Matrices and Vectors

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Nomenclature

Matrix

- A *matrix* is an array of symbols arranged in rows and columns.
- An $m \times n$ matrix has m rows and n columns. For example, the 3×4 matrix $\mathbf{A}$:

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \end{bmatrix}$$

- The *transpose* of $\mathbf{A}$, the 4×3 matrix $\mathbf{A}^{\mathbf{T}}$ has the rows and columns exchanged, i.e. element a_{ij} becomes element a_{ji} in the transpose

Vector

- A single column array is termed a *vector*.
- For example, the 3×1 vector $\mathbf{x}$:

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix}$$

- The transpose of $\mathbf{x}$ is the 1×3 *row vector* $\mathbf{x}^T$:

$$\mathbf{x} = \begin{bmatrix} x_1 & x_2 & x_3 & x_4 \end{bmatrix}$$

Matrix Notation Makes Equations Compact

- Suppose you have a solution containing a mixture of three different cytochromes at concentrations x_1, x_2 and x_3.
- You measure the absorbance of the solution at three different wavelengths $\lambda_1 \ldots \lambda_3$, obtaining results $y_1 \ldots y_3$.
- Let the absorption coefficient of cytochrome j at wavelength λ_i be a_{ij}.
- Then by Beer's Law we can write:

$$y_1 = a_{11}x_1 + a_{12}x_2 + a_{13}x_3$$
$$y_2 = a_{21}x_1 + a_{22}x_2 + a_{23}x_3$$
$$y_3 = a_{31}x_1 + a_{32}x_2 + a_{33}x_3$$

which can be written in matrix notation as:

$$\mathbf{y} = \mathbf{A}\mathbf{x}$$

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Matrix multiplication

The previous slide showed you that matrix multiplication works like this:

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3$$
$$a_{21}x_1 + a_{22}x_2 + a_{23}x_3$$
$$a_{31}x_1 + a_{32}x_2 + a_{33}x_3$$

- Note that multiplying a 3×3 matrix by a 3×1 vector produces a 3×1 result. For the result of matrix multiplication to be defined (conformable), the number of columns in the first term must be the same as the number of rows in the second term.
- Hence $\mathbf{xA}$ is not allowed, but $\mathbf{x^T A}$ is.
- What is the result of $\mathbf{x^T A}$, and is it equal to $\mathbf{Ax}$?

Special Matrices 1: Identity Matrix

This is a square n–dimensional matrix, $\mathbf{I_n}$, or simply $\mathbf{I}$, with 1s on the diagonal and zeroes elsewhere:

$$\mathbf{I_3} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Multiplication of, or by an identity matrix leaves the other multiplicand unchanged:

$$\mathbf{Ix} = \mathbf{x}; \mathbf{AI} = \mathbf{A}$$

Special Matrices 2: Null Matrix

The null matrix, $\mathbf{0}$, is any matrix (or vector) all of whose elements are 0.

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Special Matrices 3: Inverse Matrix

The identity matrix is involved in the definition of the *inverse*, denoted $\mathbf{A}^{-1}$, of a square matrix $\mathbf{A}$:

$$\mathbf{A}\mathbf{A}^{-1} = \mathbf{A}^{-1}\mathbf{A} = \mathbf{I}$$

Being square is a necessary, but not sufficient, condition for a matrix to have an inverse; if it does not have an inverse, it is said to be *singular*. If the inverse exists, it is unique.
The inverse is related to the solution of sets of equations.
Returning to our three absorbance values measured at three wavelengths:

$$\mathbf{y} = \mathbf{A}\mathbf{x}$$

If we *premultiply* both sides of the equation by $\mathbf{A}^{-1}$, we get:

$$\mathbf{A}^{-1}\mathbf{y} = \mathbf{A}^{-1}\mathbf{A}\mathbf{x} = \mathbf{I}\mathbf{x} = \mathbf{x}$$

As the inverse is unique, the solutions $\mathbf{x}$ are also unique.

Solutions of Linear Equation Systems

Solution by Gauss-Jordan Elimination

Returning to:

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}$$

We can start converting to row-echelon form by eliminating a_{21} and a_{31}.
First multiply every term in row 2 of $\mathbf{A}$ and $\mathbf{y}$ by a_{11}/a_{21}, and subtract the corresponding terms from row 1. This gives:

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ 0 & a'_{22} & a'_{23} \\ 0 & a'_{32} & a'_{33} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} y_1 \\ y'_2 \\ y'_3 \end{bmatrix}$$

Where the primes indicate terms whose values have been altered in the process.

Solution by Gauss-Jordan Elimination 2

Next multiply every term in row 3 of $\mathbf{A}$ and $\mathbf{y}$ by a_{22}/a_{32}, and subtract the corresponding terms from row 2. This gives:

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ 0 & a'_{22} & a'_{23} \\ 0 & 0 & a''_{33} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} y_1 \\ y'_2 \\ y''_3 \end{bmatrix}$$

This is *row echelon* form,and it tells us $x_3 = y''_3/a''_{33}$, from which we can use row 2 to evaluate x_2 (by *back substitution* of x_3), and so on.

Dependencies and Matrix Rank

Suppose at the last step of making the row echelon form, when eliminating a_{32}, a_{33} and y_3 disappeared at the same time, giving:

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ 0 & a'_{22} & a'_{23} \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} y_1 \\ y'_2 \\ 0 \end{bmatrix}$$

What would this mean?

Forward to answer

Problem: Analysing an Enzyme Mixture

A cell sample contains three isoenzymes for the same reaction that differ in their K_m values such that when assayed at 0.5, 2.5 and 25 mM:

- E_1 gives 0.33, 0.71 and 0.96 of its V_1;
- E_2 gives 0.17, 0.50 and 0.91 of its V_2, and
- E_3 gives 0.02, 0.11 and 0.55 of its V_3.

When the sample was assayed, the measured rates of reaction were 5.1, 13.7 and 32.2 nmol.min^{-1}

Follow the instructions on the web site for solving:

$$\mathbf{A}^{-1}\mathbf{y} = \mathbf{x}$$

to answer the following:

1. What are the V values of the three enzymes in the sample?
2. Assuming the error on a rate measurement is 2%, what is the impact on the results?
3. What could be done to improve the estimates?

Forward to answer

Solutions of Linear Equation Systems

$$\mathbf{A}\mathbf{x} = \mathbf{y}$$

	$\mathbf{y} \neq 0$	$\mathbf{y} = 0$
$\mathbf{A}$ is non–singular; rank equals dimension.	Unique non–trivial solution	Unique trivial solution; $\mathbf{x} = 0$.
$\mathbf{A}$ singular; rank less than dimension.	Infinite solutions, not including $\mathbf{x} = 0$, but dependencies between the x_i, provided equations are consistent	Infinite solutions, with dependencies, and including $\mathbf{x} = 0$.

Answers

Matrix multiplication

Given $\mathbf{A}$:

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$$

and a 3x1 vector $\mathbf{x}$, what is the result of $\mathbf{x}^{\mathbf{T}}\mathbf{A}$, and is it equal to $\mathbf{A}\mathbf{x}$?

Answer:

$$\begin{matrix} a_{11}x_1 + a_{21}x_2 + a_{31}x_3 \\ a_{12}x_1 + a_{22}x_2 + a_{32}x_3 \\ a_{13}x_1 + a_{23}x_2 + a_{33}x_3 \end{matrix}$$

which is not equal to:

$$\begin{matrix} a_{11}x_1 + a_{12}x_2 + a_{13}x_3 \\ a_{21}x_1 + a_{22}x_2 + a_{23}x_3 \\ a_{31}x_1 + a_{32}x_2 + a_{33}x_3 \end{matrix}$$

Back to question

Dependencies and Matrix Rank

Suppose at the last step of making the row echelon form, when eliminating a_{32}, a_{33} and y_3 disappeared at the same time, giving:

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ 0 & a'_{22} & a'_{23} \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} y_1 \\ y'_2 \\ 0 \end{bmatrix}$$

What would this mean?
The three rows of $\mathbf{A}$ are not independent; row 3 is some linear combination of rows 1 and 2.
Although $\mathbf{A}$ was a 3×3 matrix, its *rank* was only 2, and we can now no longer obtain a unique solution for $\mathbf{x}$.
This corresponds to $\mathbf{A}$ being singular and not having an inverse.

Back to question

Answer: Analysing an Enzyme Mixture

The answers are:

1. The three enzyme values are 11.2, 4.7 and 32.2 nmol.min^{-1} respectively.
2. The values of E$_1$ and E$_2$ in particular are very sensitive to the errors in the measurement.
3. Improvements might include:
   - Trying to find a set of substrate concentrations that gave better resolution.
   - Making measurements at additional concentrations. As there would then be more measurements than variables, a least squares solution would be necessary, as the experimental error would make the equation set inconsistent.
   - Make the measurement a different way, as the dependencies of the three enzymes on substrate, though different, are quite strongly correlated.

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