- Non-commuting matrices

$$A.B \neq B.A$$

- Diagonal matrix (*not the identity matrix*)
- If A and B commute, they are simultaneously diagonalizable.

§First example of diagonalization
Take our old problem

Feb27 Lecture

$$M = \begin{bmatrix} 4 & 2 \\ 3 & -1 \end{bmatrix}$$

$$M \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \lambda \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

$$\begin{bmatrix} 4 & 2 \\ 3 & -1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \lambda \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

$$\begin{bmatrix} 4x_1 + 2x_2 \\ 3x_1 - x_2 \end{bmatrix} = \lambda \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

$$4x_1 + 2x_2 = \lambda x_1$$
$$3x_1 - x_2 = \lambda x_2$$

$$\Rightarrow \begin{bmatrix} 4-\lambda & 2 \\ 3 & -\lambda-1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = 0$$

$$\det \begin{vmatrix} 4-\lambda & 2 \\ 3 & -\lambda-1 \end{vmatrix} = 0$$

$$(4-\lambda)(1+\lambda) + 6 = 0$$
$$-\lambda^2 + 3\lambda + 10 = 0$$
$$\lambda^2 - 3\lambda - 10 = 0$$

$$\lambda = \frac{3 \pm \sqrt{9+40}}{2} = \frac{3 \pm 7}{2}, \quad \lambda_+ = 5, \quad \lambda_- = -2$$

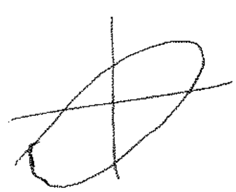
$\lambda_+ = 5$

$$\begin{bmatrix} -1 & 2 \\ 3 & -6 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = 0 \text{ and } x_1^2 + x_2^2 = 1$$

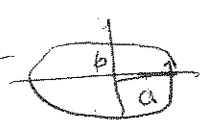
$$x_1 = 2x_2$$
$$x_1/x_2 = 2$$

§Second example: From geometry:

$$ax^2 + by^2 + 2cxy = 1 \tag{1}$$



$$\frac{x^2}{a^2} + \frac{y^2}{b^2} = 1$$



We can write this as

$$\begin{bmatrix} x & y \end{bmatrix}.A.\begin{bmatrix} x \\ y \end{bmatrix} = 1$$

$$\text{where } A = \begin{bmatrix} a & c \\ c & b \end{bmatrix}$$

Notice we can always write down a matrix M whose role is to rotate the coordinates

$$M.\begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} x' \\ y' \end{bmatrix}$$

and also its transpose... Class: $\begin{bmatrix} x \\ y \end{bmatrix} = M^T \begin{bmatrix} x' \\ y' \end{bmatrix}$ $\begin{bmatrix} x & y \end{bmatrix} . M^T = \begin{bmatrix} x' & y' \end{bmatrix}$

$M^T = M^{-1}$

Because M = Rot^n matrix

Then our equation becomes

$$\begin{bmatrix} x' & y' \end{bmatrix}.M.\begin{bmatrix} a & c \\ c & b \end{bmatrix}.M^T\begin{bmatrix} x' \\ y' \end{bmatrix} = 1 \tag{2}$$

Now we choose M such that

$$M.\begin{bmatrix} a & c \\ c & b \end{bmatrix}.M^T = \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix}. \tag{3}$$

Call

$$A_D = \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix}$$

where D is for diagonal. Now going back to our initial notation we have chosen M such that

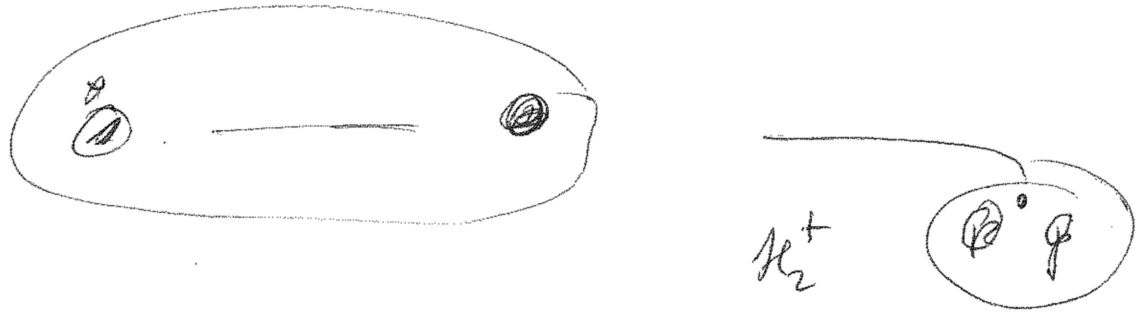
$$M.A.M^T = A_D$$

Plugging Eq. (3) into Eq. (2) we get

$$\begin{bmatrix} x' & y' \end{bmatrix}.\begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix}.\begin{bmatrix} x' \\ y' \end{bmatrix} = 1 = \lambda_1(x')^2 + \lambda_2(y')^2. \tag{4}$$

This is the equation of an ellipse.

Let us now see what we have achieved. We have rotated Eq. (1) this into an ellipse. In formal language, we have taken the quadratic form Eq. (1) and rotated it into normal coordinates- this corresponds to a change of coordinate system.



Let us think about an electron jumping between two positions. In physics this is the problem of the Hydrogen molecular ion. Let us write the Hamiltonian (energy operator) as

$$H = \begin{bmatrix} a & \Delta \\ \Delta^* & b \end{bmatrix}$$

and look for

$$H \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \lambda \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

Here a and $b \geq a$ are the energies of the two electrons if they are parked on atoms 1 and 2. Δ is a complex number corresponding to the jumping of the electron between the two atoms. Note that the H is Hermitean! This is a requirement from QM, such that the eigenvalues (λ) are real.

Solution is easy. Notice that the ground state is always lower than a for any value of Δ.

Physics 116A- Winter 2018

Mathematical Methods 116 A

S. Shastry, Feb 27 2018
Notes on Matrices

§Return to first example of diagonalization- two further comments

In our old problem

$$M = \begin{bmatrix} 4 & 2 \\ 3 & -1 \end{bmatrix}$$

$\phi = \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$ $\quad \phi^T.\phi = (\alpha^2+\beta^2)$

$\psi = \nu \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$ s.t. $\psi^T.\psi = 1$

$\psi^T.\psi = \nu^2 \phi^T.\phi = \nu^2(\alpha^2+\beta^2) = 1$

$\nu = \frac{1}{\sqrt{\alpha^2+\beta^2}}$

and

$$M \begin{bmatrix} x_1 \\ y_1 \end{bmatrix} = \lambda \begin{bmatrix} x_1 \\ y_1 \end{bmatrix}$$

we saw that there are two eigenvalues $\lambda = \lambda_{a,b}$ where $\lambda_a = 5$ and $\lambda_b = -2$ and there are two corresponding eigenvectors, let us call them ψ_a and ψ_b. We have normalized the two eigenvectors to unity. This is not strictly necessary, but helpful in most cases.

$\det(M - \lambda \mathbb{1}) = 0 \qquad \det \begin{vmatrix} 4-\lambda & 2 \\ 3 & -1-\lambda \end{vmatrix} = 0$

$\lambda_a = 5, \lambda_b = -2$

$\begin{bmatrix} 4 & 2 \\ 3 & -1 \end{bmatrix} \begin{bmatrix} x_1 \\ y_1 \end{bmatrix} = 5 \begin{bmatrix} x_1 \\ y_1 \end{bmatrix} \qquad \begin{bmatrix} 4 & 2 \\ 3 & -1 \end{bmatrix} \begin{bmatrix} x_2 \\ y_2 \end{bmatrix} = -2 \begin{bmatrix} x_2 \\ y_2 \end{bmatrix}$

$4x_1 + 2y_1 = 5x_1$

$x_1 = 2y_1 \quad \psi_a = \frac{1}{\sqrt{5}} \begin{bmatrix} 2 \\ 1 \end{bmatrix} \quad \psi_a^T.\psi_a = 1$

$4x_2 + 2y_2 = -2x_2 \qquad 3x_2 + y_2 = 0$

$\psi_b = \frac{1}{\sqrt{10}} \begin{bmatrix} 1 \\ -3 \end{bmatrix}$

From this we see that

$$\psi_a = \begin{bmatrix} \frac{2}{\sqrt{5}} \\ \frac{1}{\sqrt{5}} \end{bmatrix}, \text{and } \psi_b = \begin{bmatrix} \frac{1}{\sqrt{10}} \\ \frac{-3}{\sqrt{10}} \end{bmatrix}, \tag{1}$$

such that

$$M.\psi_a = \lambda_a \psi_a, \quad M.\psi_b = \lambda_b \psi_b, \tag{2}$$

From normalization $\psi_a^T.\psi_a = 1$ and $\psi_b^T.\psi_b = 1$

Let me define a matrix formed from the eigenvectors of M

$$W = \begin{bmatrix}\psi_a & \psi_b\end{bmatrix} = \begin{bmatrix}\frac{2}{\sqrt{5}} & \frac{1}{\sqrt{10}} \\ \frac{1}{\sqrt{5}} & \frac{-3}{\sqrt{10}}\end{bmatrix} \tag{3}$$

We have shown that the diagonal matrix of eigenvalues D can be expressed as

$$M.W = W.D, \quad \text{where } D = \begin{bmatrix}\lambda_a & 0 \\ 0 & \lambda_b\end{bmatrix}$$

More explicitly

$$\begin{bmatrix}4 & 2 \\ 3 & -1\end{bmatrix} \cdot \begin{bmatrix}\frac{2}{\sqrt{5}} & \frac{1}{\sqrt{10}} \\ \frac{1}{\sqrt{5}} & \frac{-3}{\sqrt{10}}\end{bmatrix} = \begin{bmatrix}\frac{2}{\sqrt{5}} & \frac{1}{\sqrt{10}} \\ \frac{1}{\sqrt{5}} & \frac{-3}{\sqrt{10}}\end{bmatrix} \cdot \begin{bmatrix}5 & 0 \\ 0 & -2\end{bmatrix}$$

$W^{-1}.M.W = W^{-1}.W.D = D$

$W^{-1}.M.W = D.W$ No fi!!

Check that $D.W \neq W.D$!!

This implies we have found the diagonal matrix D by computing the "similarity transformation"

$$W^{-1}.M.W = D \tag{4}$$

Comment: Rotations, i.e. orthogonal transforms is a special case of this

More Generally: (very important in QM)

If M is real symmetric, i.e. $M^T = M$, we can diagonalize it by an *orthogonal transformation*

$$\begin{aligned} O^T.M.O &= D \\ O^T &= O^{-1} \end{aligned} \tag{5}$$

If M is complex but Hermitean, i.e. $M^\dagger = M$, we can diagonalize it by an *unitary transformation*

$$\begin{aligned} U^\dagger.M.U &= D \\ U^\dagger &= U^{-1} \end{aligned} \tag{6}$$

$UU^\dagger = 1 = U^\dagger U$