Quantum Mechanics

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Determinants

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Determinant

A determinant is a quantity obtained by adding products of the elements of a square matrix. In particular, given a matrix

$$\mathbf{M} = \begin{pmatrix} M_{11} & \cdots & M_{1n} \\ \vdots & \ddots & \vdots \\ M_{n1} & \cdots & M_{nn} \end{pmatrix}$$

its determinant is written as an array of numbers (or functions)

$$M = \begin{vmatrix} M_{11} & \cdots & M_{1n} \\ \vdots & \ddots & \vdots \\ M_{n1} & \cdots & M_{nn} \end{vmatrix}$$

from which a number (or a function) can be generated

2×2 Determinant

A determinant of order 2 is evaluated as follows.

$$\begin{vmatrix} a & b \\ c & d \end{vmatrix} = ad - bc$$

For example,

$$\begin{vmatrix} -1 & -4 \\ 3 & 2 \end{vmatrix} = (-1)(2) - (-4)(3) = -1 + 12 = 11$$

$$\begin{vmatrix} x^2 & y \\ \sin z & z/x \end{vmatrix} = xz - ysinz$$

Order 3

A determinant of order 3 may be evaluated as follows

$$\begin{vmatrix} a & b & c \\ d & e & f \\ g & h & k \end{vmatrix} \rightarrow \begin{vmatrix} a & b & c \\ d & e & f \\ g & h & k \end{vmatrix}\begin{matrix} a & b \\ d & e \\ g & h \end{matrix} = aek + bfg + cdh - gec - hfa - kdb$$

For example

$$\begin{vmatrix} 3 & -1 & 2 \\ 1 & 0 & 4 \\ -2 & -4 & -3 \end{vmatrix}$$
$$= (3)(0)(-3) + (-1)(4)(-2) + (2)(1)(-4) - (-2)(0)(2) - (-4)(4)(3)$$
$$- (-3)(1)(-1) = 0 + 8 - 8 - 0 + 48 - 3 = 45$$

Cofactors

A determinant of any order may in general be evaluated using cofactors.

Let us consider a 3×3 determinant

$$\begin{vmatrix} a & b & c \\ d & e & f \\ g & h & k \end{vmatrix}$$

First, assign + and – signs alternately

$$\begin{vmatrix} + & - & + \\ - & + & - \\ + & - & + \end{vmatrix}$$

Then evaluate the minor of the element by crossing out other elements in the same row and the same column, giving rise to a determinant with order lower by one. For example, the minor of e is

$$\begin{vmatrix} a & b & c \\ d & e & f \\ g & h & k \end{vmatrix} \rightarrow \begin{vmatrix} a & c \\ g & k \end{vmatrix}$$

The cofactor of an element is its sign times its minor.

Evaluation by Cofactors

The determinant is then evaluated by summing over the elements of a row or column multiplied by their cofactors.

Thus

$$\begin{vmatrix} a & b & c \\ d & e & f \\ g & h & k \end{vmatrix}$$

for example can be evaluated as

$$a\begin{vmatrix} e & f \\ h & k \end{vmatrix} - b\begin{vmatrix} d & f \\ g & k \end{vmatrix} + c\begin{vmatrix} d & e \\ g & h \end{vmatrix} = a(ek - hf) - b(dk - gf) + c(dh - ge)$$
$$= aek + bfg + cdh - ceg - afh - bdk$$

Another way is

$$-b\begin{vmatrix} d & f \\ g & k \end{vmatrix} + e\begin{vmatrix} a & c \\ g & k \end{vmatrix} - h\begin{vmatrix} a & c \\ d & f \end{vmatrix} = -b(dk - gf) + e(ak - gc) - h(af - dc)$$
$$= aek + bfg + cdh - ceg - afh - bdk$$

There are in all 9 ways of doing this.

Evaluation by Cofactors

For order 2, a cofactor evaluation could be

$$\begin{vmatrix} a & b \\ c & d \end{vmatrix} = (-c)(b) + (d)(a) = ad - bc$$

This is one of four ways which all yield the same value.

For order 4, one of the 16 possible ways is (taking the fourth column)

$$\begin{vmatrix} a & b & c & d \\ e & f & g & h \\ k & m & n & p \\ q & r & s & t \end{vmatrix} = -d \begin{vmatrix} e & f & g \\ k & m & n \\ q & r & s \end{vmatrix} + h \begin{vmatrix} a & b & c \\ k & m & n \\ q & r & s \end{vmatrix} - p \begin{vmatrix} a & b & c \\ e & f & g \\ q & r & s \end{vmatrix} + t \begin{vmatrix} a & b & c \\ e & f & g \\ k & m & n \end{vmatrix}$$

In practice, we choose the column or row with the most zeroes to make the calculation simpler.