# THE CHEMIST'S TOOLKIT 25 Matrix methods for solving eigenvalue equations

In matrix form, an **eigenvalue equation** is

$$\boldsymbol{M}\boldsymbol{x} = \lambda \boldsymbol{x} \qquad \text{Eigenvalue equation} \qquad (25.1\text{a})$$

where $\boldsymbol{M}$ is a square matrix with $n$ rows and $n$ columns, $\lambda$ is a constant, the **eigenvalue**, and $\boldsymbol{x}$ is the **eigenvector**, an $n \times 1$ (column) matrix that satisfies the conditions of the eigenvalue equation and has the form:

$$\boldsymbol{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}$$

In general, there are $n$ eigenvalues $\lambda^{(i)}$, $i = 1, 2, \ldots, n$, and $n$ corresponding eigenvectors $\boldsymbol{x}^{(i)}$. Equation 25.1a can be rewritten as

$$(\boldsymbol{M} - \lambda \boldsymbol{1})\boldsymbol{x} = 0 \qquad (25.1\text{b})$$

where $\boldsymbol{1}$ is an $n \times n$ unit matrix, and where the property $\boldsymbol{1x} = \boldsymbol{x}$ has been used. This equation has a solution only if the determinant $|\boldsymbol{M} - \lambda\boldsymbol{1}|$ of the matrix $\boldsymbol{M} - \lambda\boldsymbol{1}$ is zero. It follows that the $n$ eigenvalues may be found from the solution of the **secular equation**:

$$|\boldsymbol{M} - \lambda\boldsymbol{1}| = 0 \qquad (25.2)$$

### Brief illustration 25.1: Simultaneous equations

Consider the matrix equation

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

rearranged into $\begin{pmatrix} 1-\lambda & 2 \\ 3 & 4-\lambda \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = 0$

From the rules of matrix multiplication, the latter form expands into

$$\begin{pmatrix} (1-\lambda)x_1 + 2x_2 \\ 3x_1 + (4-\lambda)x_2 \end{pmatrix} = 0$$

which is simply a statement of the two simultaneous equations

$$(1-\lambda)x_1 + 2x_2 = 0 \text{ and } 3x_1 + (4-\lambda)x_2 = 0$$

The condition for these two equations to have solutions is

$$|\boldsymbol{M} - \lambda\boldsymbol{1}| = \begin{vmatrix} 1-\lambda & 2 \\ 3 & 4-\lambda \end{vmatrix} = (1-\lambda)(4-\lambda) - 6 = 0$$

This condition corresponds to the quadratic equation

$$\lambda^2 - 5\lambda - 2 = 0$$

with solutions $\lambda = +5.372$ and $\lambda = -0.372$, the two eigenvalues of the original equation.

The $n$ eigenvalues found by solving the secular equations are used to find the corresponding eigenvectors. To do so, begin by considering an $n \times n$ matrix $\boldsymbol{X}$ the columns of which are formed from the eigenvectors corresponding to all the eigenvalues. Thus, if the eigenvalues are $\lambda_1, \lambda_2, \ldots$, and the corresponding eigenvectors are

$$\boldsymbol{x}^{(1)} = \begin{pmatrix} x_1^{(1)} \\ x_2^{(1)} \\ \vdots \\ x_n^{(1)} \end{pmatrix} \quad \boldsymbol{x}^{(2)} = \begin{pmatrix} x_1^{(2)} \\ x_2^{(2)} \\ \vdots \\ x_n^{(2)} \end{pmatrix} \quad \cdots \boldsymbol{x}^{(n)} = \begin{pmatrix} x_1^{(n)} \\ x_2^{(n)} \\ \vdots \\ x_n^{(n)} \end{pmatrix} \qquad (25.3\text{a})$$

then the matrix $\boldsymbol{X}$ is

$$\boldsymbol{X} = (\boldsymbol{x}^{(1)}\, \boldsymbol{x}^{(2)} \cdots \boldsymbol{x}^{(n)}) = \begin{pmatrix} x_1^{(1)} & x_1^{(2)} & \cdots & x_1^{(n)} \\ x_2^{(1)} & x_2^{(2)} & \cdots & x_2^{(n)} \\ \vdots & \vdots & & \vdots \\ x_n^{(1)} & x_n^{(2)} & \cdots & x_n^{(n)} \end{pmatrix} \qquad (25.3\text{b})$$

Similarly, form an $n \times n$ matrix $\boldsymbol{\Lambda}$ with the eigenvalues $\lambda$ along the diagonal and zeroes elsewhere:

$$\boldsymbol{\Lambda} = \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{pmatrix} \qquad (25.4)$$

Now all the eigenvalue equations $\boldsymbol{M}\boldsymbol{x}^{(i)} = \lambda_i \boldsymbol{x}^{(i)}$ may be combined into the single matrix equation

$$\boldsymbol{MX} = \boldsymbol{X\Lambda} \qquad (25.5)$$

### Brief illustration 25.2: Eigenvalue equations

In *Brief illustration* 25.1 it is established that if $\boldsymbol{M} = \begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix}$ then $\lambda_1 = +5.372$ and $\lambda_2 = -0.372$. Then, with eigenvectors $\boldsymbol{x}^{(1)} = \begin{pmatrix} x_1^{(1)} \\ x_2^{(1)} \end{pmatrix}$ and $\boldsymbol{x}^{(2)} = \begin{pmatrix} x_1^{(2)} \\ x_2^{(2)} \end{pmatrix}$ form

$$\boldsymbol{X} = \begin{pmatrix} x_1^{(1)} & x_1^{(2)} \\ x_2^{(1)} & x_2^{(2)} \end{pmatrix} \quad \boldsymbol{\Lambda} = \begin{pmatrix} 5.372 & 0 \\ 0 & -0.372 \end{pmatrix}$$

The expression $\boldsymbol{MX} = \boldsymbol{X\Lambda}$ becomes

$$\begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix}\begin{pmatrix} x_1^{(1)} & x_1^{(2100)} \\ x_2^{(1)} & x_2^{(2)} \end{pmatrix} = \begin{pmatrix} x_1^{(1)} & x_1^{(2)} \\ x_2^{(1)} & x_2^{(2)} \end{pmatrix}\begin{pmatrix} 5.372 & 0 \\ 0 & -0.372 \end{pmatrix}$$

which expands to

$$\begin{pmatrix} x_1^{(1)}+2x_2^{(1)} & x_1^{(2)}+2x_2^{(2)} \\ 3x_1^{(1)}+4x_2^{(1)} & 3x_1^{(2)}+4x_2^{(2)} \end{pmatrix} = \begin{pmatrix} 5.372x_1^{(1)} & -0.372x_1^{(2)} \\ 5.372x_2^{(1)} & -0.372x_2^{(2)} \end{pmatrix}$$

This is a compact way of writing the four equations

$$\begin{aligned} x_1^{(1)}+2x_2^{(1)} &= 5.372x_1^{(1)} \qquad & x_1^{(2)}+2x_2^{(2)} &= -0.372x_1^{(2)} \\ 3x_1^{(1)}+4x_2^{(1)} &= 5.372x_2^{(1)} \qquad & 3x_1^{(2)}+4x_2^{(2)} &= -0.372x_2^{(2)} \end{aligned}$$

corresponding to the two original simultaneous equations and their two roots.

Finally, form $\boldsymbol{X}^{-1}$ from $\boldsymbol{X}$ and multiply eqn 25.5 by it from the left:

$$\boldsymbol{X}^{-1}\boldsymbol{M}\boldsymbol{X} = \boldsymbol{X}^{-1}\boldsymbol{X}\boldsymbol{\Lambda} = \boldsymbol{\Lambda} \qquad (25.6)$$

A structure of the form $\boldsymbol{X}^{-1}\boldsymbol{M}\boldsymbol{X}$ is called a **similarity transformation**. In this case the similarity transformation $\boldsymbol{X}^{-1}\boldsymbol{M}\boldsymbol{X}$ makes $\boldsymbol{M}$ diagonal (because $\boldsymbol{\Lambda}$ is diagonal). It follows that if the matrix $\boldsymbol{X}$ that causes $\boldsymbol{X}^{-1}\boldsymbol{M}\boldsymbol{X}$ to be diagonal is known, then the problem is solved: the diagonal matrix so produced has the eigenvalues as its only nonzero elements, and the matrix $\boldsymbol{X}$ used to bring about the transformation has the corresponding eigenvectors as its columns. In practice, the eigenvalues and eigenvectors are obtained by using mathematical software.

### Brief illustration 25.3: Similarity transformations

To apply the similarity transformation to the matrix $\begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix}$ from *Brief illustration* 25.1 it is best to use mathematical software to find the form of $\boldsymbol{X}$ and $\boldsymbol{X}^{-1}$. The result is

$$\boldsymbol{X} = \begin{pmatrix} 0.416 & 0.825 \\ 0.909 & -0.566 \end{pmatrix} \qquad \boldsymbol{X}^{-1} = \begin{pmatrix} 0.574 & 0.837 \\ 0.922 & -0.422 \end{pmatrix}$$

This result can be verified by carrying out the multiplication

$$\boldsymbol{X}^{-1}\boldsymbol{M}\boldsymbol{X} = \begin{pmatrix} 0.574 & 0.837 \\ 0.922 & -0.422 \end{pmatrix}\begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix}\begin{pmatrix} 0.416 & 0.825 \\ 0.909 & -0.566 \end{pmatrix} = \begin{pmatrix} 5.372 & 0 \\ 0 & -0.372 \end{pmatrix}$$

The result is indeed the diagonal matrix $\boldsymbol{\Lambda}$ calculated in *Brief illustration* 25.2. It follows that the eigenvectors $\boldsymbol{x}^{(1)}$ and $\boldsymbol{x}^{(2)}$ are

$$\boldsymbol{x}^{(1)} = \begin{pmatrix} 0.416 \\ 0.909 \end{pmatrix} \qquad \boldsymbol{x}^{(2)} = \begin{pmatrix} 0.825 \\ -0.566 \end{pmatrix}$$