

DIAGONALIZATION OF MATRICES

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Suppose we have an operator T that has a matrix representation $T(\{v\})$ in some basis v . In some cases (not all!) it is possible to transform to a different basis u in which $T(\{u\})$ is a diagonal matrix. If the operator A transforms from the basis v to u , then we've seen that T transforms according to

$$T(\{u\}) = A^{-1}T(\{v\})A \quad (1)$$

The diagonalization problem is therefore to find the matrix A (if it exists) so that $T(\{u\})$ is diagonal.

Assuming A does exist, we can look at the situation in two ways.

- (1) The matrix representation of T is diagonal in the u basis.
- (2) The operator $A^{-1}TA$ is diagonal in the original v basis.

To prove (2), we start with the fact that T is diagonal in the u basis, so that (no implied sums in what follows):

$$Tu_i = \lambda_i u_i \quad (2)$$

$$TA v_i = \lambda_i A v_i \quad (3)$$

$$A^{-1}TA v_i = \lambda_i A^{-1}A v_i \quad (4)$$

$$= \lambda_i v_i \quad (5)$$

From the last line, we see that v_i is an eigenvector of the operator $A^{-1}TA$ with the same eigenvalue λ_i as the eigenvector u_i of the operator T . Thus we can write, in the original basis v , the equation

$$D_T \equiv A^{-1}TA \quad (6)$$

where D_T is the diagonalized version of the matrix T in the v basis. This is known as a *similarity transformation*.

All this is fine, but we still haven't seen how to find A . It turns out that the columns of A are the eigenvectors of T . We can see this from the following argument.

In the basis v , each v_i has the form of a column vector with a 1 in the i th position and zeroes everywhere else. Thus the transformation to the u basis can be written as

$$u_k = Av_k = \begin{bmatrix} A_{11} & \cdots & A_{1n} \\ \vdots & \ddots & \vdots \\ A_{n1} & \cdots & A_{nn} \end{bmatrix} \begin{bmatrix} \vdots \\ 1 \\ \vdots \end{bmatrix} = \begin{bmatrix} A_{1k} \\ \vdots \\ A_{nk} \end{bmatrix} \quad (7)$$

The 1 is in the k th position in the column vector representing v_k and picks out the elements in column k of A in the product Av_k . Since u_k is the k th eigenvector of T , the columns of A are the eigenvectors of T . Suppose we have

$$T = \begin{bmatrix} 1 & 2 \\ 3 & 1 \end{bmatrix} \quad (8)$$

The eigenvalues are found in the usual way, from the characteristic determinant, which is

$$(1 - \lambda)^2 - 6 = 0 \quad (9)$$

$$\lambda = 1 \pm \sqrt{6} \quad (10)$$

We can find the eigenvectors by solving $Tu_i = \lambda_i u_i$ for each eigenvalue, where u_i is a 2-element column vector. (I won't go through this, since it's just algebra.) Placing the eigenvectors as the columns in a matrix A , we have

$$A = \begin{bmatrix} \frac{\sqrt{6}}{3} & -\frac{\sqrt{6}}{3} \\ 1 & 1 \end{bmatrix} \quad (11)$$

The inverse of a 2×2 matrix $A = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$ is

$$A^{-1} = \frac{1}{ad - bc} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix} \quad (12)$$

So for our matrix, we have

$$A^{-1} = \begin{bmatrix} \frac{\sqrt{6}}{4} & \frac{1}{2} \\ -\frac{\sqrt{6}}{4} & \frac{1}{2} \end{bmatrix} \quad (13)$$

Doing the matrix products (just a lot of arithmetic) we get

$$A^{-1}TA = \begin{bmatrix} 1 + \sqrt{6} & 0 \\ 0 & 1 - \sqrt{6} \end{bmatrix} \quad (14)$$

The resulting matrix is diagonal, and the diagonal entries are the eigenvalues of T . It's worth verifying that the traces of $A^{-1}TA$ and T are the same (both = 2), as are the determinants (both = -5).

REFERENCES

- (1) Zwiebach, Barton, Online course *Mastering Quantum Mechanics Part 1: Wave Mechanics*. Archive available [here](#).
- (2) Landi, Giovanni & Zampini, Alessandro (2018), *Linear Algebra and Analytic Geometry for Physical Sciences*, Chapter 9.
- (3) Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press, Chapter 1.

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