

# An example of matrix diagonalization

## Rotation of a quadrupole tensor

We refer to the example of a quadrupole tensor. A quadrupole moment is represented by a second rank tensor which is a matrix.

For charges at the following positions:

+1 at  $(x,y) = (1,1)$  and  $(-1,-1)$

-1 at  $(x,y) = (-1,1)$  and  $(1,-1)$

The elements of the quadrupole tensor are obtained from

$$\Theta_{ij} = \sum_i q_i r_i r_i$$

The elements of the quadrupole tensor are:

$$\Theta_{xx} = 1(1)(1) + 1(-1)(-1) - 1(-1)(-1) - 1(1)(1) = 0$$

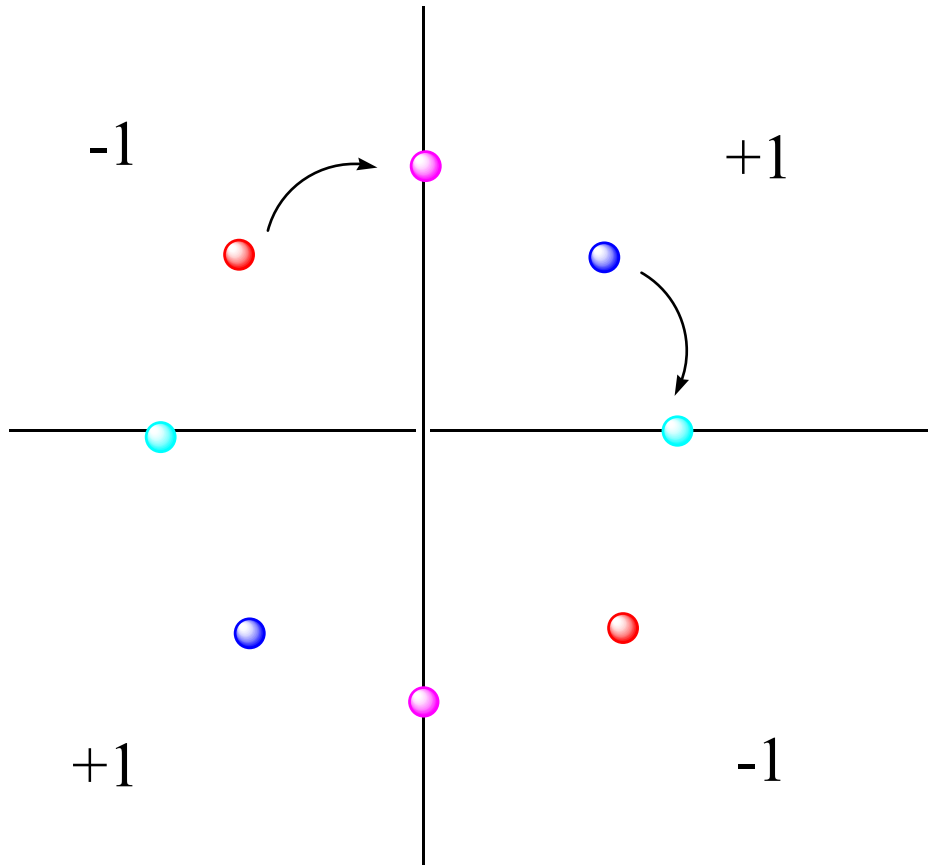
$$\Theta_{yy} = 1(1)(1) + 1(-1)(-1) - 1(-1)(-1) - 1(1)(1) = 0$$

$$\Theta_{xy} = 1(1)(1) + 1(-1)(-1) - 1(-1)(1) - 1(1)(-1) = 4$$

$$\Theta_{yx} = 1(1)(1) + 1(-1)(-1) - 1(1)(-1) - 1(-1)(1) = 4$$

$$\Theta = \begin{pmatrix} 0 & 4 \\ 4 & 0 \end{pmatrix}$$

By inspection we can see that a  $\pi/4$  rotation of the coordinate system will diagonalize the matrix.



This is shown as a rotation of the charges for simplicity. In the new coordinate system we have  
 +1 at  $(x,y) = (\sqrt{2},0)$  and  $(-\sqrt{2},0)$   
 -1 at  $(x,y) = (0,\sqrt{2})$  and  $(0,-\sqrt{2})$

$$\Theta_{ij} = \sum_i q_i r_i r_i$$

The elements of the quadrupole tensor are:

$$\Theta_{xx} = 1(\sqrt{2})(\sqrt{2}) + 1(-\sqrt{2})(-\sqrt{2}) - 1(0)(0) - 1(0)(0) = 4$$

$$\Theta_{yy} = 1(0)(0) + 1(0)(0) - 1(\sqrt{2})(\sqrt{2}) - 1(-\sqrt{2})(-\sqrt{2}) = -4$$

$$\Theta_{xy} = 1(\sqrt{2})(0) + 1(-\sqrt{2})(0) - 1(0)(\sqrt{2}) - 1(0)(-\sqrt{2}) = 0$$

$$\Theta_{yx} = 1(0)(\sqrt{2}) + 1(0)(-\sqrt{2}) - 1(\sqrt{2})(0) - 1(-\sqrt{2})(0) = 0$$

$$\Theta = \begin{pmatrix} 4 & 0 \\ 0 & -4 \end{pmatrix}$$

This problem is that of diagonalization of a matrix. We began with a non-diagonal matrix and ended up with a diagonal matrix.

We did this using a transformation of coordinate system. In this case the transformation was a rotation. The general case of a clockwise rotation of a vector by an angle  $\theta$  is:

$$\begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} x_1 \\ y_1 \end{pmatrix} = \begin{pmatrix} x_2 \\ y_2 \end{pmatrix}$$

In this case we know that the rotation occurs through an angle  $\theta = \pi/4 = 45^\circ$ . Thus,  $\cos\theta = \sin\theta = 1/\sqrt{2}$ . The rotation matrix is:

$$\begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} x_1 \\ y_1 \end{pmatrix} = \begin{pmatrix} x_2 \\ y_2 \end{pmatrix}$$

to rotate the vector  $(x_1, y_1)$  by  $45^\circ$ . We seem to know the answer. We use this example to demonstrate a general method of matrix diagonalization and to show that this method also generates a transformation matrix. The elements of the diagonalized matrix are called eigenvalues and the rows of the transformation matrix are called eigenvectors. How do we obtain these eigenvectors and eigenvalues. We wish to diagonalize the matrix  $\Theta$ . We require that:

$$(\Theta - \lambda I) \mathbf{c}^T = 0$$

$\mathbf{c}^T$  is a column vector. This is the same thing as a  $n \times 1$  column matrix. We can write this as:

$$\left( \begin{pmatrix} \Theta_{xx} & \Theta_{xy} \\ \Theta_{yx} & \Theta_{yy} \end{pmatrix} - \begin{pmatrix} \lambda_+ & 0 \\ 0 & \lambda_+ \end{pmatrix} \right) \begin{pmatrix} c_1^+ \\ c_2^+ \end{pmatrix} = 0$$

We have substituted in one possible solution that we call  $\lambda_+$ . There is a second solution that we call  $\lambda_-$ .

$$\left( \begin{pmatrix} \Theta_{xx} & \Theta_{xy} \\ \Theta_{yx} & \Theta_{yy} \end{pmatrix} - \begin{pmatrix} \lambda_- & 0 \\ 0 & \lambda_- \end{pmatrix} \right) \begin{pmatrix} c_1^- \\ c_2^- \end{pmatrix} = 0$$

The solution to the above set of equations will exist only if the determinant of the matrix  $(\Theta - \lambda \mathbf{I})$  vanishes. Using the explicit values above we have the determinant:

$$\det \begin{pmatrix} (\Theta_{xx} - \lambda) & \Theta_{xy} \\ \Theta_{yx} & (\Theta_{yy} - \lambda) \end{pmatrix} = \det \begin{pmatrix} (-\lambda) & 4 \\ 4 & (-\lambda) \end{pmatrix} = \lambda^2 - 16 = 0$$

Which results in the solution:

$$\lambda = \pm 4$$

We see that the eigenvalue matrix is:

$$\Lambda = \begin{pmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{pmatrix} = \begin{pmatrix} 4 & 0 \\ 0 & -4 \end{pmatrix}$$

This eigenvalue matrix  $\Lambda$  is exactly the same as the diagonalized matrix that we obtained above using geometric means. To obtain the eigenvectors we substitute in each eigenvalue and solve for the coefficients. We must use a normalization condition as a constraint.

$$(c_1)^2 + (c_2)^2 = 1$$

$$\begin{pmatrix} (\Theta_{xx} - \lambda) & \Theta_{xy} \\ \Theta_{yx} & (\Theta_{yy} - \lambda) \end{pmatrix} \begin{pmatrix} c_1^+ \\ c_2^+ \end{pmatrix} = \begin{pmatrix} (-4) & 4 \\ 4 & (-4) \end{pmatrix} \begin{pmatrix} c_1^+ \\ c_2^+ \end{pmatrix} = 0$$

$$(-4)c_1^+ + (4)c_2^+ = 0$$

$$c_1^+ = c_2^+$$

$$(c_1^+)^2 + (c_2^+)^2 = 2(c_1^+)^2 = 1$$

$$c_1^+ = c_2^+ = \frac{1}{\sqrt{2}}$$

First we substitute in  $\lambda_+$ .

Using the normalization condition:

Then we substitute in  $\lambda_-$ .

$$\begin{pmatrix} (\Theta_{xx} - \lambda) & \Theta_{xy} \\ \Theta_{yx} & (\Theta_{yy} - \lambda) \end{pmatrix} \begin{pmatrix} c_1^- \\ c_2^- \end{pmatrix} = \begin{pmatrix} (4) & 4 \\ 4 & (4) \end{pmatrix} \begin{pmatrix} c_1^- \\ c_2^- \end{pmatrix} = 0$$

$$(4)c_1^- + (4)c_2^- = 0$$

$$c_1^- = -c_2^-$$

Again the normalization condition is applied.

$$(c_1^-)^2 + (c_2^-)^2 = 2(c_1^-)^2 = 1$$

$$c_1^- = \frac{-1}{\sqrt{2}}, \quad c_2^- = \frac{1}{\sqrt{2}}$$

Finally, we construct a matrix of coefficients:

$$\mathbf{C} = \begin{pmatrix} c_1^+ & c_2^+ \\ c_1^- & c_2^- \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}$$

This is the transformation matrix. It is equal to the rotation matrix that we discussed above. The form of the transformation is:

$$(\Theta - \Lambda)\mathbf{C}^T = 0$$

$$\Theta\mathbf{C}^T = \Lambda\mathbf{C}^T = \mathbf{C}^T\Lambda = \mathbf{C}^{-1}\Lambda$$

$$\mathbf{C}\Theta\mathbf{C}^{-1} = \mathbf{C}\mathbf{C}^{-1}\Lambda = \Lambda$$

This procedure defines the similarity transform.

$$\mathbf{C}\Theta\mathbf{C}^{-1} = \Lambda$$

We have used the fact that  $\mathbf{C}$  is a unitary matrix and therefore its inverse is equal to its transpose.

$$\mathbf{C}^{-1} = \mathbf{C}^T$$

The similarity transform is simply a rotation in the present case.

We have transformed the coordinate system into one which is rotated by  $45^\circ$  with respect to the charges in the quadrupole.

Thus, we can show that

$$\begin{aligned} \mathbf{C}\Theta\mathbf{C}^T &= \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} 0 & 4 \\ 4 & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \\ &= \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \frac{4}{\sqrt{2}} & \frac{4}{\sqrt{2}} \\ \frac{4}{\sqrt{2}} & -\frac{4}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} 4 & 0 \\ 0 & -4 \end{pmatrix} \end{aligned}$$