Part 2: Partial Differential Equations

Most of our mathematical models in physics and engineering are built on Partial Differential Equations.

Imagine there is some quantity ψ that we would like to compute. Physical laws usually give us relationships for the derivatives of ψ, and it is up to us to compute what ψ is.

E.g. Waves in water

$$\nabla^2\psi = \frac{1}{v^2}\frac{\partial^2\psi}{\partial t^2}$$

Heat flow through a solid:

$$\nabla^2\psi = -\kappa^2\frac{\partial\psi}{\partial t}$$

Wave function of an electron:

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V(x,y,z)\psi = E\psi$$

Before solving these, we begin by revisiting a 1D problem:
<u>The Helmholtz equation in one dimension</u>
(e.g. the vibration of a guitar string)

Find $f(x)$ on the domain $0 \leq x \leq L$, where

$$-\frac{d^2 f}{dx^2} = \lambda f$$

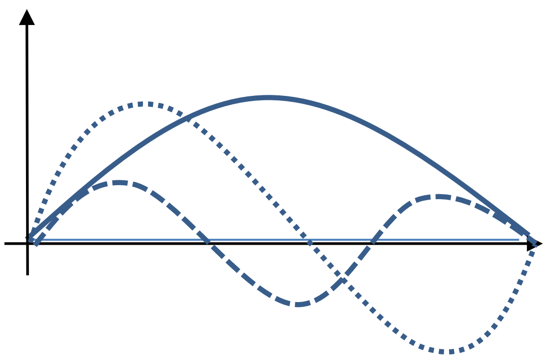
and $f(0) = f(L) = 0$.

The problem we have just solved, i.e.

Find $f(x)$ on the domain $0 \leq x \leq L$, where

$$-\frac{d^2 f}{dx^2} = \lambda f$$

and $f(0) = f(L) = 0$.



is known as a Sturm-Liouville Boundary value problem.

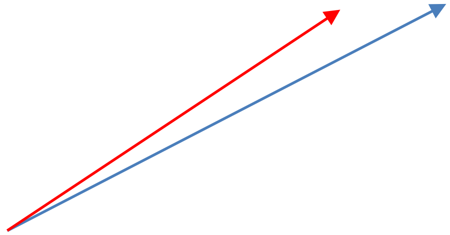
This week we will be going through the main points of S-L theory, so that we can use it to solve PDEs in higher dimensions.

- **The Inner Product for Functions**
- **Differential Operators**
- **The Sturm-Liouville Eigenvalue Problem**
- **Expansion in terms of eigenfunctions**

The Inner Product for functions and Orthogonality

The inner product for vectors

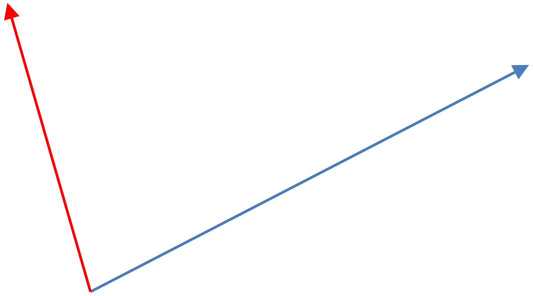
Recall the dot product between two vectors:



$$\mathbf{a} \cdot \mathbf{b}$$

This scalar quantity tells us how much two vectors are in alignment,
or, in other words, “how much” of one vector points in the direction of the other.

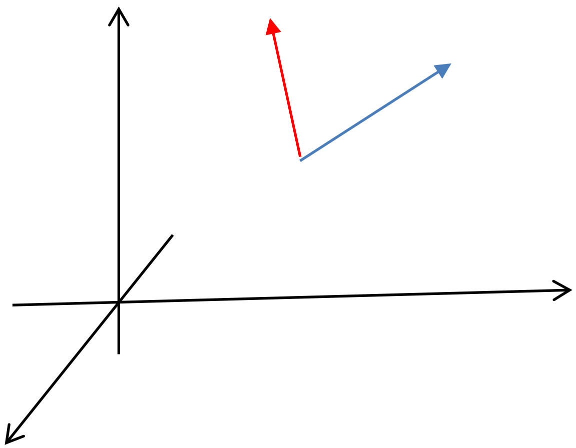
If $\mathbf{a} \cdot \mathbf{b} = 0$ then **a** and **b** are said to be *orthogonal*



The dot product is an example of an *inner product*.

The inner product

$$\mathbf{a} \cdot \mathbf{b}$$



has the following properties:

1. $\mathbf{a} \cdot \mathbf{b} = \mathbf{b} \cdot \mathbf{a}$

2. $\mathbf{a} \cdot k\mathbf{b} = k\mathbf{b} \cdot \mathbf{a}$

3. $\mathbf{a} \cdot (\mathbf{b} + \mathbf{c}) = \mathbf{a} \cdot \mathbf{b} + \mathbf{a} \cdot \mathbf{c}$

4. $\mathbf{a} \cdot \mathbf{a}$ is real and positive, and is zero iff $\boldsymbol{a} = 0$

We call $|a| = \sqrt{\boldsymbol{a} \cdot \boldsymbol{a}}$ the *vector norm* of $\boldsymbol{a}$.

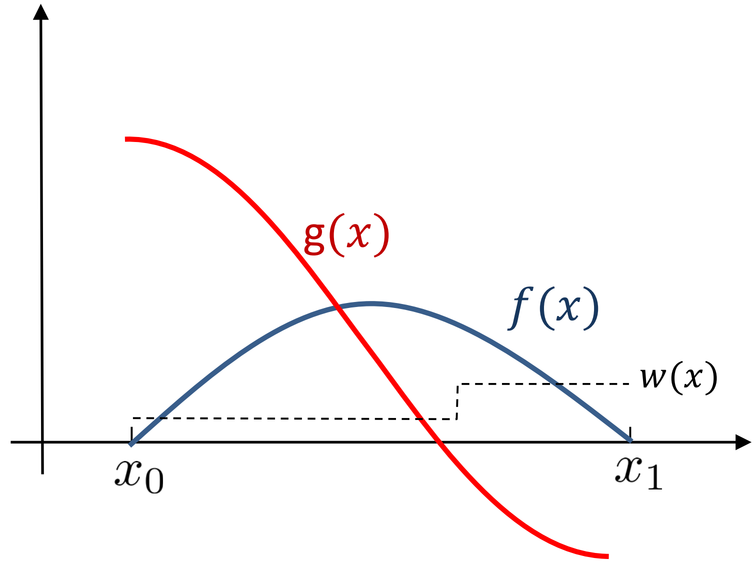
The inner product for functions

Consider two functions $f(x)$ and $g(x)$, defined on a domain $D = \{x: x_0 < x < x_1\}$

We define the *inner product* between f and g as the scalar quantity

$$\langle f, g \rangle = \int_D f^*(x) g(x)\ w(x) \mathrm{d}x$$

where $w(x)$ is a positive real function, known as the *weight function.*

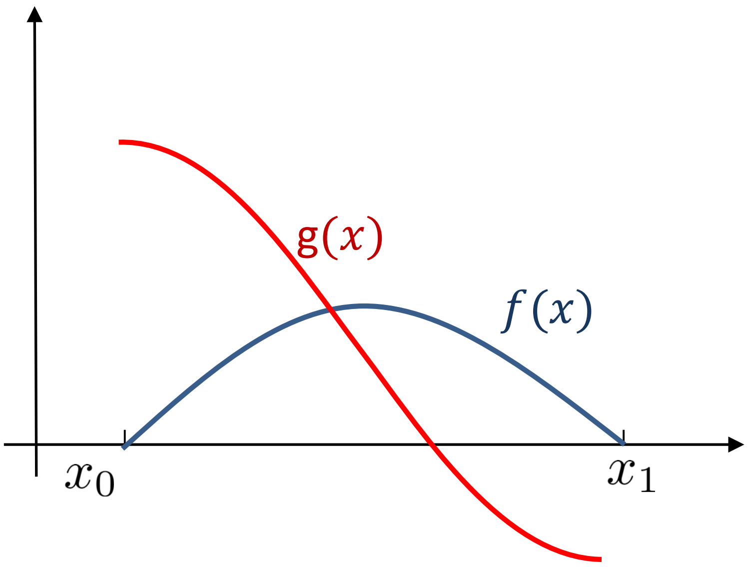


- The quantity $\langle f, g \rangle$ is a complex scalar (don't get it confused with vector notation)

- The weight function is just there to make things more general:
Most of the time $w = 1$.

The inner product

$$\langle f, g\rangle = \int_D f^*(x)g(x)\ w(x)\mathrm{d}x$$



has the following properties:

1. $\langle f, g\rangle = \langle g, f\rangle^*$

2. $\langle f, kg\rangle = k\ \langle f, g\rangle$

3. $\langle f, g + h\rangle = \langle f, g\rangle + \langle f, h\rangle$

4. $\langle f, f\rangle$ is real and positive, and is zero iff $f = 0$.

   We call $||\mathrm{f}|| \coloneqq \sqrt{\langle f, f\rangle}$ the *norm of f* on D.

We say that f and g are <u>orthogonal functions</u> if

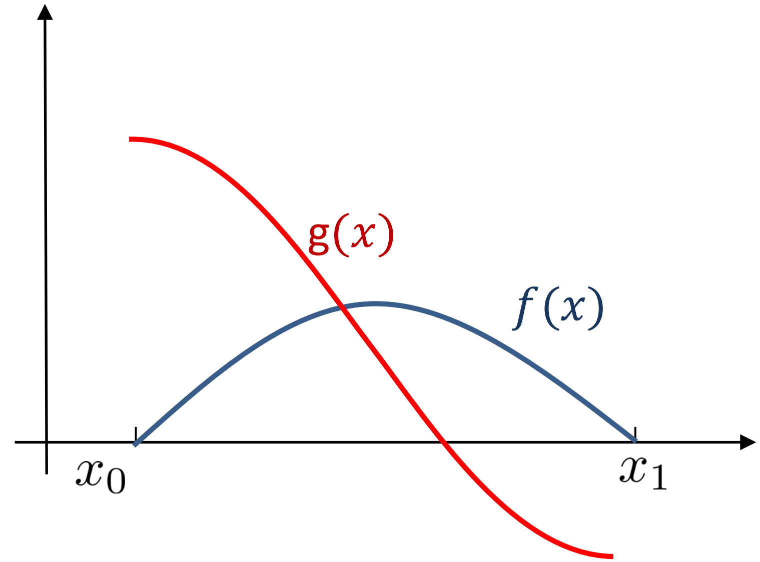
$$\langle f, g \rangle = 0$$

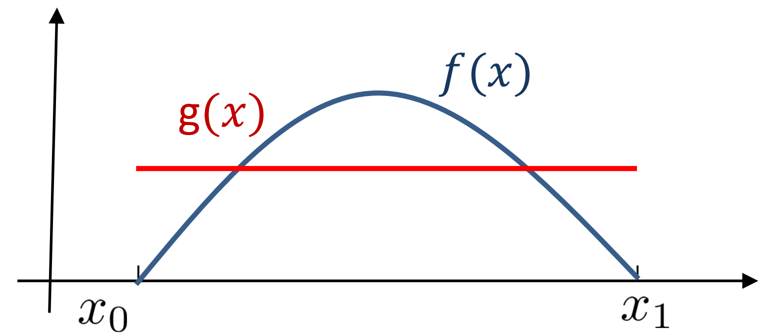
That is, if the integral of their product is zero:

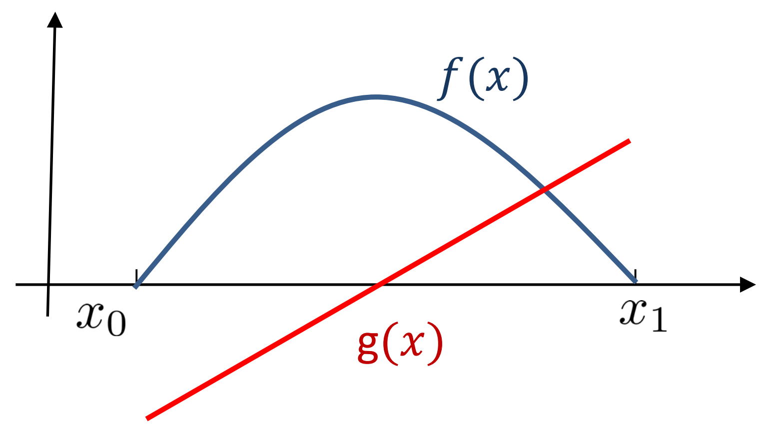
$$\int_{x_0}^{x_1} f^*(x) g(x)\ w(x) \mathrm{d}x = 0$$

Two functions f and g are orthogonal if, in some sense, there is “g”-ness in g and vice-versa.

Formally, this says that f and g are *Linearly Independent*





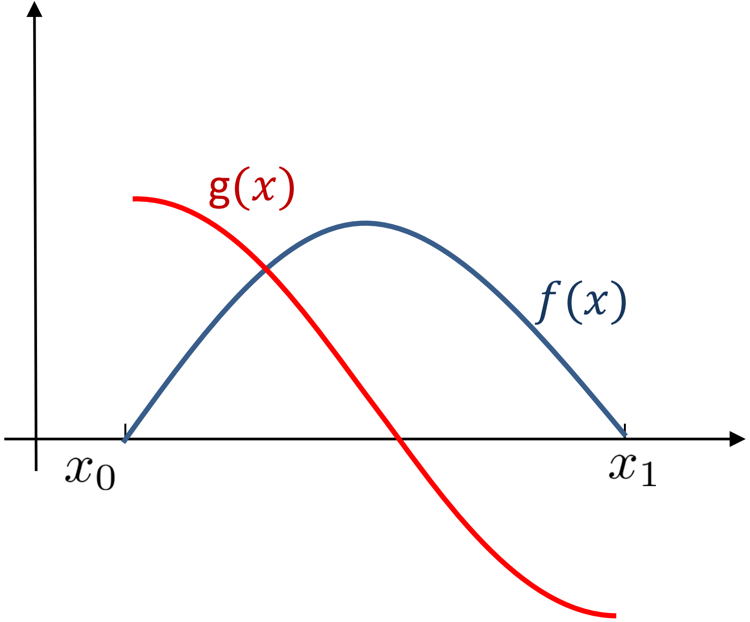


Example: Consider

$$f(x) = \sin x$$

$$g(x) = \cos x$$

with $w(x) = 1$ on $x \in [0, 2\pi]$

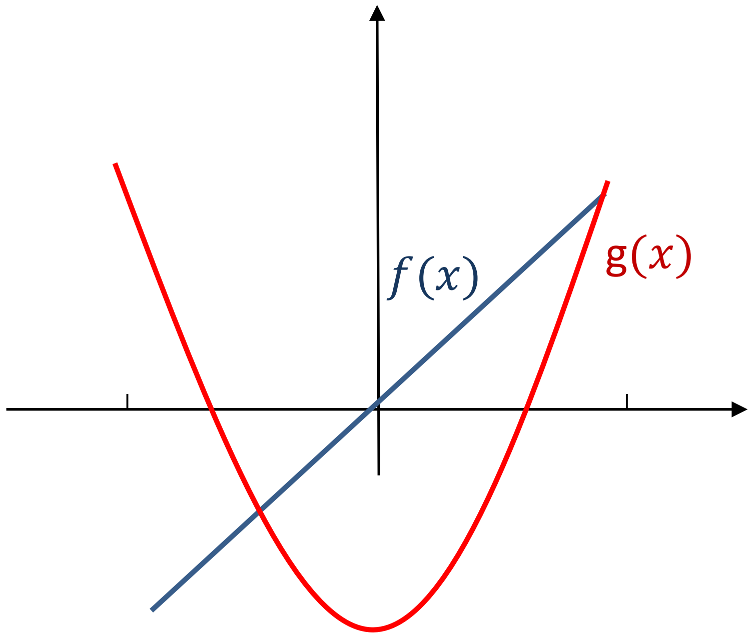


Example: Consider

$$f(x) = x$$

$$g(x) = \frac{1}{2}(3x^2 - 1)$$

with $w(x) = 1$ on $x \in [-1,1]$

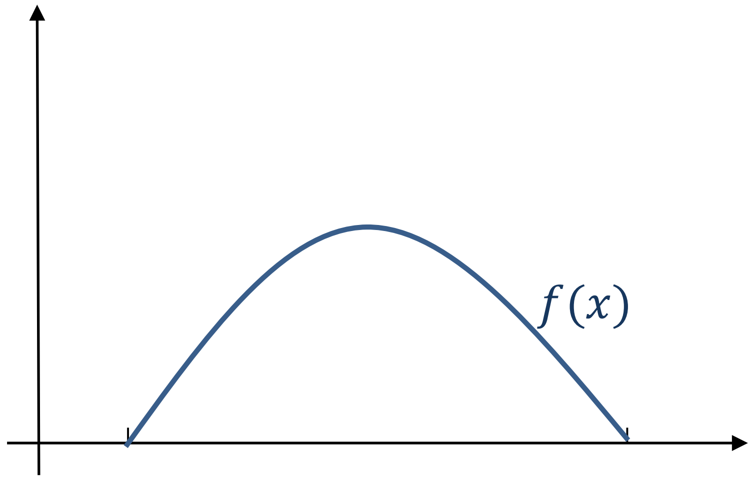


Differential Operators

An *operator* is a device for turning one function into another. For the function u, we create a new function

$$g = \mathcal{L}u$$

using the operator $\mathcal{L}$.



Examples:

The operator $\mathcal{L} = \dfrac{d}{dx}$ acts on a function f to form $\mathcal{L}f = \dfrac{df}{dx}$

$$\mathcal{L} = 2$$

$$\mathcal{L} = -\frac{d^2}{dx^2}$$

$$\mathcal{L} = e^{-x}$$

Note that the *direction from which the operator is applied can be important.*

E.g.

$$\mathcal{L} = \frac{d}{dx}$$

Applied on the left side of f gives

$$\mathcal{L}f = \frac{df}{dx}$$

But applied on the right side of f gives *another operator*:

$$f\mathcal{L} = f\frac{d}{dx}$$

Once we have an operator, we can see how it behaves
in conjunction with an inner product.

$$\langle f, \mathcal{L}g \rangle = \int_D f^*(x)\mathcal{L}g(x)\ w(x)\mathrm{d}x$$

There are three major properties that a lot of differential operators have, and which are really useful if they do have them:

1. Linearity

2. Positivity

3. Self-Adjoint-ness

An operator is linear if, for any two functions f and g :

$$\mathcal{L}(f+g) = \mathcal{L}f + \mathcal{L}g$$

$$\mathcal{L}(kf) = k\mathcal{L}f$$

for any constant k.

$$\mathcal{L} = \frac{d}{dx}$$

$$\mathcal{L} = -\frac{d^2}{dx^2}$$

$$\mathcal{L} = \frac{d^2}{dx^2}\frac{d}{dx} + \frac{d}{dx}$$

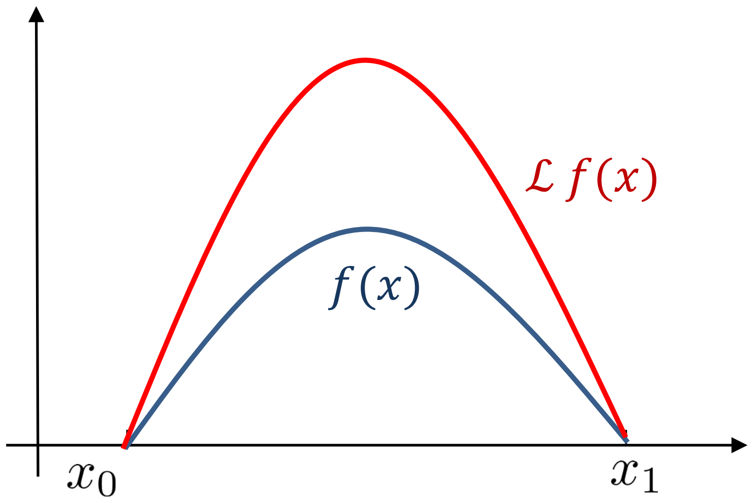
$$\mathcal{L} = \frac{d}{dx} + x$$

An operator is positive if, for any function f:

$$\langle f, \mathcal{L} f \rangle \quad \geq 0$$

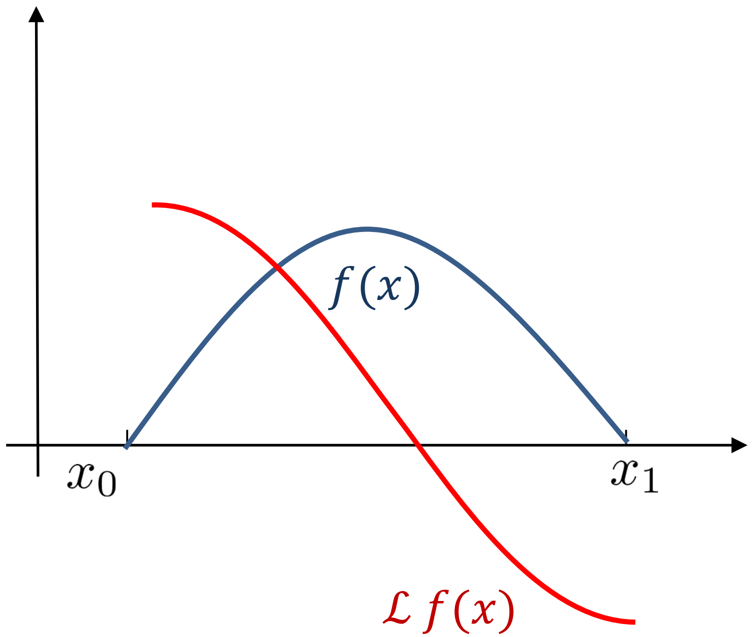
E.g. consider

$$\mathcal{L} = 2$$



An operator is self-adjoint if, for any functions f and g, we have

$$\langle f, \mathcal{L}g \rangle = \langle \mathcal{L}f, g \rangle$$



This looks complicated, but most interesting differential operators are self-adjoint.

E.g. You can prove that

$$\mathcal{L} = -\frac{d^2}{dx^2} + V(x)$$

is self-adjoint.

The Sturm-Liouville Eigenvalue Problem

The Sturm-Liouville Operator

We now introduce an important type of 2nd-order linear operator, called the Sturm-Liouville operator. This operator is defined as

$$\mathcal{L} = -\frac{1}{w(x)}\left[\frac{d}{dx}p(x)\frac{d}{dx} - q(x)\right]$$

where $p(x), w(x) > 0$ and $q(x) \geq 0$.

This looks complicated, but almost any 2nd-order DE can be put in this form.

E.g.

$$\mathcal{L} = -\frac{d^2}{dx^2}$$

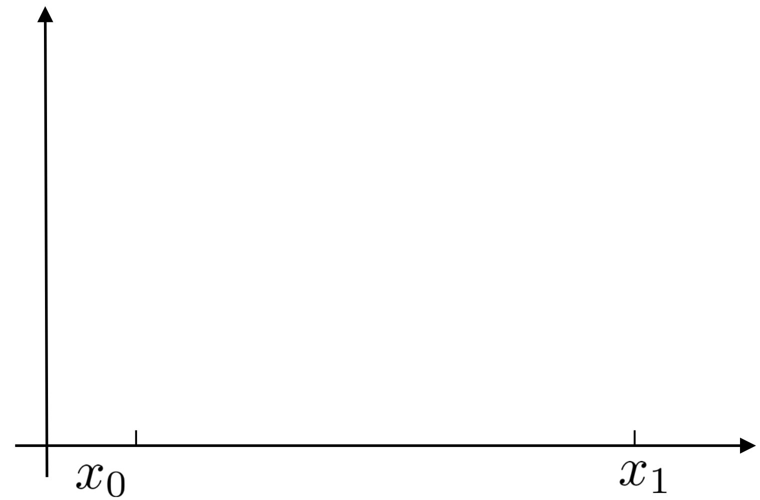
$$\mathcal{L} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$$

Any S-L operator is *linear, self-adjoint, and positive.*

$$\mathcal{L} = -\frac{1}{w(x)}\left[\frac{d}{dx}p(x)\frac{d}{dx} - q(x)\right]$$

The Sturm-Liouville eigenvalue problem

We consider the following problem on a domain $D = \{x: x_0 \leq x \leq x_1\}$:



$$\mathcal{L}\phi = \lambda\phi \quad \text{on } D$$

where $\mathcal{L}$ is the S-L differential operator.

$$\mathcal{L} = -\frac{1}{w(x)}\left[\frac{d}{dx}p(x)\frac{d}{dx} - q(x)\right]$$

Plus boundary conditions of <u>either</u> $\phi(x_0) = \phi(x_1) = 0$

<u>or</u> $\phi'(x_0) = \phi'(x_1) = 0.$

This type of problem is called an *eigenvalue problem*. The solutions form a set:

By convention: $\phi = 0$, $\lambda = 0$ is always a solution, and we omit this from the set.

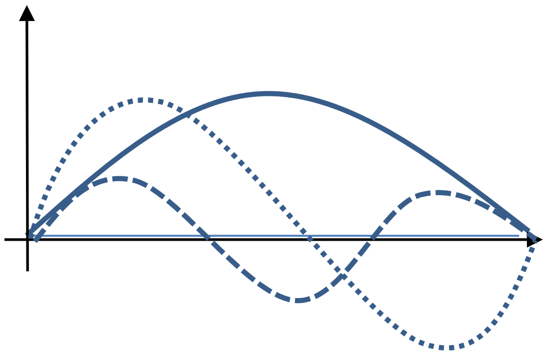
The solution ϕ_n is the eigenfunction corresponding to the eigenvalue n.

The “vibration of a guitar string” problem that we solved earlier

Find $f(x)$ on the domain $0 \leq x \leq L$, where

$$-\frac{d^2 f}{dx^2} = \lambda f$$

and $f(0) = f(L) = 0$.



is a Sturm-Liouville problem.

Other examples:
Wavefunction of an electron in a square well:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\phi = \lambda\phi$$

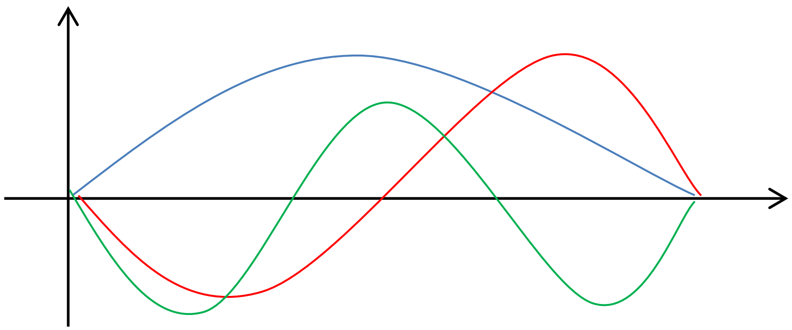
Properties of Sturm-Liouville problems

S-L problems all have the following important properties:

$$\mathcal{L}\phi = \lambda\phi \quad \text{on } D$$

1. There is an infinite set of eigenfunctions and eigenvalues

$$\{\phi_m, \lambda_m\}$$



2. All Eigenvalues are real and positive

$$0 \leq \lambda_0 \leq \lambda_1 \leq \lambda_2 \ldots$$

3. Eigenfunctions are *orthogonal*

$$\langle \phi_m, \phi_n \rangle = \delta_{n,m} ||\phi_m||^2$$

4. The Eigenfunctions form a complete set

Proof that eigenfunctions are *orthogonal:*

Proof that eigenvalues are *real and positive:*

Analytic solutions to the S-L problem

In general exact solutions are rare.
Two important examples in 1D:

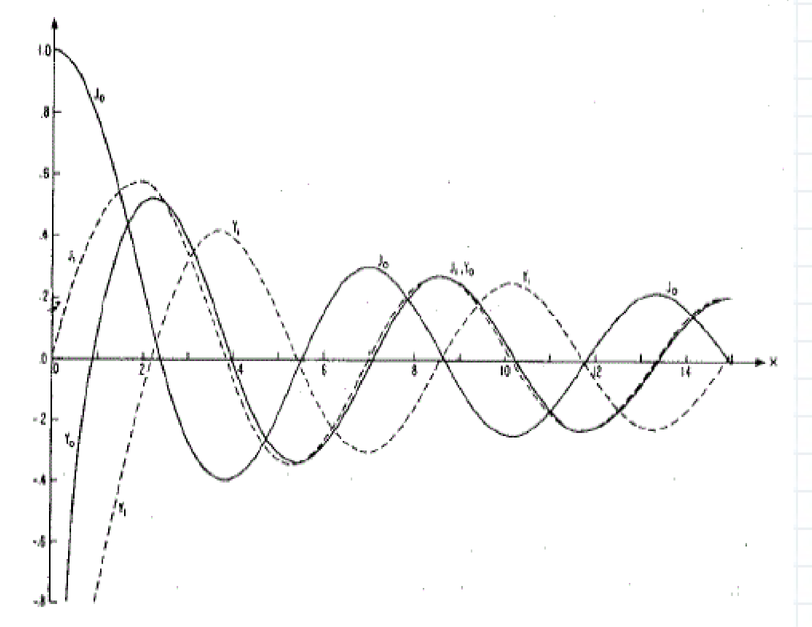
1. The Helmholtz equation

$$-\frac{d^2}{dx^2}\phi = \lambda\phi$$

2. Bessel's equation

This arises from the decomposition of the Laplacian into polar coordinates.

$$-\frac{d^2\phi}{dx^2} - \frac{1}{x}\frac{d\phi}{dx} + \frac{m^2}{x^2}\phi = \lambda\phi$$



The general solutions to this equation are *Bessel functions:*

$$\phi(x) = AJ_m(\sqrt{\lambda}x) + BY_m(\sqrt{\lambda}x)$$

Bessel functions can only be expressed as infinite series: e.g.

$$J_m(x) = \sum_{k=0}^{\infty} \frac{(-1)^k (x/2)^{2k+m}}{k!(k+m)!}$$

(To find the terms in this series we use the method of undetermined coefficients.)

E.g. Solve the S-L problem

$$-\frac{d^2\phi}{dx^2} - \frac{1}{x}\frac{d\phi}{dx} + \frac{1^2}{x^2}\phi = \lambda\phi$$

on the domain 0<x<2 with boundary conditions $\phi(0) = \phi(2) = 0$.

Expansion in terms of eigenfunctions

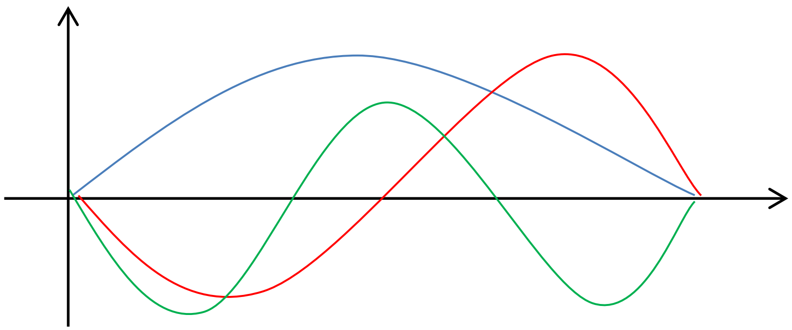
Properties of Sturm-Liouville problems

S-L problems all have the following important properties:

$$\mathcal{L}\phi = \lambda\phi \quad \text{on } D$$

1. There is an infinite set of eigenfunctions and eigenvalues

$$\{\phi_m, \lambda_m\}$$



2. All Eigenvalues are real and positive

$$0 \leq \lambda_0 \leq \lambda_1 \leq \lambda_2 \ldots$$

3. Eigenfunctions are *orthogonal*

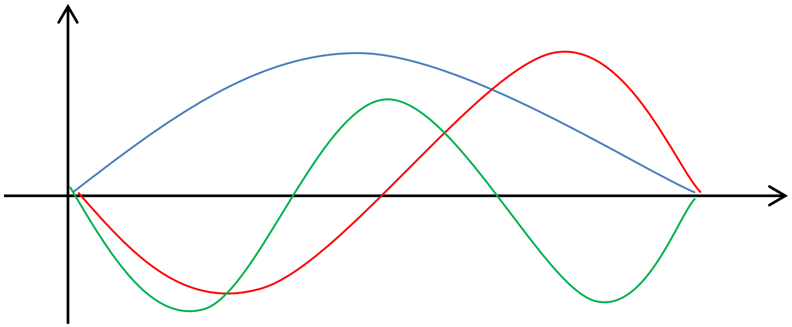
$$\langle \phi_m, \phi_n \rangle = \delta_{n,m} ||\phi_m||^2$$

4. The Eigenfunctions form a complete set

4. The Eigenfunctions form a complete set

This means that *any function* can be expanded in terms of the eigenfunctions of the S-L operator.

$$f(\mathbf{x}) = \sum_{m=0}^{\infty} c_m \phi_m(\mathbf{x})$$

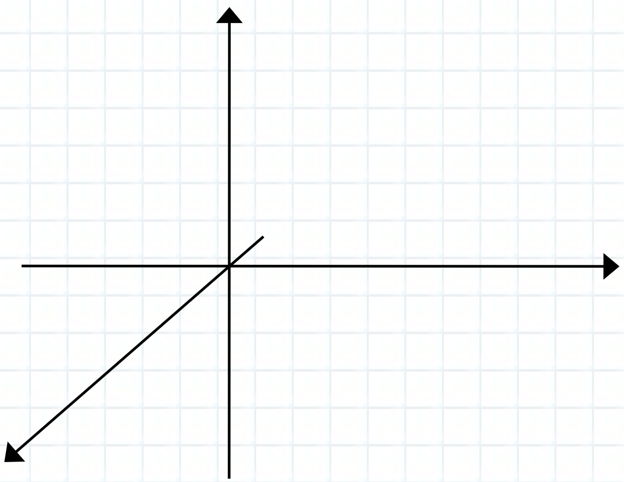


Such an expansion in known as a *generalised Fourier series.*

To find the coefficients c_m we take the inner product with an eigenfunction ϕ_n :

So

$$f(\mathbf{x}) = \sum_{m=0}^{\infty} c_m \phi_m(\mathbf{x})$$



with

$$c_m = \frac{\langle \phi_m, f \rangle}{||\phi_m||^2}$$

and hence

$$f(\mathbf{x}) = \sum_{m=0}^{\infty} \frac{\langle \phi_m, f \rangle}{||\phi_m||^2} \phi_m(\mathbf{x})$$

The coefficients c_m are known as the *projection of f* on the basis $\{\phi_n\}$.

Example:

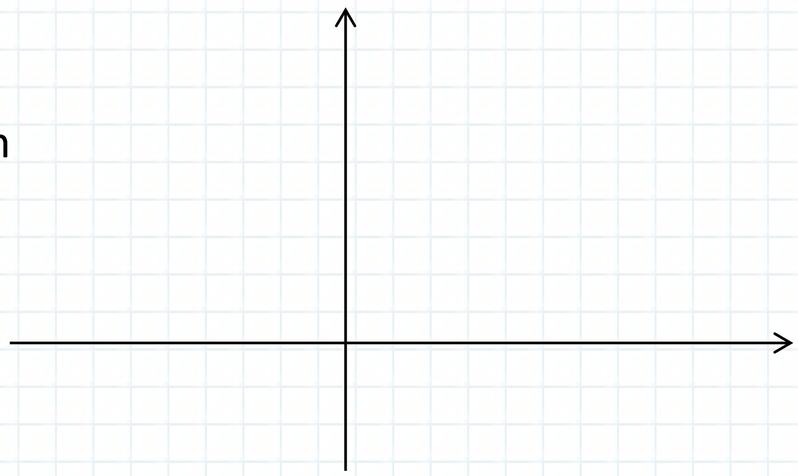
Expand the function

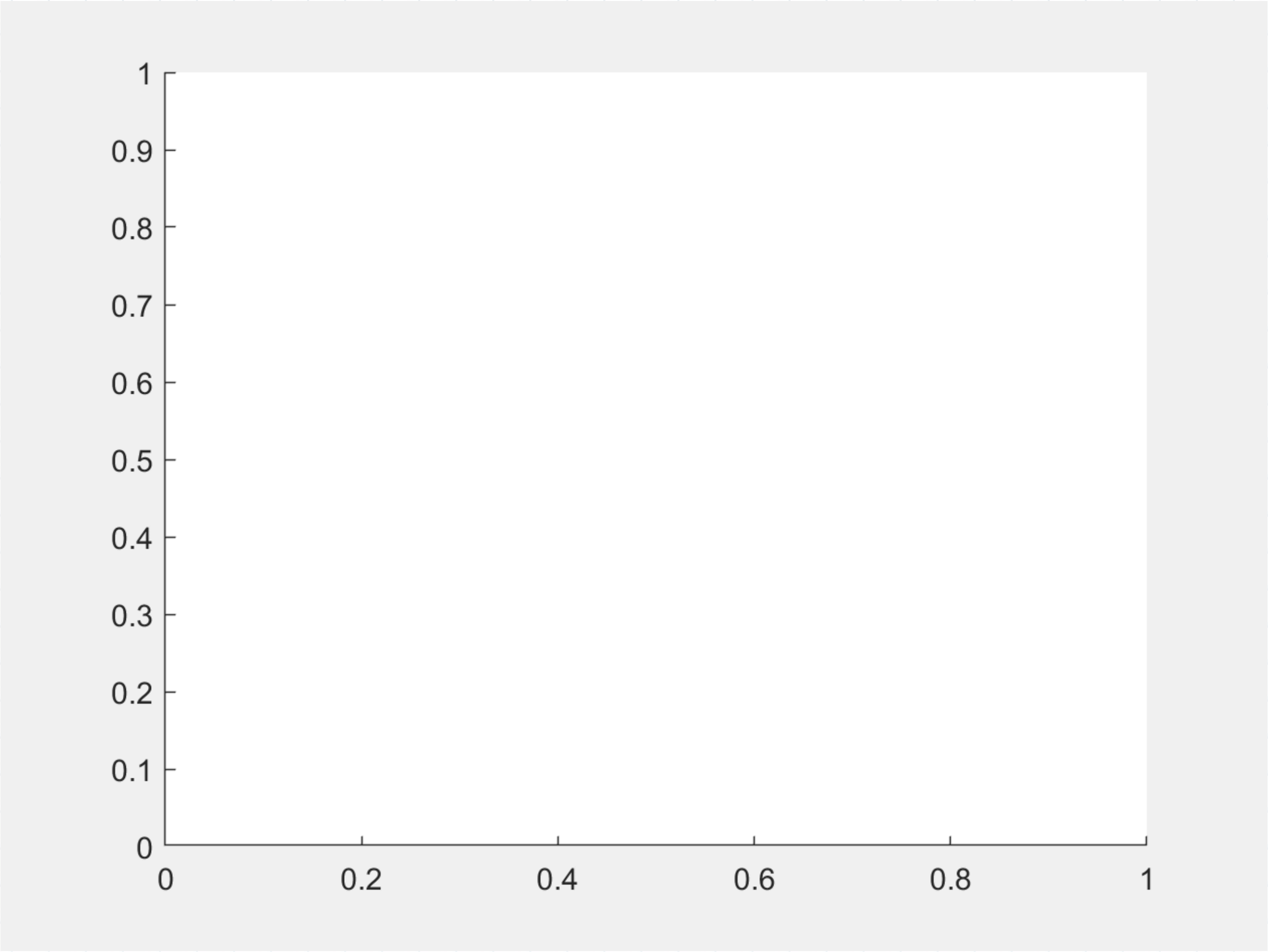
$$f(x) = \begin{cases} 1 & 0 \le x \le 1 \\ 0 & 1 \le x \le 2 \end{cases}$$

in terms of the eigenfunctions of the S-L problem

$$-\frac{d^2\phi}{dx^2} = \lambda\phi$$

with $\phi(0) = \phi(2) = 0$.




1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
0.2
0.4
0.6
0.8
1

More complicated example:

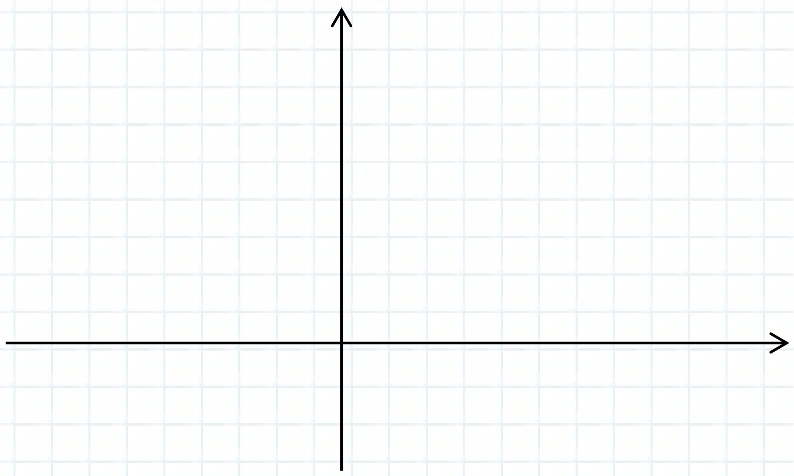
Expand the function

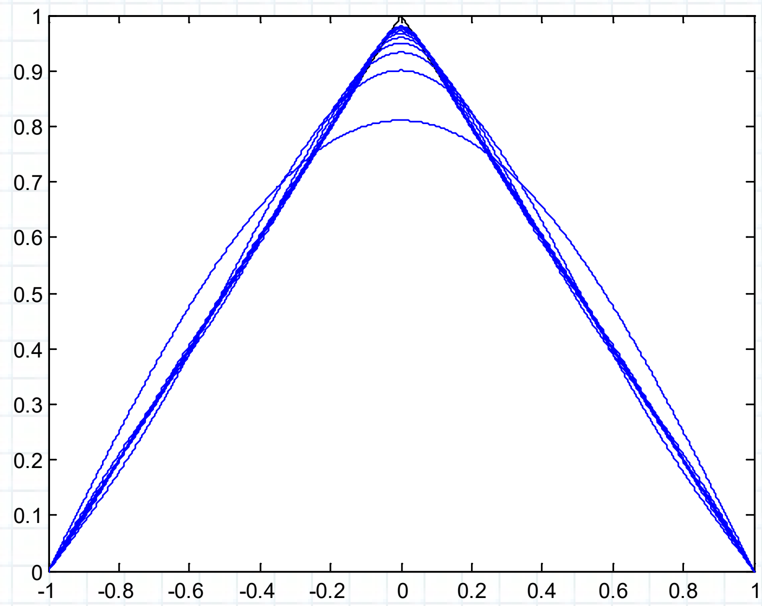
$$f(x) = \begin{cases} 1 + x & -1 \leq x \leq 0 \\ 1 - x & 0 \leq x \leq 1 \end{cases}$$

in a basis of solutions to

$$-\frac{d^2\phi}{dx^2} = \lambda\phi$$

with $\phi(-1) = \phi(1) = 0.$

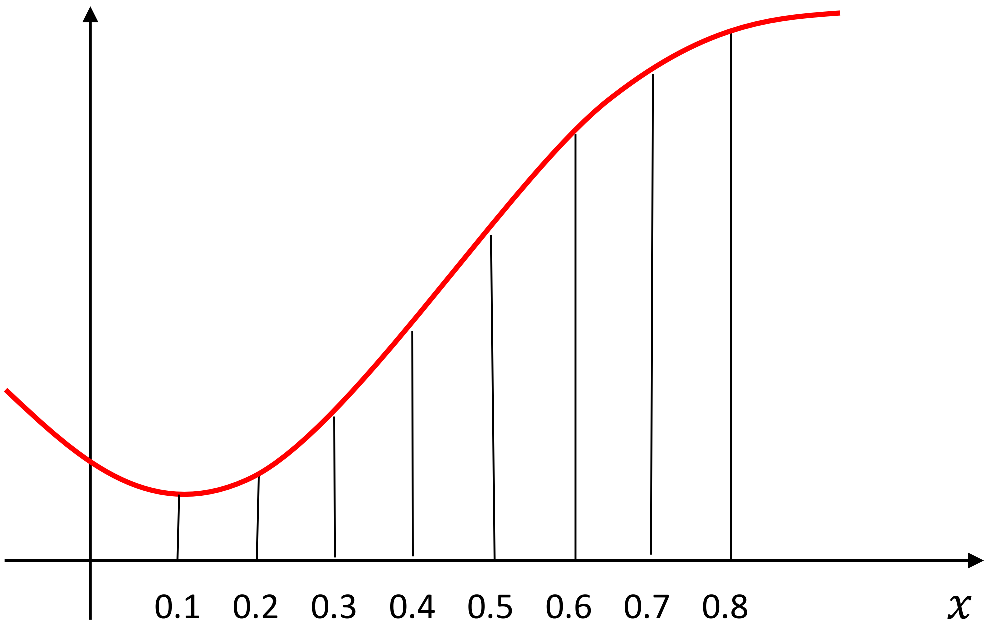




1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
-1
-0.8
-0.6
-0.4
-0.2
0
0.2
0.4
0.6
0.8
1

Representation of Functions as vectors
(Intro to infinite-dimensional Hilbert Space)

We can visualise a function $f(x)$ as being a list of values,
Each one corresponding to a different point x:



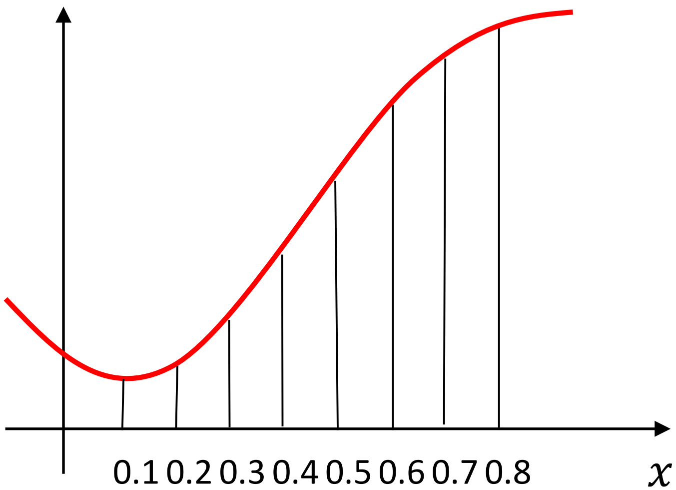
x	f(x)
0.1	1.5
0.2	1.6
0.3	2.0
0.4	3.1
0.5	4.5
0.6	5.4
0.7	6.2
0.8	6.8

We can therefore list the values of the function as a “vector”:

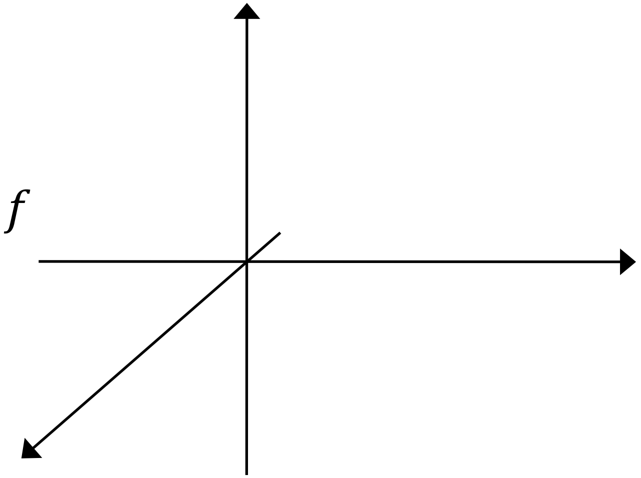
$$f = \begin{bmatrix} 1.5 \\ 1.6 \\ 2.0 \\ 3.1 \\ 4.5 \\ 5.4 \\ 6.2 \\ 6.8 \end{bmatrix}$$

Note that we still have to specify the values of x to get a full picture of f

$$x = \begin{bmatrix} 0.1 \\ 0.2 \\ 0.3 \\ 0.4 \\ 0.5 \\ 0.6 \\ 0.7 \\ 0.8 \end{bmatrix} \qquad f = \begin{bmatrix} 1.5 \\ 1.6 \\ 2.0 \\ 3.1 \\ 4.5 \\ 5.4 \\ 6.2 \\ 6.8 \end{bmatrix}$$



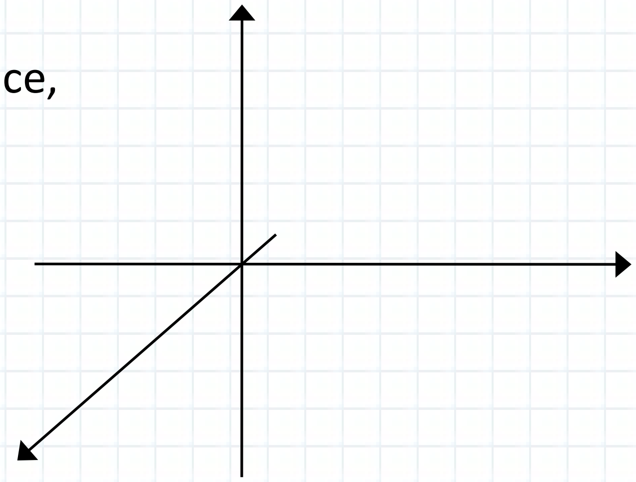
If f were only defined at 3 points, we could imagine f as a vector in 3D space.



For a continuous function we have to specify f at an Infinite number of points, and so the vector representing f would be infinite dimensional.

Hilbert spaces

We can think of f as a vector in an infinite dimensional space, known as a *Hilbert Space*.



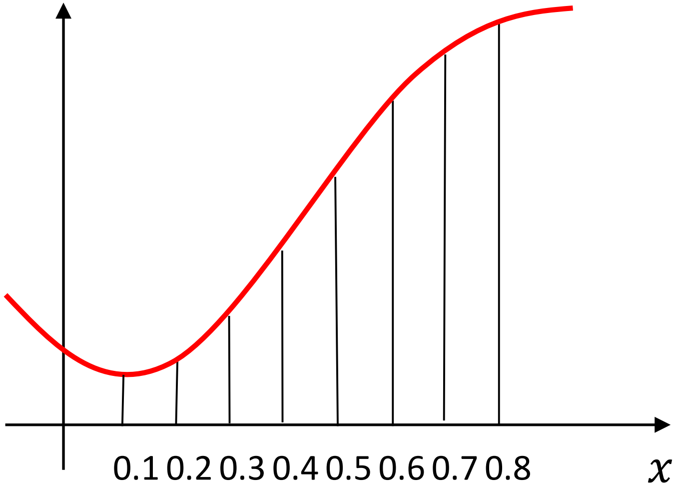
Properties of a *Hilbert Space:*

1. It has an inner product

2. The *norm* is defined and the space is *complete* with respect to the norm.

In this vector picture, linear operators become *matrices*.

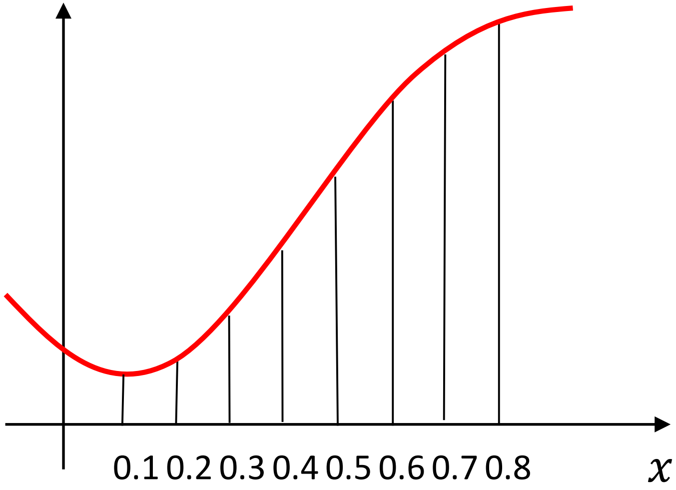
$$\mathcal{L}f = 2f(x) = \begin{bmatrix} 1.5 \\ 1.6 \\ 2.0 \\ 3.1 \\ 4.5 \\ 5.4 \\ 6.2 \\ 6.8 \end{bmatrix}$$



Self-Adjoint operators become *Hermitian matrices*.

The inner product between two functions becomes very similar to the vector inner product:

$$\begin{bmatrix} 1.5 \\ 1.6 \\ 2.0 \\ 3.1 \\ 4.5 \\ 5.4 \\ 6.2 \\ 6.8 \end{bmatrix}$$



We also have a way of representing functions in terms of
an infinite series of eigenfunctions

$$f(\mathbf{x}) = \sum_{m=0}^{\infty} c_m \phi_m(\mathbf{x}) = \sum_{m=0}^{\infty} \frac{\langle \phi_m, f \rangle}{||\phi_m||^2} \phi_m(\mathbf{x})$$

Again, we could list the coefficients c_m as a vector, and this would represent the function.

$$f = \begin{bmatrix} c_0 \\ c_1 \\ c_2 \\ c_3 \\ c_4 \\ c_5 \\ c_6 \\ \vdots \end{bmatrix}$$

Again, an operator becomes a matrix multiplication on the vector f:

In each case we can represent a function as a vector in infinite-dimensional space.

$$f = \begin{bmatrix} 1.5 \\ 1.6 \\ 2.0 \\ 3.1 \\ 4.5 \\ 5.4 \\ 6.2 \\ 6.8 \end{bmatrix} \qquad f = \begin{bmatrix} c_0 \\ c_1 \\ c_2 \\ c_3 \\ c_4 \\ c_5 \\ c_6 \\ \vdots \end{bmatrix}$$

In each case *self-adjoint operators* become equivalent to self-adjoint matrices.

Given that each vector and each matrix represents the same thing, can we abandon the particular basis that we are using, and represent functions and operators more abstractly?

Ket notation

In Quantum mechanics, physical states are represented by abstract vectors in a Hilbert space, denoted

$$|\, \psi \,\rangle$$

The state $|\psi\rangle$ represents, in abstract form, everything that can be known about the state, without specifying a particular basis.

Similarly, measurable quantities are represented by *Hermitian Operators* which act on $|\psi\rangle$.

This formulation allows us to make predictions that don't rely on a particular basis.