PHYS 516: METHODS OF COMPUTATIONAL PHYSICS

A Assignment 1- Writing like a Computational Scientist

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January 18, 2017

1 Problem

Given a 2×2 matrix

$$\boldsymbol{A} = \begin{bmatrix} a & b \\ b & a \end{bmatrix} \tag{1}$$

where a and b are real numbers, derive a closed form expression for its n^{th} power $\boldsymbol{A}^n$.

2 Solution

Consider the Eigenvalue problem,

$$\boldsymbol{A}\boldsymbol{u} = \lambda\boldsymbol{u} \tag{2}$$

where A is the given matrix, λ is the eigenvalue, and $\boldsymbol{u} = \begin{bmatrix} u \\ v \end{bmatrix}$ is the corresponding eigenvector. Eq(1) can be equivalently written as

$$\boldsymbol{A}\boldsymbol{u} - \lambda\boldsymbol{u} = 0 \tag{3}$$

$$(\boldsymbol{A} - \lambda\boldsymbol{I})\boldsymbol{u} = 0 \tag{4}$$

where $\boldsymbol{I}$ is the identity matrix of the same dimensions as $\boldsymbol{A}$. For nontrivial solutions $(u = v \neq 0)$, the matrix on the LHS must be singular. Mathematically,

$$det(\boldsymbol{A} - \lambda I) = 0 \tag{5}$$

Substituting the matrix given in this problem for A, we get

$$\begin{vmatrix} a-\lambda & b \\ b & a-\lambda \end{vmatrix} = 0 \tag{6}$$

To obtain λ, let us evaluate this determinant.

$$(a-\lambda)^2 - b^2 = 0 \tag{7}$$

$$\Rightarrow \quad (a-\lambda)^2 = b^2 \tag{8}$$

$$\Rightarrow \quad a-\lambda = \pm b \tag{9}$$

$$\Rightarrow \quad \lambda = a \pm b \tag{10}$$

Therefore, there are two eigenvalues– $\lambda_+ = a + b$ and $\lambda_- = a - b$.

Let us now evaluate the eigenvector corresponding to each of these eigenvalues. Using Eq(4)

$$\begin{bmatrix} a - \lambda_+ & b \\ b & a - \lambda_+ \end{bmatrix} \begin{bmatrix} u_+ \\ v_+ \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \tag{11}$$

Plugging in the value of λ_+, we obtain the eigenvector as

$$\begin{bmatrix} u_+ \\ v_+ \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \tag{12}$$

Similarly, the eigenvector corresponding to λ_- is obtained to be

$$\begin{bmatrix} u_+ \\ v_+ \end{bmatrix} = \begin{bmatrix} 1 \\ -1 \end{bmatrix} \tag{13}$$

Now, let us define **D** as a matrix containing the eigenvalues along it's diagonal and **U** as a matrix which contains the eigenvectors as its columns, in the same order as the eigenvalues in **D**.

$$\boldsymbol{D} = \begin{bmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{bmatrix} \tag{14}$$

$$\boldsymbol{U} = \begin{bmatrix} u_+ & u_- \\ v_+ & v_- \end{bmatrix} \tag{15}$$

Hence, using Eq(2), the above two equations can be expressed together in matrix form as

$$\boldsymbol{AU} = \boldsymbol{UD} \tag{16}$$

Right-multiplying both sides by $\boldsymbol{U}^{-1}$,

$$\boldsymbol{A} = \boldsymbol{UDU}^{-1} \tag{17}$$

Therefore,

$$\boldsymbol{A}^n = \boldsymbol{UD}^n\boldsymbol{U}^{-1} \tag{18}$$

In this problem,

$$\boldsymbol{U} = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \implies \boldsymbol{U}^{-1} = 0.5 \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \tag{19}$$

Plugging in these values,

$$\begin{bmatrix} a & b \\ b & a \end{bmatrix} = 0.5 \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} a + b & 0 \\ 0 & a - b \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \tag{20}$$

Therefore,

$$\begin{bmatrix} a & b \\ b & a \end{bmatrix}^n = 0.5 \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} (a + b)^n & 0 \\ 0 & (a - b)^n \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \tag{21}$$

$$= 0.5 \begin{bmatrix} (a + b)^n + (a - b)^n & (a + b)^n - (a - b)^n \\ (a + b)^n - (a - b)^n & (a + b)^n + (a - b)^n \end{bmatrix} \tag{22}$$