

PHYS 516: Methods of Computational Physics
ASSIGNMENT 5- Quantum Dynamics Basics

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1 Problem

Given 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 form expression for its n^{th} power \mathbf{A}^n .

2 Solution

Consider the Eigenvalue problem,

$$\mathbf{A}\mathbf{u} = \lambda\mathbf{u} \quad (2)$$

where \mathbf{A} is the given matrix, λ is the eigenvalue, and $\mathbf{u} = \begin{bmatrix} u \\ v \end{bmatrix}$ is the corresponding eigenvector.

Eq(1) can be equivalently written as

$$\mathbf{A}\mathbf{u} - \lambda\mathbf{u} = 0 \quad (3)$$

$$(\mathbf{A} - \lambda\mathbf{I})\mathbf{u} = 0 \quad (4)$$

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

$$\det(\mathbf{A} - \lambda\mathbf{I}) = 0 \quad (5)$$

Substituting the matrix given in this problem for \mathbf{A} , we get

$$\begin{vmatrix} a - \lambda & b \\ b & a - \lambda \end{vmatrix} = 0 \quad (6)$$

To obtain λ , let us evaluate this determinant.

$$(a - \lambda)^2 - b^2 = 0 \quad (7)$$

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

$$\Rightarrow a - \lambda = \pm b \quad (9)$$

$$\Rightarrow \lambda = a \pm b \quad (10)$$

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)

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

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

$$\begin{bmatrix} u_+ \\ v_+ \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \quad (12)$$

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

$$\begin{bmatrix} u_- \\ v_- \end{bmatrix} = \begin{bmatrix} 1 \\ -1 \end{bmatrix} \quad (13)$$

Now, let us define \mathbf{D} as a matrix containing the eigenvalues along its diagonal and \mathbf{U} as a matrix which contains the eigenvectors as its columns, in the same order as the eigenvalues in \mathbf{D} .

$$\mathbf{D} = \begin{bmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{bmatrix} \quad (14)$$

$$\mathbf{U} = \begin{bmatrix} u_+ & u_- \\ v_+ & v_- \end{bmatrix} \quad (15)$$

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

$$\mathbf{A}\mathbf{U} = \mathbf{U}\mathbf{D} \quad (16)$$

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

$$\mathbf{A} = \mathbf{U}\mathbf{D}\mathbf{U}^{-1} \quad (17)$$

Therefore,

$$\mathbf{A}^n = \mathbf{U}\mathbf{D}^n\mathbf{U}^{-1} \quad (18)$$

In this problem,

$$\mathbf{U} = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \implies \mathbf{U}^{-1} = 0.5 \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \quad (19)$$

Plugging in these values,

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

Therefore,

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

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