Assignments for the course
Computational Chemistry and Classical Molecular Dynamics (CCCMD):
Lectures 16 to Lecture 20 Week - 4

The assignments are listed lecture-wise and weekly. For example, Assignment (5.1) will be the first assignment after lecture 5. There are a total of 41 lectures.

16.1) State the method and the formula for estimating the maximum error in interpolating a given set of data using the Newton's forward interpolating polynomial.

16.2) What are the three elementary matrices E_1, E_2 and E_3 that are used in the Gauss elimination method? For an arbitrary matrix A, for which of the matrix or matrices E_i, is the relation $A E_i = E_i A$ valid?

16.3) Write a program that has subroutines which perform the tasks of each of the individual elementary matrices.

17.1) How is the problem of having a pivotal element having the value zero solved in the Gauss elimination method?

17.2) For a 3×3 matrix and a 4×4 matrix A, obtain $B = A^{-1}$ using your program. Using B as the new input, obtain $C = B^{-1}$. Mathematically, C = A, but numerically, the elements of A (A_{ij}) and C (C_{ij}) differ. What is the maximum difference between the elements A_{ij} and C_{ij}?

See how this difference changes when you use the program in double precision.

18.1) What is the difference between the inverse of a matrix and the diagonal form of the same matrix? If a matrix has its determinant with a value of zero, can it be diagonalized?

18.2) A 3×3 matrix C has the eigenvectors e_1, e_2 and e_3. These vectors can be expressed in three dimensions as, $e_1 = A_{11}\, i + A_{12}\, j + A_{13}\, k$; $e_2 = A_{21}\, i + A_{22}\, j + A_{23}\, k$ and so on, where, i, j and k are the unit vectors in three dimensions. Find the coefficients of the matrix that can express the unit vectors i, j and k in terms of e_1, e_2 and e_3.

18.3) Invert the following 3×3 matrix

$$\begin{bmatrix} 1 & 1 & 1 \\ 1 & 2 & 3 \\ 2 & -1 & -3 \end{bmatrix}$$

19.1) In a similarity transformation, $B = X^{-1} A X$, what is similar or the same between matrices A and B?

19.2) Find the largest eigenvalue of the matrix given in problem 18.3 using the program described in the lectures.

19.3) In the similarity transformation described in problem 19.1, $X^{-1} X = I$, the identity matrix. This implies that each row i of matrix X is orthogonal to all the columns of the same matrix X, other than the column i. Does this orthogonality imply linear independence? Conversely, does linear independence imply orthogonality? Give examples of vectors to illustrate your answer.

20.1) Find the best linear least square fit, $ax + b$, to the following data.

Xi	2.0	3.0	4.0	5.0	6.0	7.0	8.0	9.0	10.0	11.0
Yi	6.9	8.95	10.99	13.0	15.05	17.1	19.15	21.2	23.25	25.3

20.2) Find both the roots of the quadratic equation, $x^2 - 4 = 0$, using the Newton Raphson method. Find the roots of the cubic equation, $x^3 - 4x^2 - 4x + 16 = 0$, using a procedure similar to the one used for the quadratic equation.