ME 685A (2016-2017 Summer)

Assignment Policy

- **Three kinds of problems**
  (A) Practice (B) Modelling (B) Methods
  Modelling related problems are open ended seeds for potential projects. A reasonable amount of work from formulation to post-processing is expected.
  Methods related problems are to be implemented in any programming language (e.g, Fortran, C, C++, Python etc) or perhaps MATLAB (for 90% credit), and validated for at least 3 sets of data:
  (1) Data suggested in the problem,
  (2) Student's own data, and
  (3) Data given at the time of evaluation.

- **Submission**
  (1) A hard copy of a brief report, in the *beginning* of the class.
  (2) A soft copy (zip file) of the code (**in any language**) done **individually** and the pdf file of the report, to mankur@ and sunjac@ roughly two hours before the class.
  (3) Typical time for completing an assignment: 6 days; due dates strict, with mild penalties for late submission.

- The code for a problem on a particular method must not use the **corresponding** library function.

- To the extent possible the methods are to be implemented as **functions or subroutines** rather than cluttering the main program.

ME685 (2017) Assignment 1

(Full marks = 100)

Deadline:
Soft complete version (zip and pdf) with codes— 06 Jun 12:00;
Hard copy without codes— 06 Jun 14:00.

1. **Problem for variable data sets.**
   Consider the function $f : R^2 \to R$. Measuring the *size* of the input by $|x| + |y|$, and taking the size of the output as $|f(x, y)|$, determine the condition number of the problem of evaluating the function f. In which regions of the x-y plane would you expect less reliability?
   Suggested case: $f(x, y) = x - y$. (10)

2. **Problem for variable data sets.**
   Write a programme to solve the quadratic equation $ax^2 + bx + c = 0$ using the *standard formula*

   $$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

   and also by the alternative formula that you can develop by multiplying the numerator and denominator in the above with $-b \mp \sqrt{b^2 - 4ac}$ (even though the idea looks funny).
   Make your programme robust against unusual input data (values of a, b, c) that may cause numerical inaccuracies in one solution or the other. Test your programme using lots of *unusual* data sets and check whether these measures give better results than the standard formula.
   Suggested data sets: (i) $a = 6 \times 10^{30}$, $b = 5 \times 10^{30}$, $c = -4 \times 10^{30}$; (ii) $a = 1$, $b = -4$, $c = 3.999999$; (iii) $a = 10^{-30}$, $b = 10^{-30}$, $c = 10^{30}$. (10)

3. **Problem for variable data sets.**
   The first derivative of a function $f(x)$ was computed using the usual central difference formula

   $$f'(x) = \frac{f(x + h) - f(x - h)}{2h},$$

   with its usual error of the second order. After that, the need for the third derivative was felt, for which the function was evaluated at two more points, namely $x - 2h$ and $x + 2h$. Develop the formula for the third derivative in terms of these four function values (even if you have done it once in Quiz 1) and work out its order of error. Further, now that you have as many as four function values, use them to develop an alternative formula for the first derivative which will be (hopefully) more accurate.
   Still later, there arose the need for the second derivative as well, for which the usual (second order) formula needs the value of $f(x)$, which we *do not* have yet. We decide that we will not evaluate it, rather we will use the four function values that we already have to work out the second derivative. Develop a formula for this purpose and determine its error order.
   Test all your formulae against diverse functions.
   Suggested case: $f(x) = x^3 e^{-2x} \sin x$. (15)

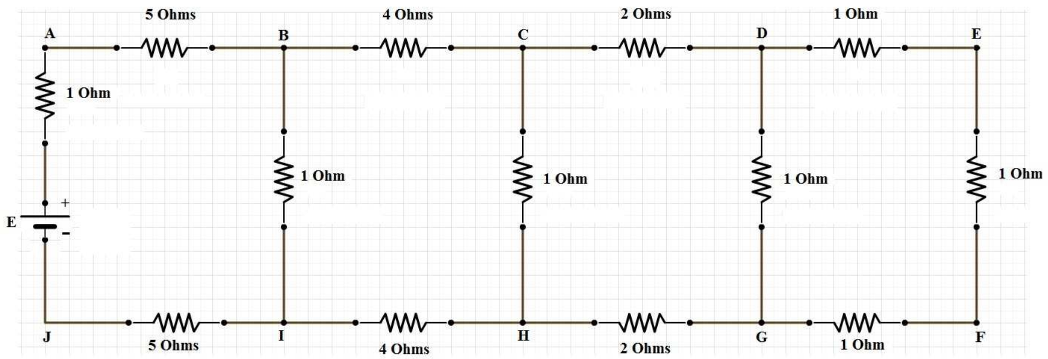
4. A surveyor reaches a remote valley to prepare records of land holdings. The valley is a narrow strip of plain land between a mountain ridge and sea, and local people use a local and antiquated system of measures. They have two distant landmarks: the lighthouse and the high peak. To mention the location of any place, they typically instruct: *so many* bans *towards the lighthouse and so many* kos *towards the high peak.* Upon careful measurement, the surveyor and his assistants found that (a) one *bans* is roughly 200 m, (b) one *kos* is around 15 km, (c) the lighthouse is 10 degrees south of east, and (d) the high peak is 5 degress west of north; and both the lighthouse and the high peak are actually far away — they are just distant direction indicators.

   The surveyor's team, obviously, uses the standard system, with unit distances of 1 km along east and along north. Now, to convert the local documents into standard system and to make sense to the locals about their intended locations, work out

   (a) a conversion formula from valley system to standard system, and (5)

   (b) another conversion formula from standard system to valley system. (5)

5. Find out the current in each branch of the circuit in terms of the emf E (in volts). (10)



   Next, instead of just four loops, suppose there are more such loops on the right side, in the same pattern. Work out the current through the battery in the case of 7, 8 and 10 such loops. (10)
   Taking advantage of the pattern of coefficients, try to make the computation *efficient.* (BONUS)

6. **Problem for variable data sets.**
   Implement a complete and robust linear system solver that will work in all kinds of cases.
   Suggested data:

   (i) $\begin{bmatrix} 3 & 2 & -1 \\ 4 & 0 & 1 \\ -1 & 3 & 2 \end{bmatrix} X = \begin{bmatrix} 3 \\ 2 \\ 9 \end{bmatrix}$ (ii) $\begin{bmatrix} 2 & 0 & -1 \\ 1 & 3 & 4 \\ -1 & 1 & 2 \end{bmatrix} X = \begin{bmatrix} 4 \\ 11 \\ 1 \end{bmatrix}$

   (iii) $\begin{bmatrix} 1 & 2 & -1 \\ 3 & 3 & 1 \\ 4 & 2 & -3 \\ 1 & 0 & 2 \end{bmatrix} X = \begin{bmatrix} 2 \\ 3 \\ 4 \\ 1 \end{bmatrix}$ (iv) $\begin{bmatrix} 2 & 3 & 5 & 4 \\ 1 & 9 & 10 & 3 \\ 3 & -3 & 0 & 5 \end{bmatrix} X = \begin{bmatrix} 2 \\ 3 \\ 0 \end{bmatrix}$ (35)

ME685 (2017) Assignment 2

(Full marks = 100)

Deadline:
Soft complete version (zip and pdf) with codes— 19 Jun 12:00;
Hard copy without codes— 19 Jun 14:00.

1. **Problem for variable data sets.**
   Given four data points, determine the interpolating cubic polynomial using

   (a) the monomial basis,

   (b) the Lagrange basis,

   (c) the Newton basis.

   Show that the three representations give the same polynomial.
   Suggested data: $(-1, 4), (0, 3), (2, 7), (8, 11)$. (20)

2. **Problem for variable data sets.**
   Use Richardson extrapolation to improve the estimate of the first derivative of a function $f(x)$ at a given point. Compare the predicted value with the actual analytical derivative.
   Suggested case:

$$f(x) = \frac{\sin(2x + \pi/3)\sqrt{3x^2 + 2x - 4}}{\ln(2x + 4)} \quad \text{at} \quad x = 2\,.$$

(15)

3. **Problem for variable data sets.**
   Write a programme to approximate any given function using an 8th degree interpolating polynomial. With the same data, develop a cubic spline approximation and compare the two. Which method gives a better representation in the given domain?
   Suggested case:

$$p(t) = \cos(10\cos^{-1} t + \pi/6) + \ln(2t + 5) \quad \text{over} \quad [-0.3, 0.8]\,.$$

(15)

4. Consider the problem of finding a root of the function $h(x) = 30 \sin x + x^3 - 5$ with two points 0 and 1.44 identified with opposite signs of the function. (Up to two places of decimal is enough.)

   (a) Use the method of false position with these two points as starting values to find the root.

   (b) Use the Newton-Raphson method, starting with 0, to find the root and note the comparative performance.

   (c) Attempt the Newton-Raphson method, starting with 1.42, 1.44 and 1.46, and explain your experience of the first four iterations in each case.

(20)

5. Starting from $\mathbf{x} = [1 \;\; 1 \;\; 1]^T$, solve the system of equations

$$16x_1^4 + 16x_2^4 + x_3^4 = 15, \quad x_1^2 + x_2^2 + x_3^2 = 3, \quad x_1^3 - x_2 = 0$$

by Newton's method. (10)

6. Consider the function $f : R^2 \rightarrow R$ defined by

$$f(\mathbf{x}) = 2x_1^2 - x_1^4 + x_1^6/6 + x_1 x_2 + x_2^2/2 \;.$$

Find out the stationary points and classify them as minimum, maximum and saddle points. Using a penalty for constraint violation, minimize $f(x)$ in the domain defined by

$$2x_1^2 - 12x_1 - x_2 + 23 \leq 0\,.$$

Verify and display your results with a contour plot. (20)

ME685 (2017) Assignment 3

(Full marks = 100)

Deadline:
Soft complete version (zip and pdf) with codes— 29 Jun 12:00;
Hard copy without codes— 29 Jun 14:00.

1. **Problem for variable data sets.**
   Bracket a minimum of function $f(x)$ and use bisection method to locate the minimum precisely.
   Suggested function: $f(x) = x^4 - 14x^3 + 60x^2 - 70x$. (15)

2. We wish to fit the model function $f(t, \mathbf{x}) = x_1 + x_2 t + x_3 t^2 + x_4 e^{x_5 t}$ to the following data.

t	0	0.25	0.50	0.75	1	1.25	1.5	1.75	2
f	20	51.58	68.73	75.46	74.36	67.09	54.73	37.98	17.28

   The problem is to find the optimal values of x_i's that minimize the error from the data points in the least square sense. Use the following two methods to solve the problem.

   (a) Use Levenberg-Marquardt method to solve the nonlinear least squares problem (in five parameters) as elaborated in class. (15)

   (b) Notice that the problem becomes a linear least square problem (in four parameters) if we assume a value for x_5. Hence assume a **zero** value of x_5 initially and solve the linear problem for the remaining x_i's, perhaps using a solver developed for the previous assignments. Evaluate the net error as $g(x_5)$ which is implicitly a function of x_5. This becomes one function evaluation. Use the one-dimensional minimizer developed for problem 1 to solve for the optimal value of x_5 and the corresponding values of the other parameters (x_1 to x_4). (15)

3. **Problem for variable data sets.**
   Implement the power method to find the dominant eigenvalue and the corresponding eigenvector of the matrix. After finding the dominant eigenvalue, deflate the matrix and find the second largest eigenvalue. (15)

   Suggested data: $\begin{bmatrix} 2 & 3 & 2 & 4 \\ 3 & 3 & 4 & 1 \\ 2 & 6 & 1 & 2 \\ 4 & 1 & 2 & 0 \end{bmatrix}$.

4. **Problem for variable data sets.**
Compute all the roots of the polynomial of the form $p(\lambda) = \lambda^n + a_{n-1}\lambda^{n-1} + ... + a_1\lambda + a_0$ by applying the QR method on the companion matrix

$$\begin{bmatrix} 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & 1 & \dots & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & 1 \\ -a_0 & -a_1 & -a_2 & \dots & -a_{n-1} \end{bmatrix},$$

the eigenvalues of which are the same as the roots of the polynomial. (15)
Suggested case: $p(x) = x^4 - 13x^3 + 35x^2 - 40x + 24$.

5. Consider the spring-mass system shown in the following figure,

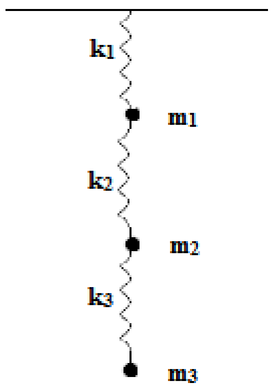


Figure 1: Spring-Mass System of Q.5.

where $m_1 = 2; m_2 = 3; m_3 = 4; k_1 = k_2 = k_3 = 1$. Derive the system of equations for the vibration of the masses. Find out the natural frequencies and vibration modes of the system by formulating the generalized eigenvalue problem. Combine power method and the inverse iteration method to your advantage. You may use shift and deflation wherever required. (25)

ME685 (2017) Assignment 4

(Full marks = 100)

Deadline:
Soft complete version (zip and pdf) with codes— 13 Jul 12:00;
Hard copy without codes— 13 Jul 14:00.

1. Use trapezoidal rule to evaluate definite integrals of test functions and compare results with different values of step size h. Plot the variation of absolute error against the step size. Implement Romberg integration and examine its effectiveness and efficiency. (15)
   Suggested data: $\int_0^1 \frac{4}{1+x^2} dx$. [The analytical solution is π.]

2. Using Gaussian quadrature, evaluate the elliptic integral

   $$K(x) = \int_0^{\pi/2} \frac{d\theta}{\sqrt{1 - x^2 \sin^2 \theta}}$$

   for several values of x in the interval $0 \leq x < 1$ and plot $K(x)$ smoothly. (15)

3. Evaluate the double integral $\int \int e^{-xy}\, dx\, dy$ over

   (a) the unit square, and

   (b) the quarter of the unit circle in the first quadrant.

   [Gauss quadrature with 2×2, 2×3, 3×2 or 3×3 grid of quadrature points may be used.] (10)

4. Use Euler's, Improved Euler's and fourth order Runge-Kutta methods with step size $h = 0.1$ (in all the cases) to solve the initial value problem $y' = (4x + y - 1)^2, y(0) = -1$ for $0 \leq x \leq 1$ and compare the results with $y = 1 - 4x + 2\tan(2x - \frac{\pi}{4})$ which is the analytical solution. (15)

5. The population dynamics of rabbits (y_1) and foxes (y_2) is given by the Lotka-Volterra predator-prey system

$$y_1' = ay_1 - by_1y_2, \quad y_2' = cy_1y_2 - dy_2.$$

For suitable values of parameters, find out the set(s) of initial conditions for which no change takes place in future, i.e. $y_1' = y_2' = 0$. For several *other* initial conditions $(y_1(0),\, y_2(0))$, work out the way rabbits and foxes grow/decay. (15)
Suggested parameter values: $a = 6$, $b = 1$, $c = 2$, $d = 8$ (in some suitable units like 'per hundred per month' etc).
Suggested initial conditions: (i) small, large; (ii) small, small; (iii) large, small; (iv) large, large; in some suitable units (like hundreds, thousands etc).

6. Consider a reaction vessel containing three chemical species with mole fractions x_1, x_2 and x_3. The first decays to form the second, while that in turn decyas to form the third. The rate coefficients for the two reactions are k_1 and k_2, respectively. Model the processes. Examine the stiffness of the system and develop an appropriate solver to simulate the processes in the vessel against time. (15)
Suggested coefficients: $k_1 = 1$; $k_2 = 1000$, 100, 10, 1, 0.1, etc.
Suggested set of initial conditions: $x_1 = 1/2$, $x_2 = 2/5$, $x_3 = 1/10$.
Hint: $x_1' = -k_1x_1$ since x_1 is only decaying.

7. Solve the two-point boundary value problem

$$y'' = 10y^3 + 3y + t^2,\ 0 \le t \le 1$$

with boundary conditions $y(0) = 0$, $y(1) = 1$ using

   (a) Shooting method, and
   (b) Finite difference method.

You may use the programs developed in the previous assignments or suitable library routines for solving the resulting **sub-problems**.

(15)