

There is a strong analogy:

function \longleftrightarrow vector
operator \longleftrightarrow matrix

We know $f(x)$ if we know its value for every x . In practice, one can say we *know* a function $f(x)$ if we know its value for *many* points x that span the range we're interested in.

Suppose we evaluate $f(x)$ at many points x , $x = \dots, 0.00, 0.01, 0.02, 0.03, \dots$ and we arrange the values $\dots f(0.00), f(0.01), f(0.02), f(0.03), \dots$ in a vector. Let's call that vector \vec{f} and represent it as:

$$\begin{pmatrix} \dots \\ f(0.00) \\ f(0.01) \\ f(0.02) \\ f(0.03) \\ \dots \end{pmatrix}$$

We can calculate the integral on the left-hand side below (the so-called *overlap* integral of $f(x)$ and $g(x)$) to a good approximation using vectors:

$$\begin{aligned} \int f(x) g(x) dx &= 0.01 \times (\dots \\ &+ f(0.00) \cdot g(0.00) + f(0.01) \cdot g(0.01) \\ &+ f(0.02) \cdot g(0.02) + f(0.03) \cdot g(0.03) \\ &+ \dots) \\ &= 0.01 \times \vec{f} \cdot \vec{g} \end{aligned}$$

Integrals of products of functions are just like *scalar products of vectors* !

Functions are like vectors with an infinite number of components.

quantum mechanics / *matrix mechanics* / *wave mechanics*

The analogy goes much further. In matrix-vector algebra, one often uses a set of *unit length orthogonal vectors* as a basis for representing other vectors (see next page). Likewise, one can use a set of *orthonormal functions* as a basis for representing other functions.

Complete orthonormal set of vectors in 3D space:

$$\vec{u}_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad \vec{u}_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad \vec{u}_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

For any 3D vector we can write

$$\begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = c_1\vec{u}_1 + c_2\vec{u}_2 + c_3\vec{u}_3 = \sum_{n=1}^3 c_n\vec{u}_n$$

Many choices of orthonormal basis set of vectors are possible, for ex.:

$$\vec{u}'_1 = \begin{pmatrix} \sqrt{2}/2 \\ \sqrt{2}/2 \\ 0 \end{pmatrix}, \quad \vec{u}'_2 = \begin{pmatrix} \sqrt{2}/2 \\ -\sqrt{2}/2 \\ 0 \end{pmatrix}, \quad \vec{u}'_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

for which we can write

$$\begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = c'_1\vec{u}'_1 + c'_2\vec{u}'_2 + c'_3\vec{u}'_3 = \sum_{n=1}^3 c'_n\vec{u}'_n$$