FUNCTIONS AS (AND) VECTORS

- Think of a function over the integers 1 to 5, for example f(x)=x!

- The vector

$$\begin{bmatrix} 1 \\ 2 \\ 6 \\ 24 \\ 120 \end{bmatrix}$$

completely represents this function.

- With ‘usual’ functions over the real numbers it is a bit more unusual and more difficult to visualize because the vector is infinitely long but in principle it is exactly the same.

LINEAR ALGEBRA DEALS WITH VECTOR SPACES

- Any function can be expressed in a suitable basis.
- The normal function space of real (or complex) numbers is the Hilbert space.
- A function can thought of as a mapping $x \rightarrow y$

In the Hilbert space a function is a single vector.
The equivalent of the basis (x,y,z…) is the infinite x vector.
The equivalent of the weights is components in each dimension is y.

LINEAR ALGEBRA: FUNCTION SPACES

- Now that is very useful !

It can guide us, for example, if we want to convert algebraic equations to matrix equations which can be solved on the computer. Algebraic equations are, for example, differential equations like wave or diffusion equations.

- Normally we do not work in the infinite Hilbert space but take finite bases which we can treat numerically.

- By the way, who was Hilbert ?

MAIN EQUATION

A function can be expressed in a basis Ψ as

$$f(x) = \sum_k a_k \Psi_k(x)$$

The $\Psi_k(x)$ are called basis (expansion) functions. The weights a_k are the only unknowns and are found by solving above matrix equation.

Then we have the representation of a function in a given basis.

This is very powerful

It allows one to choose some universal set of functions in terms of which all other (well-behaved) functions can be represented just as a set of coefficients.

Think of the spaces made up of Fourier components, finite elements, atomic orbitals.

THE BASIS FUNCTIONS Ψ

If the $\Psi_k(x)$ fulfill

$$\int_{-\infty}^{\infty} \Psi_k^*(x)\Psi_j(x)dx = 0 \quad (k \neq j)$$

they are called orthogonal.

Think of s , p, d, f functions (spherical harmonics) and other solutions of important equations.

Orthogonality is a good feature because the basis functions are then independent of each other, just like x,y,z are perpendicular to each other and do not mix.

LINEAR ALGEBRA: FUNCTION SPACES

If they also fulfill

$$< \Psi_k(x), \Psi_j(x) > \; = \; \int_{-\infty}^{\infty} \Psi_k^*(x)\Psi_j(x)dx = 1 \;\; (k = j)$$

they are called orthonormal.

- The condition that the integral is 1 can easily be achieved by normalization.
- The orthogonality can not so easily be guaranteed but there are procedures to create mixtures of non-orthogonal functions to make them orthogonal.
- It is be normally better if they are orthogonal from the beginning.