

PHYS516 ASSIGNMENT 1—COMPUTING & MATH PREPARATION

Due January 18 (Wed), 2023

Part 1: Set Up a Computing Environment (This Part Will Not Be Graded)

In the subsequent assignments, you will need to edit, compile and run C programs. In this part, you will *compile and run the accompanying C program, [mean.c](#), on a computer of your choice (e.g., your laptop), so that you are prepared for future homeworks (no need to submit anything for this part)*. For example, this is what I typed on my MacBook terminal (blue font) as well as output from the program (gray font):

```
$ cc -o mean mean.c -lm
$ ./mean
Input the number of MC trials
1000000
MC estimate for PI = 3.141064
```

Part 2: Write Like a Computational Scientist (Only This Part Will Be Graded)

(Goal) This assignment warms you up for subsequent assignments throughout the semester. In some of the assignments, you will be asked to derive mathematical formulae, in which it is required to clearly state all assumptions and explicitly explain all logical inference steps. The goal of this assignment is to learn how to formally write a logical proof, which you will use for completing the assignments in this class as well as for writing your thesis and journal papers as a professional computational scientist.

(Preparation) Read *Chapter 1.5 of Discrete Mathematics and Its Applications* (by K. H. Rosen, McGraw-Hill, [rosen-proof.pdf](#) in the assignment package) and learn the style of proof in the examples. (For the definitions of some terminologies, please see my lecture note on “logic and proof”, [Logic.pdf](#).) In your future assignments, you will need to write your proofs at the level of example 14 on page 1-64 (do not just write equations without defining all symbols and explaining their logical connections in English). In particular, each step of your proof should be one of the legitimate inference rules listed in Tables 1 and 2 in Rosen’s textbook. See also the lecture note on “Minimal introduction to linear algebra”, [MinLinAlg.pdf](#). Some useful tips are found in assignment guidelines, [AsgnGuide.pdf](#), for useful tips.

(Assignment) For a 2×2 matrix

$$\mathbf{A} = \begin{bmatrix} a & b \\ b & a \end{bmatrix}, \quad (1)$$

where a and b are real numbers, derive a closed formula for its n -th power \mathbf{A}^n (n is a positive integer). *Submit your answer along with its complete readable derivation.* (This problem may be too easy, but just writing the answer is not sufficient. You need to describe every derivation step in your own words and equations.)

(Hint) The derivation steps are outlined below. This is just to give you an idea. Do not refer to these equations and just fill the gaps in your submission. Your derivation must be self-contained (e.g., all symbols need be defined before used) and understandable on its own.

Consider the eigenvalue problem,

$$\begin{bmatrix} a & b \\ b & a \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} = \varepsilon \begin{bmatrix} u \\ v \end{bmatrix} \quad (2)$$

or equivalently

$$\begin{bmatrix} \varepsilon - a & -b \\ -b & \varepsilon - a \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \quad (3)$$

where ε is an eigenvalue and

$$\begin{bmatrix} u \\ v \end{bmatrix}$$

is the corresponding eigenvector.

For nontrivial solutions (*i.e.*, other than $u = v = 0$), the determinant of the matrix in Eq. (3) should be zero. (Otherwise, one can invert Eq. (3) to obtain $u = v = 0$.) Hence,

$$\begin{vmatrix} \varepsilon - a & -b \\ -b & \varepsilon - a \end{vmatrix} = 0. \quad (4)$$

Let ε_+ and ε_- be the two solutions (*i.e.*, eigenvalues) of Eq. (4) and

$$\begin{bmatrix} u_+ \\ v_+ \end{bmatrix} \text{ and } \begin{bmatrix} u_- \\ v_- \end{bmatrix}$$

be the corresponding eigenvectors that satisfy Eq. (2).

Now, define a 2×2 matrix,

$$U = \begin{bmatrix} u_+ & u_- \\ v_+ & v_- \end{bmatrix}. \quad (5)$$

Equation (2) for the two solutions can be combined into a matrix form as

$$\mathbf{A}U = U\mathbf{D} \quad (6)$$

or

$$\mathbf{A} = U\mathbf{D}U^{-1}, \quad (7)$$

where we have defined a diagonal matrix as

$$\mathbf{D} = \begin{bmatrix} \varepsilon_+ & 0 \\ 0 & \varepsilon_- \end{bmatrix}. \quad (8)$$

The n -th power of \mathbf{A} is then obtained as

$$\mathbf{A}^n = (U\mathbf{D}U^{-1})^n = U\mathbf{D}^nU^{-1}. \quad (9)$$

(Comment) While this assignment is rather simple, this is a specific example of the spectral method, or *eigen decomposition* in Eq. (7), that we will continue to use throughout the class in order to evaluate various functions $f(\mathbf{A})$ of matrix \mathbf{A} .