Determinants

Singular Matrices

what's the inverse of the following matrix

$$\underset{=}{Q} = \begin{pmatrix} 1 & 1 & 1 \\ 0 & 1 & 2 \\ 1 & -1 & -3 \end{pmatrix}$$

Using Gaussian Elimination:

$$\left(\begin{array}{ccc|ccc} 1 & 1 & 1 & 1 & 0 & 0 \\ 0 & 1 & 2 & 0 & 1 & 0 \\ 1 & -1 & -3 & 0 & 0 & 1 \end{array}\right)$$

subtract 1^{st} row from 3^{rd}:

$$\left(\begin{array}{ccc|ccc} 1 & 1 & 1 & 1 & 0 & 0 \\ 0 & 1 & 2 & 0 & 1 & 0 \\ 0 & -2 & -4 & -1 & 0 & 1 \end{array}\right)$$

Add $2\times$ 2^{nd} row to 3^{rd}:

$$\left(\begin{array}{ccc|ccc} 1 & 1 & 1 & 1 & 0 & 0 \\ 0 & 1 & 2 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 & 2 & 1 \end{array}\right)$$

This is a problem. The row of 0s on the left means we will <u>never</u> be able to turn it into the identity matrix. This is a <u>non-invertible</u> matrix. there is no $\underset{=}{Q}^{-1}$ such that

$$\underset{=}{Q}\,\underset{=}{Q}^{-1} = \underset{=}{I}$$

A non-invertible matrix is called <u>singular</u>. The problem is that one row can be written as a combination of the other 2:

$$(1 \;\; -1 \;\; -3) = (1 \;\; 1 \;\; 1) - 2(0 \;\; 1 \;\; 2)$$

Stated more generally, one row can be expressed in terms of all of the others:

$$(q_{11}, q_{12}, \ldots, q_{1n}) = c_2 (q_{21}, q_{22}, \ldots q_{2n}) + \cdots + c_n (q_{n1}, q_{n2} \ldots q_{nn})$$

And even more generally, if we write:

$$\sum_{i=1}^{n} c_i (q_{i1}, q_{i2}, \ldots q_{in}) = 0$$

Then for any singular matrix, there are some c_i values $\neq 0$ which satisfy this eqn.

If $\underline{\underline{Q}}$ is singular, then we'll also have singular matrices when we

- switch 2 rows in Q
- mutiply any row by a constant
- Add two rows and put the result in one of them
- transpose Q

Let's try the last of these..

$$\underline{\underline{Q}}^T = \begin{pmatrix} 1 & 0 & 1 \\ 1 & 1 & -1 \\ 1 & 2 & -3 \end{pmatrix}$$

$$\left(\begin{array}{ccc|ccc} 1 & 0 & 1 & 1 & 0 & 0 \\ 1 & 1 & -1 & 0 & 1 & 0 \\ 1 & 2 & -3 & 0 & 0 & 1 \end{array}\right)$$

Subtract row 1 from rows 2 & 3:

$$\left(\begin{array}{ccc|ccc} 1 & 0 & 1 & 1 & 0 & 0 \\ 0 & 1 & -2 & -1 & 1 & 0 \\ 0 & 2 & -4 & -1 & 0 & 1 \end{array}\right)$$

Subtract $2\times$ 2^{nd} row from 3^{rd}:

$$\left(\begin{array}{ccc|ccc} 1 & 0 & 1 & 1 & 0 & 0 \\ 0 & 1 & -2 & -1 & 1 & 0 \\ 0 & 0 & 0 & 1 & -2 & 1 \end{array}\right) \longleftarrow \text{Still singular}$$

Also note that because the transpose gets us a singular matrix, swapping columns, etc. also maintains singularity.

The Determinant (formally)

we want this value to determine if a matrix is singular or not. Singular $\rightarrow$ $\det(\underline{Q}) = 0$

- The identity matrix is not singular $\underline{I}^{-1} = \underline{I}$
  so: $\det I \equiv 1$

- Multiplying a row by a constant multiplies the determinant by that constant
  $$\det(cA) = c\det(A)$$

  - If $c = 0$ $\longrightarrow$ row will be 0, so $\det(\ )$ will also be 0

  - If we have a diagonal matrix,
    $$\det\begin{pmatrix} 2 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 5 \end{pmatrix} = 2\cdot3\cdot5 = 30$$

    the determinant of a diagonal matrix is the product of the diagonal values.

$$\det\begin{pmatrix} 2 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 5 \end{pmatrix} = \begin{vmatrix} 2 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 5 \end{vmatrix}$$ ← straight lines means determinant

- Adding the values of one row to another doesn't change the value of det (Q)

$$\begin{vmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix} = \begin{vmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{vmatrix} = \begin{vmatrix} 1 & 1 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{vmatrix}$$

- This means we can add or subtract any multiple of a row from another row and the determinant won't change:

$$\begin{vmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix} = 1 \qquad \begin{vmatrix} 1 & 0 & 0 \\ 0 & -2 & 0 \\ 0 & 0 & 1 \end{vmatrix} = -2$$

$$\begin{vmatrix} 1 & -2 & 0 \\ 0 & -2 & 0 \\ 0 & 0 & 1 \end{vmatrix} = -2 \qquad \begin{vmatrix} 1 & -2 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix} = 1$$

We can go further and say that any matrix with all zeros below the diagonal (or above) has a determinant equal to product of diagonals:

$$Q = \begin{vmatrix} 1 & a & b \\ 0 & 1 & c \\ 0 & 0 & 1 \end{vmatrix} = \begin{vmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix} = 1$$

- Switching 2 rows changes the sign of the determinant

- $|\underline{A}| = |\underline{A}^T|$ ← transpose has same determinant

∴ all we've said about rows applies to columns also.

Using Gaussian Elimination to get $|\underline{A}|$

$$|\underline{A}| = \begin{vmatrix} a & b \\ c & d \end{vmatrix} = \begin{vmatrix} a & b \\ c-\frac{c}{a}a & d-\frac{c}{a}b \end{vmatrix}$$

$$= \begin{vmatrix} a & b \\ 0 & d-\frac{c}{a}b \end{vmatrix}$$

product of diagonals:

$$a\left(d-\frac{c}{a}b\right) = ad-cb$$

Taken to larger matrices, this (i.e. gaussian elimination) gives us back our previous rules on divide & conquer:

$$\begin{vmatrix} a & b & c \\ d & e & f \\ g & h & i \end{vmatrix} = a\begin{vmatrix} e & f \\ h & i \end{vmatrix} - b\begin{vmatrix} d & f \\ g & i \end{vmatrix} + c\begin{vmatrix} d & e \\ g & h \end{vmatrix}$$

Some chemical Applications: Slater Determinants
General Linear systems

$$\begin{aligned} x + y - z &= 6 \\ 3x - y + z &= -3 \\ -x + y + 2z &= -10 \end{aligned}$$

Solving Linear Systems - two ways

$$\begin{aligned} x + y - z &= 6 \\ 3x - y + z &= -3 \\ -x + y + 2z &= -10 \end{aligned}$$

1. Treat coefficients as a determinant

$$D = \begin{vmatrix} 1 & 1 & -1 \\ 3 & -1 & 1 \\ -1 & 1 & 2 \end{vmatrix}$$

2. Multiply 1^{st} column by x, this changes values of Determinant

$$xD = \begin{vmatrix} x & 1 & -1 \\ 3x & -1 & 1 \\ -x & 1 & 2 \end{vmatrix}$$

3. Multiply 2^{nd} column by y and then add to 1^{st} column (this doesn't change overall determinant value):

$$xD = \begin{vmatrix} x+y & 1 & -1 \\ 3x-y & -1 & 1 \\ -x+y & 1 & 2 \end{vmatrix}$$

4. Do the same thing for z & 3^{rd} column:

$$xD = \begin{vmatrix} x+y-z & 1 & -1 \\ 3x-y+z & -1 & 1 \\ -x+y+2z & 1 & 2 \end{vmatrix}$$

5. Use the original equations to replace 1^{st} column:

$$xD = \begin{vmatrix} 6 & 1 & -1 \\ -3 & -1 & 1 \\ -10 & 1 & 2 \end{vmatrix}$$

6. Divide both sides by original determinant

$$x = \begin{vmatrix} 6 & 1 & -1 \\ -3 & -1 & 1 \\ -10 & 1 & 2 \end{vmatrix} \Bigg/ \begin{vmatrix} 1 & 1 & -1 \\ 3 & -1 & 1 \\ -1 & 1 & 2 \end{vmatrix}$$

This procedure is called <u>Cramer's rule</u>

To get y & z we'd simply move the result column to columns 2 & 3:

$$y = \begin{vmatrix} 1 & 6 & -1 \\ 3 & -3 & 1 \\ -1 & -10 & 2 \end{vmatrix} \Big/ \begin{vmatrix} 1 & 1 & -1 \\ 3 & -1 & 1 \\ -1 & 1 & 2 \end{vmatrix}$$

$$z = \begin{vmatrix} 1 & 1 & 6 \\ 3 & -1 & -3 \\ -1 & 1 & -10 \end{vmatrix} \Big/ \begin{vmatrix} 1 & 1 & -1 \\ 3 & -1 & 1 \\ -1 & 1 & 2 \end{vmatrix}$$

Solving these gives us:

$$x = 3/4$$
$$y = 5/12$$
$$z = -29/6$$

Cramer's rule is tedious, but works well. We just have to get very good at determinants

A short detour into inverses

We've done these already using Gauss Elimination (Be-comes very tedious when matrices get big.)

A simpler way:

$$\underline{\underline{A}}^{-1} = \frac{\underline{\underline{A}}_{cof}^{T}}{|\underline{\underline{A}}|}$$

$\underline{\underline{A}}_{cof}^{T}$ ← transpose of cofactor matrix

$|\underline{\underline{A}}|$ ← Determinant of matrix

Since $|\underline{\underline{A}}|$ is the determinant, $\underline{\underline{A}}^{-1}$ only exists when $|\underline{\underline{A}}| \neq 0$

$\underline{\underline{A}}_{cof}$ is a matrix of cofactors

$$\underline{\underline{A}}_{cof} = \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix}$$

where

$$A_{ij} = (-1)^{i+j} M_{ij}$$

M_{ij} ← minor of element a_{ij}

$$A_{21} = (-1)^{2+1} \begin{vmatrix} a_{12} & a_{13} \\ a_{32} & a_{33} \end{vmatrix} = (-1)(a_{12}a_{33} - a_{13}a_{32})$$

← just like a determinant

Let's do an example:

$$\underline{\underline{A}} = \begin{pmatrix} 1 & 1 & -1 \\ 3 & -1 & 1 \\ -1 & 1 & 2 \end{pmatrix}$$

$$|\underline{\underline{A}}| = 1\begin{vmatrix} -1 & 1 \\ 1 & 2 \end{vmatrix} - 1\begin{vmatrix} 3 & 1 \\ -1 & 2 \end{vmatrix} - 1\begin{vmatrix} 3 & -1 \\ -1 & 1 \end{vmatrix}$$

$$= -3 - 7 - 2 = -12$$

$$\underline{\underline{A}}_{cof} = \begin{pmatrix} -3 & -7 & 2 \\ -3 & 1 & -2 \\ 0 & -4 & -4 \end{pmatrix}$$

The transpose of this is easy:

$$\underline{\underline{A}}^T_{cof} = \begin{pmatrix} -3 & -3 & 0 \\ -7 & 1 & -4 \\ 2 & -2 & -4 \end{pmatrix}$$

$$\underline{\underline{A}}^{-1} = \frac{1}{-12}\begin{pmatrix} -3 & -3 & 0 \\ -7 & 1 & -4 \\ 2 & -2 & -4 \end{pmatrix} = \begin{pmatrix} 1/4 & 1/4 & 0 \\ 7/12 & -1/12 & 1/3 \\ -1/6 & 1/6 & 1/3 \end{pmatrix}$$

To <u>Check</u>:

$$\underline{\underline{A}}^{-1}\cdot\underline{\underline{A}} = \begin{pmatrix} 1/4 & 1/4 & 0 \\ 7/12 & -1/12 & 1/3 \\ -1/6 & 1/6 & 1/3 \end{pmatrix}\begin{pmatrix} 1 & 1 & -1 \\ 3 & -1 & 1 \\ -1 & 1 & 2 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

<u>Now</u>:

$$\begin{aligned} x + y - z &= 6 \\ 3x - y + z &= -3 \\ -x + y + 2z &= -10 \end{aligned} \Rightarrow \begin{pmatrix} 1 & 1 & -1 \\ 3 & -1 & 1 \\ -1 & 1 & 2 \end{pmatrix}\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 6 \\ -3 \\ -10 \end{pmatrix}$$

$$\underline{\underline{A}} \cdot \vec{x} = \vec{b}$$

$$\underline{\underline{A}}^{-1}\cdot\underline{\underline{A}} \cdot \vec{x} = \underline{\underline{A}}^{-1}\cdot\vec{b}$$

$$\underline{\underline{I}} \cdot \vec{x} = \underline{\underline{A}}^{-1}\cdot\vec{b}$$

$$\vec{x} = \underline{\underline{A}}^{-1}\cdot\vec{b}$$

$$\underline{\underline{A}}^{-1}\cdot\vec{b} = \begin{pmatrix} 1/4 & 1/4 & 0 \\ 7/12 & -1/12 & 1/3 \\ -1/6 & 1/6 & 1/3 \end{pmatrix}\begin{pmatrix} 6 \\ -3 \\ -10 \end{pmatrix}$$

$$\vec{x} = \begin{pmatrix} 6/4 - 3/4 \\ 42/12 + 3/12 - 10/3 \\ -1 - 1/2 - 10/3 \end{pmatrix} = \begin{pmatrix} 3/4 \\ 5/12 \\ -29/6 \end{pmatrix} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

Trace

The trace of a matrix is the sum of its diagonal elements:

$$Tr[\underline{\underline{A}}] = \sum_{i=1}^{n} a_{ii}$$

Example:

$$\underline{\underline{A}} = \begin{pmatrix} 2 & 1 & 0 \\ 4 & 3 & 2 \\ 7 & 1 & -1 \end{pmatrix} \qquad Tr[\underline{\underline{A}}] = 2+3+(-1) = 4$$

Complex Vectors

$$|\vec{u}\rangle = \vec{u} = u_1\hat{i} + u_2\hat{j}$$

where u_1 & u_2 are complex numbers, so the rules for some vector operations change a bit:

The inner product of complex vectors is one way of multiplying two of these to give real lengths:

complex conjugate

transpose

$$\langle\vec{u}|\vec{v}\rangle = (\vec{u}^*)^T \cdot \vec{v} = u_1^* v_1 + u_2^* v_2$$

$$|\vec{u}| = \langle\vec{u}|\vec{u}\rangle^{1/2} = (u_1^* u_1 + u_2^* u_2)^{1/2}$$

An example of why the matrix inverse is so important:

$$2x + y + 3z = 4$$
$$2x - 2y - z = 1$$
$$-2x + 4y + 1 = 1$$

we want this

$$\begin{pmatrix} 2 & 1 & 3 \\ 2 & -2 & -1 \\ -2 & 4 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 4 \\ 1 \\ 1 \end{pmatrix}$$

$$\underline{A} \cdot \vec{x} = \vec{b}$$

Left multiply by $\underline{A}^{-1}$

$$\underline{A}^{-1} \cdot \underline{A} \cdot \vec{x} = \underline{A}^{-1} \cdot \vec{b}$$

$$\underline{I} \cdot \vec{x} = \underline{A}^{-1} \cdot \vec{b}$$

$$\vec{x} = \underline{A}^{-1} \cdot \vec{b}$$

so if we can find $\underline{A}^{-1}$ this linear system is easily solved

$|\underline{A}| = 16$

$$\underline{A}^{-1} = \begin{pmatrix} \frac{1}{8} & \frac{11}{16} & \frac{5}{16} \\ 0 & 1/2 & 1/2 \\ 1/4 & -5/8 & -3/8 \end{pmatrix}$$

$$\underline{A}_{cof} = \begin{pmatrix} 2 & 0 & 4 \\ 11 & 8 & -5 \\ 5 & 8 & -3 \end{pmatrix}$$

So

$$\vec{x} = \begin{pmatrix} \frac{1}{8} & \frac{11}{16} & \frac{5}{16} \\ 0 & 1/2 & 1/2 \\ 1/4 & -5/8 & -3/8 \end{pmatrix} \begin{pmatrix} 4 \\ 1 \\ 1 \end{pmatrix}$$

$$x = \frac{1}{2} + 11/16 + 5/16 = 3/2$$

$$y = 0 + 1/2 + 1/2 = 1$$

$$z = 1 - 5/8 - 3/8 = 0$$

You can get the same answer in many ways but for large linear systems (10×10) the inverse is usually the fastest.

Unitary Transformation

Linear transformation: $\underline{\underline{A}}(\alpha \vec{u} + \beta \vec{v}) = \alpha \underline{\underline{A}}\vec{u} + \beta \underline{\underline{A}}\vec{v}$

A unitary transformation is a special linear transformation that preserves the length of a vector (even a complex vector!)

Example: rotation of a molecule preserves bond lengths

complex conjugate

transpose

$$\langle \underline{\underline{A}} \cdot \vec{u} | = (\underline{\underline{A}} \cdot \vec{u})^{*T}$$ ← new vector

$$| \underline{\underline{A}} \cdot \vec{u} \rangle = \underline{\underline{A}} \cdot \vec{u}$$

If a matrix $\underline{\underline{A}}$ is unitary; length of $\vec{u}$ is preserved

$$\langle \underline{\underline{A}} \cdot \vec{u} | \underline{\underline{A}} \cdot \vec{u} \rangle = \langle \vec{u} | \vec{u} \rangle = (\vec{u}^*)^T \cdot \vec{u}$$

$$\parallel \qquad\qquad\qquad \parallel$$

$$(\underline{\underline{A}}^* \vec{u}^*)^T \cdot (\underline{\underline{A}} \cdot \vec{u}) = \vec{u}^{*T} \cdot \underline{\underline{A}}^{*T} \cdot \underline{\underline{A}} \cdot \vec{u}$$

true only iff:

$$(\underline{\underline{A}}^*)^T \cdot \underline{\underline{A}} = \underline{\underline{I}}$$

or

$$(\underline{\underline{A}}^*)^T = \underline{\underline{A}}^{-1}$$

$$(\underline{\underline{A}}^*)^T \equiv \underline{\underline{A}}^\dagger$$ ← Hermitian transpose of $\underline{\underline{A}}$

or

Hermitian conjugate

In general, the determinant of a unitary transform is 1, and all rows & columns form an orthogonal set.

Example Show $\underline{\underline{A}} = \frac{1}{5}\begin{pmatrix} -1+2i & -4-2i \\ 2-4i & -2-i \end{pmatrix}$

is unitary

$$\underline{\underline{A}}^{\dagger} = (\underline{\underline{A}}^{*})^{T} = \frac{1}{5}\begin{pmatrix} -1-2i & 2+4i \\ -4+2i & -2+i \end{pmatrix}$$

$$\underline{\underline{A}}^{\dagger} A = \frac{1}{25}\begin{pmatrix} -1-2i & 2+4i \\ -4+2i & -2+i \end{pmatrix}\begin{pmatrix} -1+2i & -4-2i \\ 2-4i & -2-i \end{pmatrix}$$

$$= \frac{1}{25}\begin{pmatrix} 25 & 0 \\ 0 & 25 \end{pmatrix} = \underline{\underline{I}}$$

Hilbert Space

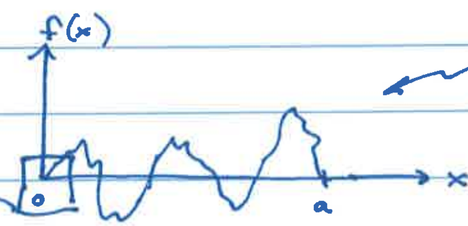
In artesian coordinates, a vector is a set of components (v_x, v_y, v_z). Any vector can be written in terms of the 3 unit vectors or the basis set for this space:

$$\vec{V} = \begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix} = v_x \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} + v_y \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} + v_z \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

$$= v_x \hat{\imath} + v_y \hat{\jmath} + v_z \hat{k}$$

$\hat{\imath}, \hat{\jmath}, \hat{k}$ form a complete basis for 3D space, i.e. they span the vector space.

Hilbert spaces have many dimensions. Consider the function $(f(x))$ on a fixed domain $0 \rightarrow a$



an arbitrary function $f(x)$

We could describe $f(x)$ as a vector where each element was a small chunk of the line along x:

$$f(x) = 0.1 \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ \vdots \end{pmatrix} + 0.3 \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix} + 0.4 \begin{pmatrix} 0 \\ 0 \\ 1 \\ \vdots \end{pmatrix} + \ldots$$

This is not very efficient or sensible, because

We'd need to know Δx to describe the function and if we decide to change Δx (i.e. for a rapidly-varying function), we have to change all of our coefficients

However, we could also write $f(x)$ in terms of other functions

$$f(x) = 0.1 \underbrace{\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ \vdots \end{pmatrix}}_{\text{represents } \sqrt{\frac{2}{a}} \sin\frac{\pi x}{a}} + 0.2 \underbrace{\begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix}}_{\text{represents } \sqrt{\frac{2}{a}} \sin\frac{2\pi x}{a}} + 0.1 \underbrace{\begin{pmatrix} 0 \\ 0 \\ 1 \\ \vdots \end{pmatrix}}_{\text{represents } \sqrt{\frac{2}{a}} \sin\frac{3\pi x}{a}} + \dots$$

A Hilbert space is a function space where each function is treated as an independent vector

$$f(x) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{a}} \sin\frac{n\pi x}{a} \quad \longleftarrow \text{expansion of } f(x) \text{ in the basis functions}$$

$$= \sum_{n=1}^{\infty} c_n \, |n\rangle$$

c_n: coefficients that describe $f(x)$ in this space

I picked $|n\rangle = \sqrt{\frac{2}{a}} \sin\frac{n\pi x}{a}$ for a few reasons.

All of these functions $\to 0$ at $x = 0$ & a

$\therefore$ All $f(x)$ we can represent also do this

There are an infinite number of these functions, so the Hilbert space is an <u>infinite dimensional</u> vector space.

Consider a <u>vector</u> dot product

$$\vec{V} \cdot \vec{u} = V_x u_x + V_y u_y + V_z u_z$$

In a Hilbert space we do something similar.

$$\int_0^a f^*(x)\, g(x)\, dx \quad \longleftarrow \text{How is this like a vector product?}$$

$$f^*(x) = \sum_{n=1}^{\infty} c_n^* \langle n|$$

← complex conjugate of basis function $|n\rangle$

← complex conjugate of coefficient c_n

$$g(x) = \sum_{m=1}^{\infty} g_m |m\rangle$$

← $g(x)$ is a different function so the coefficients are different

$$\int_0^a f^*(x)\, g(x)\, dx = \int_0^a \left(\sum_{n=1}^{\infty} c_n^* \langle n|\right)\left(\sum_{m=1}^{\infty} g_m |m\rangle\right) dx$$

$$= \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} c_n^* g_m \int_0^a \langle n|m\rangle\, dx$$

The functions $\sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$ and $\sqrt{\frac{2}{a}} \sin \frac{m\pi x}{a}$

have this neat property $\int_0^a \langle n|m\rangle\, dx = \frac{2}{a} \int \sin \frac{n\pi x}{a} \sin \frac{m\pi x}{a}\, dx$

$$= \begin{cases} 1 & \text{if } n = m \\ 0 & \text{if } n \neq m \end{cases}$$

So: $\int_0^a f^*(x)\, g(x)\, dx = \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} c_n^* g_m \; \delta_{nm}$

Kronecker delta $= \begin{cases} 1 & n = m \\ 0 & n \neq m \end{cases}$

we call these functions orthogonal basis functions.

$$\int f^*(x)\, g(x)\, dx = \sum_{n=1}^{\infty} c_n^* g_n$$

massively complicated integral

just like a dot product (and very simple)

Other Hilbert space expansions

$$|n\rangle = e^{2\pi i n \theta} \leftarrow \text{Fourier Transform}$$

used in NMR, IR and mass-spectrometry

$$f(\theta,\phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} c_{lm} Y_l^m(\theta,\phi) \leftarrow$$ spherical harmonics (orbitals)

$$(1-x)^{\alpha}(1+x)^{\beta} \leftarrow$$ Jacobi polynomials (orthogonal on [-1, 1])

$$P_n(x) = \frac{1}{2^n\, n!} \frac{d^n}{dx^n}\left[(x^2-1)^n\right] \leftarrow$$ Legendre Polynomials

Important in rotational or microwave spectroscopy.