Diagonalization

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1 Main Idea

Given a matrix $A \in M(n \times n)$, is it possible to find a basis in which the associated linear transformation is represented by a diagonal matrix? In other words, can we find an invertible matrix S such that

$$D = S^{-1} A S \tag{1}$$

is diagonal? Writing

$$D = \begin{pmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_n \end{pmatrix} \quad \text{and} \quad S = \begin{pmatrix} | & & | \\ \boldsymbol{v}_1 & \cdots & \boldsymbol{v}_n \\ | & & | \end{pmatrix} ,$$

i.e. $\boldsymbol{v}_1, \dots, \boldsymbol{v}_n$ are the columns of the matrix S, equation (1) can be written $SD = AS$, or

$$\begin{pmatrix} | & & | \\ \lambda_1 \boldsymbol{v}_1 & \cdots & \lambda_n \boldsymbol{v}_n \\ | & & | \end{pmatrix} = A \begin{pmatrix} | & & | \\ \boldsymbol{v}_1 & \cdots & \boldsymbol{v}_n \\ | & & | \end{pmatrix} .$$

If we separate this matrix equation n column vector equations, we get

$$\lambda_1 \boldsymbol{v}_1 = A \boldsymbol{v}_1 \, , \dots , \lambda_n \boldsymbol{v}_n = A \boldsymbol{v}_n \, .$$

In other words, the entries on the diagonal of D are the eigenvalues of A, and the columns of S are the corresponding eigenvectors. Therefore, our task is the following:

> Find n eigenvalues, and n linearly independent eigenvectors of A.

2 Computing Eigenvalues and Eigenvectors

As an example, let's consider the matrix

$$A = \begin{pmatrix} 0 & -i & i \\ i & 0 & -i \\ -i & i & 0 \end{pmatrix} .$$

Step 1: Compute and factor the characteristic polynomial

The characteristic polynomial is defined

$$p_A(\lambda) = \det(A - \lambda I)\,.$$

It is zero if and only if $A - \lambda I$ is singular, i.e. if and only if the equation $A\boldsymbol{v} = \lambda \boldsymbol{v}$ has a nontrivial solution, i.e. if and only if λ is an eigenvalue. In order to find the zeros, try to write the characteristic polynomial as a product of linear factors:

$$p_A(\lambda) = \pm(\lambda - \lambda_1)\cdots(\lambda - \lambda_n)\,.$$

Notice that some linear factor $\lambda - \lambda_k$ may occur more than once. In that case it is crucial that the dimension of the corresponding eigenspace, i.e. the dimension of the solution space of the linear system $(A - \lambda_k I)\boldsymbol{v}_k = 0$ has the same multiplicity. If its dimension is less than the multiplicity of the eigenvalue, the matrix cannot be diagonalized.

In our example,

$$\begin{aligned} p_A(\lambda) &= \begin{vmatrix} -\lambda & -i & i \\ i & -\lambda & -i \\ -i & i & -\lambda \end{vmatrix} \\ &= -\lambda^3 + (-i)^3 + i^3 - 3\,(-\lambda)\,i\,(-i) \\ &= -\lambda\,(\lambda^2 - 3) \\ &= -\lambda\,(\lambda + \sqrt{3})\,(\lambda - \sqrt{3})\,. \end{aligned}$$

Therefore the three eigenvalues are $\lambda_1 = 0$, $\lambda_2 = -\sqrt{3}$, $\lambda_2 = \sqrt{3}$. Since the eigenvalues are distinct, we already know that the matrix must be diagonalizable.

Step 2: Compute the eigenvectors for each eigenvalue

For each of the λ_k where $k = 1, \dots, n$ we have to solve the homogeneous equation

$$(A - \lambda_k)\boldsymbol{v}_k = 0\,.$$

In this example,

$$(A - \lambda_1)\boldsymbol{v}_1 = \begin{pmatrix} 0 & -i & i \\ i & 0 & -i \\ -i & i & 0 \end{pmatrix} = 0\,.$$

After row-reduction, we obtain the matrix

$$\begin{pmatrix} 1 & 0 & -1 \\ 0 & 1 & -1 \\ 0 & 0 & 0 \end{pmatrix},$$

thus the first eigenvector is $\boldsymbol{v}_1 = (-1,-1,-1)^T$. Next,

$$(A-\lambda_2)\boldsymbol{v}_2 = \begin{pmatrix} \sqrt{3} & -i & i \\ i & \sqrt{3} & -i \\ -i & i & \sqrt{3} \end{pmatrix} = 0\,.$$

Let's row-reduce this matrix:

$$\begin{pmatrix} \sqrt{3} & -i & i \\ i & \sqrt{3} & -i \\ -i & i & \sqrt{3} \end{pmatrix} \xrightarrow[\substack{i\text{R2}\to\text{R2} \\ i\text{R3}\to\text{R3}}]{\text{R1}/\sqrt{3}\to\text{R1}} \begin{pmatrix} 1 & -\frac{i}{\sqrt{3}} & \frac{i}{\sqrt{3}} \\ -1 & \sqrt{3}i & 1 \\ 1 & -1 & \sqrt{3}i \end{pmatrix} \xrightarrow[\text{R2+R3}\to\text{R3}]{\text{R1+R2}\to\text{R2}}$$

$$\begin{pmatrix} 1 & -\frac{i}{\sqrt{3}} & \frac{i}{\sqrt{3}} \\ 0 & \frac{2}{\sqrt{3}}i & 1+\frac{i}{\sqrt{3}} \\ 0 & \sqrt{3}i-1 & 1+\sqrt{3}i \end{pmatrix} \xrightarrow[\text{R3}/(\sqrt{3}i-1)\to\text{R3}]{-\frac{\sqrt{3}}{2}i\text{R2}\to\text{R2}} \begin{pmatrix} 1 & -\frac{i}{\sqrt{3}} & \frac{i}{\sqrt{3}} \\ 0 & 1 & \frac{1}{2}-\frac{\sqrt{3}}{2}i \\ 0 & 1 & \frac{1}{2}-\frac{\sqrt{3}}{2}i \end{pmatrix}$$

$$\xrightarrow[\text{R2}-\text{R3}\to\text{R3}]{\text{R1}-\frac{i}{\sqrt{3}}\text{R2}\to\text{R1}} \begin{pmatrix} 1 & 0 & \frac{1}{2}+\frac{\sqrt{3}}{2}i \\ 0 & 1 & \frac{1}{2}-\frac{\sqrt{3}}{2}i \\ 0 & 0 & 0 \end{pmatrix}$$

Therefore,

$$\boldsymbol{v}_2 = \begin{pmatrix} \frac{1}{2}+\frac{\sqrt{3}}{2}i \\ \frac{1}{2}-\frac{\sqrt{3}}{2}i \\ -1 \end{pmatrix}, \qquad \boldsymbol{v}_3 = \begin{pmatrix} \frac{1}{2}-\frac{\sqrt{3}}{2}i \\ \frac{1}{2}+\frac{\sqrt{3}}{2}i \\ -1 \end{pmatrix},$$

where the computation for $\boldsymbol{v}_3$ is very similar to the previous one. Hence, we can write

$$D = \begin{pmatrix} 0 & 0 & 0 \\ 0 & -\sqrt{3} & 0 \\ 0 & 0 & \sqrt{3} \end{pmatrix}, \qquad S = \begin{pmatrix} -1 & \frac{1}{2}+\frac{\sqrt{3}}{2}i & \frac{1}{2}-\frac{\sqrt{3}}{2}i \\ -1 & \frac{1}{2}-\frac{\sqrt{3}}{2}i & \frac{1}{2}+\frac{\sqrt{3}}{2}i \\ -1 & -1 & -1 \end{pmatrix}.$$

Step 3: Check your solution

It is easiest to check that $SD = AS$, because this does not require the computation of a matrix inverse. In this example,

$$SD = \begin{pmatrix} -1 & \frac{1}{2}+\frac{\sqrt{3}}{2}i & \frac{1}{2}-\frac{\sqrt{3}}{2}i \\ -1 & \frac{1}{2}-\frac{\sqrt{3}}{2}i & \frac{1}{2}+\frac{\sqrt{3}}{2}i \\ -1 & -1 & -1 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 \\ 0 & -\sqrt{3} & 0 \\ 0 & 0 & \sqrt{3} \end{pmatrix} = \begin{pmatrix} 0 & -\frac{\sqrt{3}}{2}-\frac{3}{2}i & \frac{\sqrt{3}}{2}-\frac{3}{2}i \\ 0 & -\frac{\sqrt{3}}{2}+\frac{3}{2}i & \frac{\sqrt{3}}{2}+\frac{3}{2}i \\ 0 & \sqrt{3} & -\sqrt{3} \end{pmatrix}$$

$$AS = \begin{pmatrix} 0 & -i & i \\ i & 0 & -i \\ -i & i & 0 \end{pmatrix} \begin{pmatrix} -1 & \frac{1}{2}+\frac{\sqrt{3}}{2}i & \frac{1}{2}-\frac{\sqrt{3}}{2}i \\ -1 & \frac{1}{2}-\frac{\sqrt{3}}{2}i & \frac{1}{2}+\frac{\sqrt{3}}{2}i \\ -1 & -1 & -1 \end{pmatrix} = \begin{pmatrix} 0 & -\frac{\sqrt{3}}{2}-\frac{3}{2}i & \frac{\sqrt{3}}{2}-\frac{3}{2}i \\ 0 & -\frac{\sqrt{3}}{2}+\frac{3}{2}i & \frac{\sqrt{3}}{2}+\frac{3}{2}i \\ 0 & \sqrt{3} & -\sqrt{3} \end{pmatrix}.$$