ENGR20005
Numerical Methods in Engineering

Workshop 5

Part A: Pre-Lecture Problems

Please try to attempt 5.1 before Lecture 09 and 5.2 before Lecture 10.

5.1 Starting from **Lecture09M05.m** fit the Lagrange interpolating polynomial with data obtained from the function $f(x) = 1 - e^{-(x/\sigma)^2}$ sampled at

$$x = 0, 0.1, 0.3, 0.5, 0.8, 1.0, 1.1, 2.0, 3.0, 3.5, 4.0, 4.5, 4.8, 5$$

Try this for $\sigma = 0.5$ and 0.1

5.2 Use quadratic splines to interpolate data for the following points. Start from **Lecture10M01.m**. Compare with the interpolation functions you can obtain using the **interp1()** function from MATLAB.

Part B: MATLAB Livescripts

5.3 The livescript *ENGR20005_Workshop5p3.mlx* runs through the convergence of iterative methods and how to accelerate this process.

(a) Read through the livescript and understand what each command does.

(b) Modify the livescript to solve the following system of equations

$$\begin{aligned} 2x - 4y + 4z &= 12 \\ 3x + y - 8z &= 4 \\ -5x + 11y + z &= -32 \end{aligned} \tag{5.1}$$

Does the method converge? Can you explain why.

5.4 The livescript *ENGR20005_Workshop5p4.mlx* runs through the use of MATLAB functions to perform least squares regression. Read through the livescript and make sure you understand what each line of code does.

5.5 The livescript *ENGR20005_Workshop5p5.mlx* runs through least squares regression.

(a) Read through the livescript and make sure you understand what each line of code does.

(b) Modify the livescript to perform quadratic and cubic least squares regression.

Part C: Problems

5.6 In the livescript *ENGR20005_Workshop5p3.mlx*, you would have seen that successive over-relaxation applied to the Gauss–Seidel method doesn't converge for all $0 < \omega < 2$. In the special case when $[A]$ is symmetric positive definite, it can be shown that $\rho([P]) < 1$ for all $0 < \omega < 2$, ensuring convergence for any initial guess $\{x\}^{(0)}$.

Consider the following system of linear equations

$$\begin{aligned} 2x - \quad y \quad\quad &= 1 \\ -x + \ 2y - \quad z &= 4 \\ -y + 2z &= 7 \end{aligned} \tag{5.2}$$

Recall that a matrix $[A]$ as positive definite if and only if

$$\{z\}^{\mathrm{T}}[A]\{z\} > 0$$

for any $\{z\} \in \mathbb{R}^n$ excluding the zero vector.

(a) Determine the matrix $[A]$ and the vector $\{c\}$.

(b) Prove that $[A]$ is positive definite.

(c) Apply the Gauss–Seidel method to solve Eq. (5.2).

(d) Apply successive over-relaxation to your answer in (c) and determine the spectral radius for $0 \leq \omega \leq 2$. Plot your results and use this to find the optimal relaxation factor ω_{opt}.

(e) Solve Eq. (5.2) using successive over-relaxation and verify that ω_{opt} is the optimal value of ω.

5.7 When determining the least squares regression, our goal is to minimise the squared error S. We do this by computing the parameters a_i such that the gradient is zero.

$$\frac{\partial S}{\partial a_i} = 0 \tag{5.3}$$

However, for complicated models, the resulting set of equations are nonlinear.

(a) Apply the Newton–Raphson method to Eq. (5.3) and show that the parameter vector $\{a\}$ can be found by the iterative formula

$$\{a\}^{(n+1)} = \{a\}^{(n)} - ([H]^{(n)})^{-1}\{d\}^{(n)} \tag{5.4}$$

where $d_i = \partial S/\partial a_i$ and $[H]$ is the *Hessian matrix* of S, given by

$$[H] = \begin{bmatrix} \frac{\partial^2 S}{\partial a_1^2} & \frac{\partial^2 S}{\partial a_1 \partial a_2} & \cdots & \frac{\partial^2 S}{\partial a_1 \partial a_n} \\ \frac{\partial^2 S}{\partial a_2 \partial a_1} & \frac{\partial^2 S}{\partial a_2^2} & \cdots & \frac{\partial^2 S}{\partial a_2 \partial a_n} \\ \vdots & & \ddots & \vdots \\ \frac{\partial^2 S}{\partial a_n \partial a_1} & \frac{\partial^2 S}{\partial a_n \partial a_2} & \cdots & \frac{\partial^2 S}{\partial a_n^2} \end{bmatrix} \tag{5.5}$$

(b) Show that another way of writing Eq. (5.4) is

$$[H]^{(n)}(\{a\}^{(n+1)} - \{a\}^{(n)}) = -\{d\}^{(n)} \tag{5.6}$$

From a computational perspective, why is Eq. (5.6) a better way of writing Eq. (5.4)?

(c) Apply Eq. (5.6) to a power function $y = ax^b$.

(d) Write a MATLAB function (`.m` file) to implement your answer to (c).

(e) Consider the following data set

x	y
0.7860	1.0113
1.5916	4.4279
2.1917	11.4360
2.9606	22.2894
3.6441	37.0793
4.2554	56.9877
5.0294	81.0653

Use your answer to part (d) to fit a power function of the form $y = ax^b$. Compare your answer with the linearization of nonlinear relationship technique you learnt in lectures.

5.8 * From lectures, you would have seen that fixed point iteration and the Newton–Raphson method have linear and quadratic orders of convergence respectively. In case you don't believe it, we'll conduct some numerical experiments to verify this.

Hopefully, you still have your MATLAB functions from workshops 2 and 3. In case you don't, the data is provided in *ENGR20005_Workshop5p6.mat*.

(a) The error at step i is given by

$$E_i = |x_i - x_r|$$

where x_r is the root. Write a MATLAB function (`.m` file) that determines the error of each method.

(b) Plot the error of the $(i+1)^{\text{st}}$ iteration against the error in the i^{th} iteration. i.e. E_{i+1} vs E_i.

(c) The theoretical analyses conducted in lectures have shown that these methods obey a power law, $E_{i+1} = aE_i^b$. Perform a log transformation on the data and fit a linear curve to determine the parameters a and b.

(d) Check your answer to part (c) with MATLAB's inbuilt functions and your answer to Q. 5.7. Are there any differences? Do you know why?

(e) Do your results here match with what you have seen in lectures? What can you conclude about the order of convergence of the Secant and Bracketing methods?