresponding value of the objective function $f(\alpha^*)$, and the design point $\vec{x}^1$.

(c) Describe and show clearly how you can implement the Secant Method to perform one-dimensional optimization for the problem described in part (b) (i.e., finding the minimum of the objective function $f(\alpha)$). With the procedure you have described, calculate the optimum value of α (i.e., α^*), corresponding value of the objective function $f(\alpha^*)$, and the design point $\vec{x}^1$. For the Secant Method, use the end points of the initial interval given in part (b) as the starting values and use a convergence criterion of $(\epsilon_n)_r = \frac{|\alpha_{n+1} - \alpha_n|}{|\alpha_n|} < 10^{-8}$ (n is the iteration number).

Question 3 (25 points)
An objective function of two design variables $\vec{x} = \{x_1, x_2\}$ is defined as:

$$f(x_1, x_2) = \frac{1}{30}(8x_1^2 - x_1x_2 + 0.5x_2^2) + x_1e^{-(x_1^2+x_2^2)} \tag{3}$$

Calculate the minimum objective function value and the corresponding design variables by using (i) **Steepest Descent** and (ii) **BFGS Variable Metric (Quasi-Newton)** Methods. For each method, use the initial design point $\vec{x}^0 = \{1.0, 1.0\}$ and limit the maximum number of iterations to 100.

Use the convergence criterion $\left|f(\vec{x}^k) - f(\vec{x}^{k-1})\right| \leq 10^{-10}$ and make sure to satisfy this at 4 successive iterations. **For each method:**
(a) Tabulate the values of the design variables and the objective function as a function of the iteration number k.
(b) Plot the convergence history of the objective function ($f(\vec{x}^k)$ vs. iteration number k).
(c) Comment on the convergence of the two methods.

Question 4 (25 points)
An alternative way of finding the coefficients of an n^{th} degree Lagrange polynomial approximation ($L_n(x) = a_0 + a_1 x + a_2 x^2 + ... + a_n x^n$) to a given $f(x)$ function within a specified interval $[p, q]$ is to solve a linear system of equations $Ay = b$ where A is an $(n + 1 \times n + 1)$ matrix whose elements are given by the equation

$$a_{i+1,\ j+1} = (x_i)^j \quad (i, j = 0, 1, 2, ..., n).$$

Here x_i $(i = 0, 1, 2, ..., n)$ represents the points where the function values are specified and $y = \{a_0, a_1, a_2, ..., a_n\}^T$ is the variable vector. The RHS vector is $b = \{b_0, b_1, ..., b_n\}^T$ and each component of this vector represents the function values evaluated at the corresponding x_i locations.

(a) Construct the matrix form of the linear system of equations (i.e., obtain A matrix and the b vector) for

$$x_i = \left(\frac{p+q}{2}\right) + \left(\frac{p-q}{2}\right) cos\left[\left(\frac{2i+1}{2n+2}\right)\pi\right]$$

and

$$b_i = f(x_i) = \frac{1}{1 + x_i + x_i^2}$$

for $i = 0, 1, ..., n$ where $n = 3$, $p = 1$, and $q = 4$.

(b) Use Gauss elimination with partial pivoting to solve the linear system of equations ($Ay = b$) obtained in part (a) to determine the solution vector y (coefficients of the polynomial). Your program should take A matrix and the right hand side vector b as inputs and return the solution vector y as output.

(c) Using the computer routine you have developed for Gauss-Seidel scheme with over/under relaxation, solve the linear problem obtained in part (a) to determine the solution vector y (coefficients of the polynomial). Your routine should take A (the coefficient matrix), b (the right hand side vector), ω (the relaxation factor), $NMAX$ (maximum number of iterations allowed), and p (tolerance to stop the iteration process) as inputs. Your output should include the solution vector y. In your program, define the residual vector $r^{(k)} = b - Ay^{(k)}$ where k indicates the iteration number. Stop your iteration process if

$$\frac{||r^k||_2}{||r^0||_2} \leq 10^{-p} \qquad or \qquad k \geq NMAX$$

where $NMAX = 400$ and $p = 8$. Obtain the solution with $\omega = 1.0, 1.5$, and 1.75 using the initial solution vector $y^0 = \{1., 1., 1., 1.\}$ for each case. Give the solution vector (with at least 8 decimal places for each component) and the number of iterations performed for each case.

(d) For the given problem, which method (Gauss elimination or Gauss-Seidel) would you prefer to use for solving the linear system of equations? Explain your answer.