# ENGR20005
# Numerical Methods in Engineering

Workshop 8

## Part A: Pre-Lecture Problems

Please try to attempt 8.1 before Lecture 15 and 8.2 before Lecture 16.
Don't worry if you cannot finish them. I plan to go through them in the "live" lectures

8.1 For many engineering applications, insights into the physics of the problem can be obtained by solving differential equations. A very simple form of a differential equation is

$$\frac{df}{dx} = r(x). \tag{8.1}$$

In a typical problem, you are usually given $r(x)$ and asked to find $f(x)$. You also usually know the value of $f(x)$ at the boundaries of the domain $x \in [a, b]$, e.g. $f(x = a) = 1$. In the example below, we will show you how you can use derivative matrices covered in Lecture 14 to solve Eq. (8.1). This is a very similar but simplified problem compared to the the examples in Lecture 15.

In the exercise below, we will show you how you can find an approximation for $f(x)$ by solving Eq. (8.1). We will "cheat" a bit by calculating $r(x)$ from a known $f(x)$ and use $r(x)$ to get back $f(x)$. This is only for illustrative purposes to show you that the method works. In a real life problem, you usually do not know $f(x)$ but you would know $r(x)$ and you would use it in Eq. (8.1) to get the unknown $f(x)$.

Let's consider the function

$$f(x) = e^{-x^2}. \tag{8.2}$$

For the $f(x)$ given in Eq. (8.2), the value of $f(x)$ at $x = 0$ is $f(x = 0) = 1$.

(a) Differentiate this function and show that

$$df/dx = -2xe^{-x^2}. \tag{8.3}$$

(b) Use the code that constructs the derivative matrix from Workshop 7.2 (using 1st order forward and backward and 2nd order central difference approximation) and calculate the derivative matrix, $[D]$, to differentiate $f(x)$ for an equally spaced mesh for $x \in [0, 5]$.

(c) Use $[D]$, to calculate the derivative of $f(x)$,

$$\{f'\} = [D]\{f\}, \tag{8.4}$$

where $\{f'\}$ is a column vector of the derivatives at the grid points and $\{f\}$ is a column vector consisting of the value of the function at the grid points. Check with Eq. (8.3) to get confidence that your $[D]$ matrix is correct.

(d) Now see if you can solve Eq. (8.4) to get back $f(x)$ i.e. compute

$$\{f\} = [D]^{-1}\{f'\}. \tag{8.5}$$

If you like you can use the \ operator or the `linsolve()`, `inv()` functions in MATLAB. Can you find $\{f\}$? Can you explain why?

(e) Now try to solve Eq. (8.4) but now specify the condition at $x = 0$, i.e. $f(x = 0) = 1$. Can you get a solution for $f(x)$? What is the difference between 8.1d and 8.1e? Can you explain why you can get the solution with one but not the other?

8.2 In the previous example, you learnt how to solve differential equation in one dimension, i.e. the solution $f(x)$ only depends on one variable $x$. However in many engineering problems, the solution depends on more than one variable, i.e. they are of two (or more!) dimensions. An example of a two-dimensional differential equation which you might be asked to solve to get a solution to an engineering problem would look something like

$$u_x = \frac{\partial u}{\partial x} = p(x, y). \tag{8.6}$$

$\partial/\partial x$ is the derivative in the $x$ direction assuming that $y$ is constant. In a typical problem, you are usually given $p(x, y)$ and asked to find $u(x, y)$. Note that $p(x, y)$ and $u(x, y)$ are usually functions of two variables, $x$ and $y$. You also usually know the value of $u(x, y)$ at the boundaries of the domain $x \in [a, b]$, $y \in [c, d]$, e.g. $u(x = a, y) = g(y)$.

In the exercise below, similar to 8.1, we will show you how you can find $u(x, y)$ by solving Eq. (8.6). We will "cheat" a bit by calculating $p(x, y)$ from a known $u(x, y)$ and use $p(x, y)$ to get back $u(x, y)$. Again, like the question above, this is only for illustrative purposes to show you that the method works. In a real life problem, you usually do not know $u(x, y)$ but you would know $p(x, y)$ and you would use it in Eq. (8.6) to find the unknown $u(x, y)$.

In this question, you will first learn how to calculate partial derivatives of a two-dimensional function using matrix-vector multiplication

$$\{u_x\} = [D_x]\{u\}.$$

$\{u\}$ is a column vector of two-dimensional function $u(x,y)$, $\{u_x\}$ is a column vector of $\partial u(x,y)/\partial x$ and $[D_x]$ is the derivative matrix in the $x$ direction. You will then use $[D_x]$ to solve Eq. (8.6)

(a) As was shown in lectures, the derivative of a function $u_x(x) = \partial u/\partial x(x)$ of a function $u(x)$ can be calculated using the second order central, forward and backward difference schemes

$$\begin{aligned} u_x(x_i) &= \frac{u_{i+1} - u_{i-1}}{2\Delta_x} \\ u_x(x_0) &= \frac{u_1 - u_0}{\Delta_x} \\ u_x(x_{N_x-1}) &= \frac{u_{N_x-1} - u_{N_x-2}}{\Delta_x}. \end{aligned}$$

The above equations can be written more concisely in matrix form as $\{u_x\} = [D_x]\{u\}$. The explicit structure for the matrix equations for $N_x = 2$, 3 and $N_x = 6$ are shown below

$$\{u_x\} = \begin{Bmatrix} u_x(x_0) \\ u_x(x_1) \end{Bmatrix} = \frac{1}{2\Delta_x}\begin{bmatrix} \mathbf{-2} & \mathbf{2} \\ \mathbf{-2} & \mathbf{2} \end{bmatrix}\begin{Bmatrix} u_0 \\ u_1 \end{Bmatrix}$$

$$\{u_x\} = \begin{Bmatrix} u_x(x_0) \\ u_x(x_1) \\ u_x(x_2) \end{Bmatrix} = \frac{1}{2\Delta_x}\begin{bmatrix} \mathbf{-2} & \mathbf{2} & 0 \\ \mathbf{-1} & 0 & \mathbf{1} \\ 0 & \mathbf{-2} & \mathbf{2} \end{bmatrix}\begin{Bmatrix} u_0 \\ u_1 \\ u_2 \end{Bmatrix}$$

$$\{u_x\} = \begin{Bmatrix} u_x(x_0) \\ u_x(x_1) \\ u_x(x_2) \\ u_x(x_3) \\ u_x(x_4) \\ u_x(x_5) \end{Bmatrix} = \frac{1}{2\Delta_x}\begin{bmatrix} \mathbf{-2} & \mathbf{2} & 0 & 0 & 0 & 0 \\ \mathbf{-1} & 0 & \mathbf{1} & 0 & 0 & 0 \\ 0 & \mathbf{-1} & 0 & \mathbf{1} & 0 & 0 \\ 0 & 0 & \mathbf{-1} & 0 & \mathbf{1} & 0 \\ 0 & 0 & 0 & \mathbf{-1} & 0 & \mathbf{1} \\ 0 & 0 & 0 & 0 & \mathbf{-2} & \mathbf{2} \end{bmatrix}\begin{Bmatrix} u_0 \\ u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \end{Bmatrix} \tag{8.7}$$

(b) Write a MATLAB program to compute the $[D]$ matrix and use it to calculate and plot the derivative of

$$u(x) = e^{-x^2} \tag{8.8}$$

by performing the matrix multiplication, $\{u_x\} = [D]\{u\}$, in MATLAB. Use the domain $x \in [0, 5]$. For $N_x = 6$

$$[D] = \frac{1}{2\Delta_x}\begin{bmatrix} \mathbf{-2} & \mathbf{2} & 0 & 0 & 0 & 0 \\ \mathbf{-1} & 0 & \mathbf{1} & 0 & 0 & 0 \\ 0 & \mathbf{-1} & 0 & \mathbf{1} & 0 & 0 \\ 0 & 0 & \mathbf{-1} & 0 & \mathbf{1} & 0 \\ 0 & 0 & 0 & \mathbf{-1} & 0 & \mathbf{1} \\ 0 & 0 & 0 & 0 & \mathbf{-2} & \mathbf{2} \end{bmatrix}$$

Check that your answer is correct by comparing with the exact solution $u_x(x) = -2xe^{-x^2}$. How many grid points do you need to use to get a good approximation for $u_x(x)$?

(c) Suppose now that you have a two-dimensional function

$$u(x, y) = y^3 e^{-x^2} \tag{8.9}$$

For this exercise, we will assume the domain $y \in [0, 1]$ and $x \in [0, 5]$. Write a computer program to calculate $\partial u/\partial x$ using a derivative matrix. For this part of the exercise, assume that the data for $u(x, y)$ is organised where the data in the $y$ direction is the rows of the matrix and $x$ is in columns. For example, for a grid with $N_x$ and $N_y$ data points, the data for $u(x, y)$ will be organised as follows

$$[u] = \begin{bmatrix} u(x_0, y_0) & u(x_1, y_0) & .... & u(x_{Nx-1}, y_0) \\ u(x_0, y_1) & u(x_1, y_1) & .... & u(x_{Nx-1}, y_1) \\ \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots \\ u(x_0, y_{Ny-1}) & u(x_1, y_{Ny-1}) & .... & u(x_{Nx-1}, y_{Ny-1}) \end{bmatrix}$$

For $N_x = 6$ and $N_y = 3$ this matrix is

$$[u] = \begin{bmatrix} u(x_0, y_0) & u(x_1, y_0) & u(x_2, y_0) & u(x_3, y_0) & u(x_4, y_0) & u(x_5, y_0) \\ u(x_0, y_1) & u(x_1, y_1) & u(x_2, y_1) & u(x_3, y_1) & u(x_4, y_1) & u(x_5, y_1) \\ u(x_0, y_2) & u(x_1, y_2) & u(x_2, y_2) & u(x_3, y_2) & u(x_4, y_2) & u(x_5, y_2) \end{bmatrix} \tag{8.10}$$

For this part of the question, write a MATLAB program that would take the data for every row (since you are only differentiating in the $x$ direction and assuming $y$ is constant and apply your derivative matrix for every row. Compare with the analytical solution

$$\frac{\partial u}{\partial x} = -2xy^3 e^{-x^2} \tag{8.11}$$

(d) For reasons that should become apparent latter on, we would like to organise the data for $u(x, y)$ in a one-dimensional vector where we start with the first row and turn into a column followed be the 2nd row and so on. For the matrix in Eq. (8.10) when turn into a vector should look like

$$
\{u\} = \left\{ \begin{matrix} u(x_0, y_0) \\ u(x_1, y_0) \\ u(x_2, y_0) \\ u(x_3, y_0) \\ u(x_4, y_0) \\ u(x_5, y_0) \\ u(x_0, y_1) \\ u(x_1, y_1) \\ u(x_2, y_1) \\ u(x_3, y_1) \\ u(x_4, y_1) \\ u(x_5, y_1) \\ u(x_0, y_2) \\ u(x_1, y_2) \\ u(x_2, y_2) \\ u(x_3, y_2) \\ u(x_4, y_2) \\ u(x_5, y_2) \end{matrix} \right\} \tag{8.12}
$$

and for $N_x = 6$ and $N_y = 2$ the vector would look like

$$
\{u\} = \left\{ \begin{matrix} u(x_0, y_0) \\ u(x_1, y_0) \\ u(x_2, y_0) \\ u(x_3, y_0) \\ u(x_4, y_0) \\ u(x_5, y_0) \\ u(x_0, y_1) \\ u(x_1, y_1) \\ u(x_2, y_1) \\ u(x_3, y_1) \\ u(x_4, y_1) \\ u(x_5, y_1) \end{matrix} \right\} \tag{8.13}
$$

Convince yourself that the derivative matrix to calculate $u_x$ if $u(x, y)$ is organised as a vector for $N_x = 6$ and $N_y = 2$ (see Eq. (8.13)) is given below

$$\begin{Bmatrix} u_x(x_0,y_0)\\ u_x(x_1,y_0)\\ u_x(x_2,y_0)\\ u_x(x_3,y_0)\\ u_x(x_4,y_0)\\ u_x(x_5,y_0)\\ u_x(x_0,y_1)\\ u_x(x_1,y_1)\\ u_x(x_2,y_1)\\ u_x(x_3,y_1)\\ u_x(x_4,y_1)\\ u_x(x_5,y_1) \end{Bmatrix} = \frac{1}{2\Delta_x} \begin{bmatrix} \mathbf{-2} & \mathbf{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\ \mathbf{1} & 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\ 0 & \mathbf{1} & 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & \mathbf{1} & 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & \mathbf{1} & 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & \mathbf{-2} & \mathbf{2} & 0 & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{-2} & \mathbf{2} & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 & \mathbf{1} & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 & \mathbf{1} & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 & \mathbf{1} & 0\\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 & \mathbf{1}\\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{-2} & \mathbf{2} \end{bmatrix} \begin{Bmatrix} u(x_0,y_0)\\ u(x_1,y_0)\\ u(x_2,y_0)\\ u(x_3,y_0)\\ u(x_4,y_0)\\ u(x_5,y_0)\\ u(x_0,y_1)\\ u(x_1,y_1)\\ u(x_2,y_1)\\ u(x_3,y_1)\\ u(x_4,y_1)\\ u(x_5,y_1) \end{Bmatrix}$$

Note that for $N_x = 6$ and $N_y = 2$

$$[D_x] = \frac{1}{2\Delta_x} \begin{bmatrix} \mathbf{-2} & \mathbf{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\ \mathbf{1} & 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\ 0 & \mathbf{1} & 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & \mathbf{1} & 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & \mathbf{1} & 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & \mathbf{-2} & \mathbf{2} & 0 & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{-2} & \mathbf{2} & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 & \mathbf{1} & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 & \mathbf{1} & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 & \mathbf{1} & 0\\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 & \mathbf{1}\\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{-2} & \mathbf{2} \end{bmatrix}$$

(e) The result above can be generalized to calculate the partial derivatives on a $N_x \times N_y$ mesh

$$u_x(x_i, y_i) = [I] \otimes [D]\{u\}\{u_x\} = [I] \otimes [D]\{u\} \tag{8.14}$$

where $[D_x] = [I] \otimes [D]$. $\otimes$ is some operation on the one-dimensional derivative matrix $[D]$ and the identity matrix $[I]$ that produces the correct two-dimensional derivative matrix. The operation $\otimes$ on two matrices is called the *Kronecker product* which is implemented in MATLAB using the `kron()` function. For an $m \times n$ matrix $[A]$ and a $p \times q$ matrix $[B]$ is defined as

$$[A] \otimes [B] = \begin{pmatrix} a_{11}[B] & \cdots & a_{1n}[B] \\ \vdots & \ddots & \vdots \\ a_{n1}[B] & \cdots & a_{nn}[B]. \end{pmatrix} \tag{8.15}$$

Write a computer program that calculates the $u_x$ if the data for $u(x, y)$ is arranged in column vector form e.g. Eq. (8.13). Prove that this program works by computing

$$\{u_x\} = [D_x]\{u\}$$

and compare with Eq. (8.9).

(f) Now see if you can get back $u(x, y)$ by solving

$$[D]\{u\} = \{p\} \tag{8.16}$$

where $\{p\}$ is a vector of values from Eq. Eq. (8.9). Can you find $\{u\}$? Can you explain why?

(g) Now try to solve Eq. (8.16) but now specify the condition at $x = 0$, i.e. $u(x = 0, y) = y^3$. Can you get a solution for $u(x, y)$? What is the difference between 8.2f and 8.2g? Can you explain why you can get the solution, $u(x, y)$, with one but not the other?

## Part B: MATLAB Livescripts

8.3 The livescript *ENGR20005_Workshop8p3.mlx* runs through the use of MATLAB functions to differentiate functions.

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

(b) Modify the livescript to take derivatives of the functions

i. $f(x) = \cos(x^2)$

ii. $\phi(x, y) = \exp(x^2 + y^2)$

8.4 The livescript *ENGR20005_Workshop8p4.mlx* runs through numerical differentiation.

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

(b) Modify the livescript to evaluate the derivative of

$$f(x) = \cos(x^2) \tag{8.17}$$

between $0 \le x \le 1$. Use as many points as you deem fit.

8.5 The livescript *ENGR20005_Workshop8p5.mlx* runs through spectral differentiation.

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

(b) Modify the livescript to evaluate the derivative of Eq. (8.17) between $-1 \leq x \leq 1$. Use as many points as you deem fit.

## Part C: Problems

8.6 In Workshop 6 you tested different interpolation schemes to interpolate the data for temperature in a lake given by the table below.

| $z$ depth of lake (m) | $T(^oC)$ |
|---|---|
| 0.0 | 22.8 |
| 2.3 | 22.8 |
| 4.9 | 22.8 |
| 9.1 | 20.6 |
| 13.7 | 13.9 |
| 18.3 | 11.7 |
| 22.9 | 11.1 |
| 27.2 | 11.1 |

A thermocline is a region in the lake where the warmer upper water (epilimnion) is prevented from mixing with the water at a deeper level (hypolimnion). The thermocline essentially prevents the interchange of nutrients between the epilimnion and hypolimnion and produces two separate environments for the inhabitants of the lake. The location of the thermocline can be defined as the inflection point of the temperature-depth curve, that is the point where $d^2T/dz^2 = 0$.

Use the central difference scheme to calculate $d^2T/dz^2$. Plot $d^2T/dz^2$ vs $z$ and see if you can identify the location of the thermocline by just looking at the graph (ie look at the value $z$ where $d^2T/dz^2 = 0$ ). Note that you could have used root finding methods to find $z$ where $d^2T/dz^2 = 0$. But you do not need to do that for this question.

8.7 (a) * For each of the following functions, use a 10 point central difference and spectral difference method to approximate the derivative for $x \in [-1, 1]$.

i. $f_1(x) = |x^3|$

ii. $f_2(x) = \exp(-x^{-2})$

iii. $f_3(x) = \frac{1}{1+x^2}$

iv. $f_4(x) = x^{10}$

Compare your answers with the exact derivatives

i. $f_1'(x) = 3x|x|$

ii. $f_2'(x) = \frac{2f_2(x)}{x^3}$

iii. $f_3'(x) = -2xf_3(x)^2$

iv. $f_4'(x) = 10x^9$

(b) * Repeat the previous problem with $N = 1, \ldots, 30$ points and determine error in each case. Plot the error as a function of the number of points. Compare the convergence of each method.

8.8 Determine the truncation error of the following schemes

(a) 4th order central difference

$$\left(\frac{df}{dx}\right)_i = \frac{f(x_{i-2}) - 8f(x_{i-1}) + 8f(x_{i+1}) - f(x_{i+2})}{12\Delta}$$

(b) 4th order Padé scheme

$$\left(\frac{df}{dx}\right)_{i-1} + 4\left(\frac{df}{dx}\right)_i + \left(\frac{df}{dx}\right)_{i+1} = \frac{3[f(x_{i+1}) - f(x_{i-1})]}{\Delta}$$

(c) 6th order Padé scheme

$$\left(\frac{df}{dx}\right)_{i-1} + 3\left(\frac{df}{dx}\right)_i + \left(\frac{df}{dx}\right)_{i+1} = \frac{f(x_{i+2}) + 28f(x_{i+1}) - 28f(x_{i-1}) - f(x_{i-2})}{12\Delta}$$

8.9 The central difference formula is defined as

$$\left(\frac{df}{dx}\right)_i = \frac{f(x_{i+1}) - f(x_{i-1})}{2\Delta} \tag{8.18}$$

(a) For exact derivatives, the product rule is given by

$$\frac{d(fg)}{dx} = f\frac{dg}{dx} + g\frac{df}{dx} \tag{8.19}$$

Does this hold with a central difference scheme?

(b) Show that

$$\left(\frac{d(fg)}{dx}\right)_i = \bar{f}_i\left(\frac{dg}{dx}\right)_i + \bar{g}_i\left(\frac{df}{dx}\right)_i \tag{8.20}$$

where the overbar denotes the average over the adjcent elements.

$$\bar{f}_i = \frac{1}{2}[f(x_{i+1}) + f(x_{i-1})]$$

8.10 Consider the function

$$f(\xi) = \xi^7 \tag{8.21}$$

(a) Use spectral differentiation to determine the derivative of Eq. (8.21) in the interval $\xi \in [-1, 1]$.

(b) Determine a mapping from the interval $x \in [2, 10]$ to the standard interval $\xi \in [-1, 1]$.

(c) Use your answer in part (b) and the chain rule to determine the derivative of

$$g(x) = x^7$$

in the interval $x \in [2, 10]$.