II. Sturm-Liouville Theory

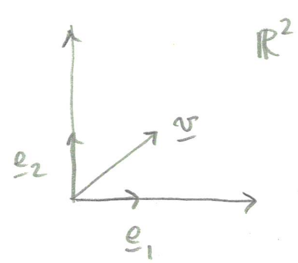
* The procedure we just did is quite general, and can be used to solve many homogeneous, linear PDEs in a variety of geometries. All of these solutions can be summarized by what is called "Sturm-Liouville theory." Hopefully learning this theory will help you see how we can use separation of variables (and many more techniques like Fourier Series) to solve many PDEs in transport in a variety of geometries (i.e. not just cartesian/rectangular coordinates)

* Note for 1st year: I don't have any HW on this right now, so just enjoy!

* Note about depth: This material really could constitute an entire course (and does!). This is just a brief overview.

A. Function Spaces

* Recall that in our discussion of coordinate systems, we talked about the concept of a vector space.



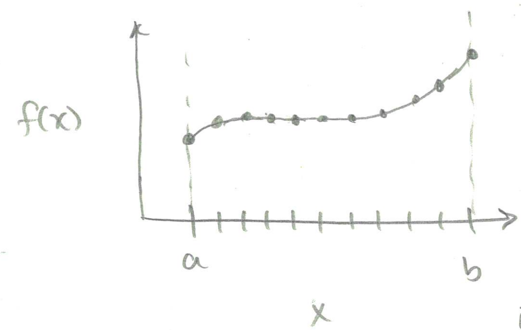
↙ For example, $\mathbb{R}^2$.

$\underline{v}$: a vector in $\mathbb{R}^2$

$\underline{e}_1, \underline{e}_2$: a basis set for $\mathbb{R}^2$ that spans the vector space

* There is an interesting connection between vectors and functions. A vector is a multidimensional object: $\underline{f} = [f_1, f_2, \ldots, f_n]$ ← an n-dimensional vector $\underline{f}$.

what if I found $\underline{f}$ by evaluating a function on the domain $[a, b]$ at n points



$i = 1, 2, \ldots n$

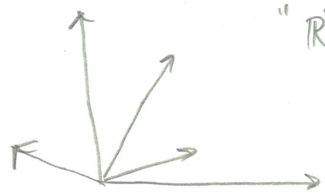
$x_i = a + \left(\frac{b-a}{n-1}\right) i$

Now, if I take the limit $n \to \infty$ of $\underline{f}$ I will get $f(x)$! So, a function is in some sense an infinite dimensional vector!

* obviously, more math is needed to make this analogy rigorous. We don't have time for that here, plus we're engineers, we want to use the result!

* Once we have this function - vector analogy in mind, we want to know if there are other useful linear-Algebra-like objects that apply to functions. The answer is of course, yes, or why would we be talking about them?

* Just like there are vector spaces, there are function spaces! These are hard to draw, because they are infinitely dimensional:



"$\mathbb{R}^\infty$" ← not actually a function space.

Some examples include:

There are many of these because of singularities that appear in the $n \to \infty$ limit!

$C(a,b)$: space of continuous functions on $x \in [a,b]$

$C^n(a,b)$: space of functions whose n^{th} derivative is are continuous on $x \in (a,b)$

$L_1(a,b)$: space of functions whose (Lebesgue) integral exists, i.e $\int_a^b f(x)\,dx < \infty$

$L_2(a,b)$: Space of functions whose square absolute values are (Lebesgue) integrable $\int_a^b |f(x)|^2 dx < \infty$

* The most important function space is L_2. What makes L_2 so important, is that it allows us to define an "inner product" for functions. In other words, it permits the use of a "dot product."

vector inner product: $(\underline{v}, \underline{w}) = \underline{v} \cdot \underline{w}$

$= \sum_i v_i w_i$ ← sum of components.

function inner product: $$(f,g) = \int_a^b f(x)\, g(x)\, dx$$

$$= \lim_{n\to\infty} \sum_{i=1}^{n} f_i g_i \Delta x$$

$\uparrow$ $\Delta x = \frac{b-a}{n-1}$

* Having an inner product, allows us to extend the definition of <u>orthogonality</u>.

<u>vectors</u>: if $(\underline{v}, \underline{w}) = 0$, we say vectors $\underline{v}$ & $\underline{w}$ are orthogonal

<u>functions</u>: if functions $(f,g) = 0$, we say functions f & g are orthogonal

recall: $(f,g) = \int_a^b f(x)\, g(x)\, dx$

* Finally, just like in finite vector spaces, it can be very useful to know a basis set of functions in a function space.

<u>vectors</u>: $$\underline{v} = \sum_{i=1}^{n} c_i \underline{e}_i$$

basis vectors

components

In a finite vector space, we can write any vector as a linear combination of basis vectors, so long as the basis vectors span the vector space.

* Analogously for functions we can write (with certain restrictions we don't have time to go into):

<u>functions</u>: $$f(x) = \sum_{i=1}^{\infty} c_i \varphi_i(x)$$

basis function

coefficients

we call such a linear combination a "generalized Fourier Series." Note that it is an infinite series that must converge for this to hold (provides restrictions). This is very powerful! Now, we can write any function f as a generalized fourier series!

* Note about the c_i: The c_i are known as "generalized Fourier coefficients." How can we find them?

$$f(x) = \sum_{i=1}^{\infty} c_i \varphi_i(x)$$

take inner product w/ $\varphi_j(x)$

$$(\varphi_j, f) = \sum_{i=1}^{\infty} c_i (\varphi_j, \varphi_i)$$

if basis is orthogonal

$(\varphi_j, \varphi_i) = 0$ when $i \neq j$

$$(\varphi_j, f) = c_j (\varphi_j, \varphi_j)$$

$$\boxed{c_j = \frac{(\varphi_j, f)}{(\varphi_j, \varphi_j)}}$$

← we did this during separation of variables!

* Finally, any function space that has an inner product, a norm, and can represent functions using a generalized Fourier series (i.e. is "complete") is called a "Hilbert space". $L_2(a,b)$ is a Hilbert space, but there are others, too.

B. Linear operators

* In finite dimensional spaces, we want to solve linear algebra problems that look like

$$\underline{\underline{A}}\,\underline{x} = b$$

$\underline{\underline{A}}$ is a linear operator. It turns the vector $\underline{x}$ into another vector $\underline{b}$. $\underline{x} \rightarrow \boxed{A} \rightarrow \underline{b}$

* Analogously, for our infinite dimensional vectors (functions) we want to solve problems like

$$\frac{d^2}{dx^2} f(x) = g(x)$$ (ie differential equations!)

we can also write this (linear) differential equation as a linear operator:

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

linear differential operator

Just like above, we can think about the operator as a factory that turns f into g:

$$f \rightarrow \boxed{\mathcal{L}} \rightarrow g$$

* In a finite dimensional vector space, operators (e.g. $\underline{\underline{A}}$) are matrices. What is the equivalent in infinite dimensional spaces? Linear differential operators are like infinite dimensional matrices.

* Consider this illustrative example:

· what are the finite difference equations for

$$\frac{d^2 f}{dx^2} = 0 \qquad f(a) = f(b) = 0$$

on the domain (a, b) with $n = 6$ grid points?

$i=$	0	1	2	3	4	5
$x=$	a	x_1	x_2	x_3	x_4	b
$f=$	f_0	f_1	f_2	f_3	f_4	f_5

$$\frac{d^2 f}{dx^2} \approx \frac{f_{i-1} - 2f_i + f_{i+1}}{\Delta x^2}$$

$\underline{i=0}$: $f_0 = 0$ $\qquad$ $\underline{i=1}$: $\frac{f_0 - 2f_1 + f_2}{\Delta x^2} = 0$ $\qquad$ $\underline{i=2}$: $\frac{f_1 - 2f_2 + f_3}{\Delta x^2} = 0$

$\underline{i=3}$: $\frac{f_2 - 2f_3 + f_4}{\Delta x^2}$ $\qquad$ $\underline{i=4}$: $\frac{f_3 - 2f_4 + f_5}{\Delta x^2} = 0$ $\qquad$ $\underline{i=5}$: $f_5 = 0$

re-writing as a matrix:

$$\frac{1}{\Delta x^2}\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 & 0 \\ 0 & 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} f_0 \\ f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$\underline{\underline{\Delta_2}}\, \underline{f} = \underline{0}$$

* If we take $\lim_{n \to \infty} \underline{\underline{\Delta_2}}$ we get $\frac{d^2}{dx^2}$ with $f(a) = f(b) = 0$

* Note that the differential operator <u>includes</u> <u>the boundary conditions</u>. A different set of BCs will give a different operator!

C. Eigenvalue problems

* With the concepts of function spaces and linear operators in place, we are prepared to talk about eigenvalue problems. Eigenvalue problems are important for at least two reasons:

  (1) They naturally occur in many places, such as separation of variables.

  (2) They will lead to the concept of a "natural" basis set of a given linear operator.

* Recall from linear algebra, that an eigenvalue problem has the form

$$\underline{\underline{A}}\,\underline{x} = \lambda\,\underline{x}$$

operator, eigenvector, eigenvalue

* An infinite dimensional eigenvalue problem has the same form:

$$\text{operator} \to \mathcal{L} f = \lambda f \leftarrow \text{eigenfunction}$$

$\nwarrow$ eigenvalue

For example:

$$\frac{d^2 f}{dx^2} = -c^2 f \qquad f(a)=0, \; f(b)=0$$

is an eigenvalue problem we solved in I.

* Besides the fact that eigenvalue problems are common, the resulting eigenfunctions are a natural basis set for expressing solutions. ← solving the EV prob, lets us find a complete basis set!

The EV prob doesn't just give any basis set, it gives the "best" basis set in some sense.

* to understand what this means, recall from linear algebra that finite dimensional operators can be diagonalized using a spectral decomposition

$$\underline{\underline{A}}\,\underline{x} = \lambda \underline{x}$$

$$\underline{\underline{A}}\,\underline{x}_i = \lambda_i \underline{x}_i \quad \text{for } i = 1, 2, \cdots, n$$

for certain properties of the $n \times n$ matrix $\underline{\underline{A}}$, there are n distinct eigenvalues and eigenvectors

These can be re-written as:

$$\underline{\underline{X}} = [\underline{x}_1, \underline{x}_2, \cdots, \underline{x}_n]$$

columns are eigenvectors

$$\underline{\underline{\Lambda}} = \begin{bmatrix} \lambda_1 & 0 & 0 & \cdots & 0 \\ 0 & \lambda_2 & 0 & \cdots & 0 \\ \vdots & & & & \\ 0 & 0 & 0 & \cdots & \lambda_n \end{bmatrix}$$

diagonal matrix of spectrum of eigenvalues

$$\underline{\underline{A}}\,\underline{\underline{X}} = \underline{\underline{X}}\,\underline{\underline{\Lambda}} \quad \text{or} \quad \boxed{\underline{\underline{A}} = \underline{\underline{X}}\,\underline{\underline{\Lambda}}\,\underline{\underline{X}}^{-1}}$$

$\underline{\underline{X}}^{-1}$ $\underline{\underline{X}}^{-1}$

spectral decomposition

* This spectral decomposition is sometimes called a "normal mode" decomposition. It is widely used in science/engineering (phonons, orbitals, etc). The eigenvectors are the "normal modes", that is they are the orthogonal basis vectors!

* The conditions that allow us to do a spectral decomposition of $\underline{\underline{A}}$, show that the eigenvectors, $\underline{x}_1, \underline{x}_2, \cdots, \underline{x}_n$ form a complete, orthogonal basis set for the function space of interest! This allows us to transform the coordinates of the problem into its "natural coordinates".

* Suppose I have the linear problem:

$$\underline{\underline{A}}\,\underline{y} = \underline{b}$$

Instead of expressing y in any old basis set, I write it in the basis of the eigenvectors of $\underline{\underline{A}}$.

$$\underline{y} = \sum_i \underbrace{y_i'}_{\text{coeffs}} \underbrace{\underline{x}_i}_{\text{eigenvectors}} = \underbrace{\underline{\underline{X}}}_{\text{Matrix of eigenvectors}}\ \underbrace{\underline{y}'}_{\text{vector w/ coeffs } y_i'}$$

I can do the same for b

$$\underline{b} = \sum_i b_i' \underline{x}_i = \underline{\underline{X}}\,\underline{b}'$$

$$\underline{\underline{A}}\,\underline{y} = b \Rightarrow \underline{\underline{A}}\,(\underline{\underline{X}}\,\underline{y}') = \underline{\underline{X}}\,b'$$

$$\Rightarrow (\underline{\underline{X}}\,\underline{\underline{\Lambda}}\,\underbrace{\underline{\underline{X}}^{-1})(\underline{\underline{X}}}_{\underline{\underline{X}}^{-1}\underline{\underline{X}} = I}\,\underline{y}') = \underline{\underline{X}}\,\underline{b}'$$

$$\Rightarrow \underline{\underline{X}}\,\underline{\underline{\Lambda}}\,\underline{y}' = \underline{\underline{X}}\,\underline{b}'$$

left multiply by $\underline{\underline{X}}^{-1}$

$$\Rightarrow \underbrace{\underline{\underline{X}}^{-1}\underline{\underline{X}}}_{I}\,\underline{\underline{\Lambda}}\,\underline{y}' = \underbrace{\underline{\underline{X}}^{-1}\underline{\underline{X}}}_{I}\,b'$$

$$\boxed{\underline{\underline{\Lambda}}\,\underline{y}' = \underline{b}'}$$

diagonal, all coefficients can be trivially solved for.

$$\boxed{\lambda_i y_i' = b_i'}$$

* takeaway: If I can express my vectors as a sum in the eigenvector basis set, my problem gets much more simple. The eigenvector basis set is like a magic basis set that simplifies the problem & uncouples the modes.

D. Sturm-Liouville Eigenvalue problem

* OK, so what does this have to do with PDEs? What if we could write solutions to PDEs in the basis set that corresponds to the linear operator? Would that make our problem easier? How can we find this basis set?

* In other words, we want to write:

$$f(x) = \sum_{i=1}^{\infty} c_i \varphi_i(x)$$

← these are eigenfunctions of the differential operator + BCs.

* The answer to the first question (does this make our problem easier) is yes! Now our differential equation will be "diagonal" and can be more easily solved.

Example:

$$\frac{\partial \phi}{\partial t} = \frac{\partial^2 \phi}{\partial y^2}$$

← we know the eigenfunctions are $\sin(n\pi y)$

$$\phi = \sum_{n=1}^{\infty} c_n \sin(n\pi y),$$ substitute in

$$\frac{\partial}{\partial t}\left[\sum_{n=1}^{\infty} c_n \sin(n\pi y)\right] = \frac{\partial^2}{\partial y^2}\left[\sum_{n=1}^{\infty} c_n \sin(n\pi y)\right]$$

$\frac{\partial^2}{\partial y^2}(\sin n\pi y)$

$$\sum_{n=1}^{\infty}\left(\frac{\partial c_n}{\partial t}\right)\sin(n\pi y) = \sum_{n=1}^{\infty} c_n \cdot (-n^2\pi^2)\sin(n\pi y)$$

$$\frac{\partial c_n}{\partial t} = -c_n n^2 \pi^2 \Rightarrow c_n = A_n \exp(-n^2\pi^2 t)$$

$$\phi = \sum_{n=1}^{\infty} A_n \exp(-n^2\pi^2 t)\sin(n\pi y)$$

↑ This is our same solution from before, but <u>much</u> faster! This idea is the basis for the "finite Fourier transform" method of solving PDE. (Equiv. to sep. of vars. see Deen ch. 5)

* Ok, so this is great & all, but what are the different eigenfunctions beyond $\sin(n\pi x)$? What are the eigenproblems I am going to have to solve?

* It turns out that two mathematicians (Sturm & Liouville) in the 1800's worked out a way to compactly summarize most of the relevant eigenvalue problems into a single eigenvalue problem:

$$\frac{1}{w(x)}\left[\frac{d}{dx}\left(p(x)\frac{d\varphi(x)}{dx}\right) + q(x)\varphi(x)\right] = -\lambda^2 \varphi(x)$$

on $x \in [a,b]$ with Boundary conditions

$$\alpha\varphi(a) + \beta\varphi'(a) = 0$$
$$\gamma\varphi(b) + \delta\varphi'(b) = 0$$

or, in operator notation

$$\mathcal{L}\varphi = \Lambda\varphi$$

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

$$\Lambda = -\lambda^2$$

* This is called the "Sturm-Liouville problem" (SLP).

* There is a lot we could talk about here, but we'll just say that it can be proven that the SLP gives real eigenvalues and a complete set of orthogonal eigenfunctions in a function space called $L_{2w}(a,b)$. $L_{2w}(a,b)$ is like $L_2(a,b)$, except its inner product has a weighting function, $w(x)$:

$$(f,g) = \int_a^b f(x)\, g(x)\, \underset{\substack{\uparrow \\ \text{weight}}}{w(x)}\, dx$$

* Let's look at some example EVPs that are special cases of the SLP.

Ex: $\dfrac{d^2 f}{dx^2} = -\lambda^2 f \quad f(a) = f(b) = 0$

$p(x) = 1, \quad q(x) = 0, \quad w(x) = 1$

$\alpha = 1, \quad \beta = 0, \quad \gamma = 1, \quad \delta = 0$

$\Rightarrow$ this gives $\sin(\lambda x)$ as eigenfunctions!

Ex2. What about cylindrical coordinates?

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{df}{dr}\right) = -\lambda^2 f \quad \swarrow \text{comes from } \nabla^2 f = 0$$

$$\left.\frac{df}{dr}\right|_{r=0} = 0, \quad f(r=R) = 0$$

$p(r) = r, \quad w(r) = r, \quad q(r) = 0$

$\alpha = 0, \quad \beta = 1, \quad \gamma = 1, \quad \delta = 0$

what are the eigen functions here? Bessel functions, $J_0(\lambda r)$

Aside:

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{df}{dr}\right) + \lambda^2 f = 0$$

$$\frac{1}{r}\left[\frac{df}{dr} + r\frac{d^2f}{dr}\right] + \lambda^2 f = 0 \quad \leftarrow \text{mult by } r^2$$

$$r^2\frac{d^2f}{dr} + r\frac{df}{dr} + \lambda^2 r^2 f = 0 \quad \leftarrow \text{Bessel's equation of order 0.}$$

Bessel's Equation:

$$x^2\frac{d^2f}{dx^2} + x\frac{df}{dx} + (x^2 - m^2) f = 0$$

m is the "order" of Bessel's equation

let $x = \lambda r$

General solution to Bessel's Equation:

$$f = c_1 J_m(x) + c_2 Y_m(x)$$

J_m: Bessel function 1st kind of order m — "sin"

Y_m: Bessel function 2nd kind of order m. — "cos"

* Show python plot of Bessel functions.

EX 3. what about spherical coordinates?

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{df}{dr}\right) = -\lambda^2 f \qquad \frac{df}{dr}(r=0) = 0 \quad f(r=R) = 0$$

$$p(r) = w(r) = r^2 \qquad q(r) = 0$$

$$\alpha = 0, \quad \beta = 1, \quad \gamma = 1, \quad \delta = 0$$

what are the eigenfunctions here? spherical Bessel functions, $j_0(\lambda r)$

$$\frac{\sin(\lambda r)}{\lambda r}$$

Aside:

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{df}{dr}\right) = -\lambda^2 f$$

$$\frac{1}{r^2}\left[2r\frac{df}{dr} + r^2\frac{d^2f}{dr^2}\right] + \lambda^2 f = 0$$

$$2r\frac{df}{dr} + r^2\frac{d^2f}{dr^2} + \lambda^2 r^2 f = 0$$

$$r^2\frac{d^2f}{dr^2} + 2r\frac{df}{dr} + \lambda^2 r^2 f = 0$$

← spherical Bessels equation of order 0

spherical Bessel's equation:

$$x^2\frac{d^2f}{dx^2} + 2x\frac{df}{dx} + \left(x^2 - n(n-1)\right)f = 0$$

let $x = \lambda r$

General solution to spherical Bessel's equation

$$f = c_1 j_n(x) + c_2 y_n(x)$$

The Bessel functions & spherical Bessel functions are related!

$$j_n(x) = \sqrt{\frac{\pi}{2x}}\, J_{n+1/2}(x)$$

$$y_n(x) = \sqrt{\frac{\pi}{2x}}\, Y_{n+1/2}(x)$$

The zeroth order spherical Bessel equation can also be written as:

$$j_0 = \frac{\sin x}{x} \qquad y_0 = -\frac{\cos x}{x}$$

* Show plot of spherical Bessel functions

* I could go on. There are more types of special functions (eigenfunctions) for different geometries and boundary conditions. Here is a useful summary from Deen.

* If time it could be nice to explain the origin of Legendre polynomials → the EVP for the ϕ coordinate in $\nabla^2 f = -\lambda^2 f$. The product of sines & cosines which are the eigenfunctions for Θ & Legendre polynomials give rise to spherical harmonics : Y_{nm}, ie. orbitals.

E. Final Comments

* So, what did we find out?

  - functions are like infinite-dimensional vectors that live in an infinite-dimensional vector space
  - we can generalize the concept of an inner product and of basis vectors to write a generalized Fourier series
  - Solving an eigenvalue problem will give us a basis set for our generalized Fourier series. This is, in some sense, the "best" basis set.
  - The Sturm-Liouville eigenvalue problem summarizes all of our relevant cases. Its solution gives a complete set of orthogonal basis functions. These eigenfunctions include sine/cosine, Bessel functions, spherical Bessel functions & Legendre polynomials.