BE.430 Tutorial:
Linear Operator Theory and Eigenfunction Expansion

(adapted from Douglas Lauffenburger)
9/22/2004

Motivating problem

In class, we encountered partial differential equations describing transient systems with chemical diffusion. We learned about the method of separation of variables to solve the PDE. However, many problems involve homogeneous reactions in the system or complicated coordinate systems, making the governing PDE more complicated and maybe requiring a more sophisticated method to solve it, such as this one:

$$\frac{\partial c}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial c}{\partial r}\right) - \alpha^2 c \qquad \text{with B.C.s } \left.\frac{\partial c}{\partial r}\right|_{r=0} = 0 \text{ and } c(r=1) = 1 \qquad (1)$$

This is a typical diffusion-reaction problem in spherical coordinates with first-order consumption (recognize it?). Solving this PDE with separation of variables can be somewhat confusing and cumbersome. Here, we introduce the linear operator theory and the eigenfunction expansion method, which build the basis of all methods of solving linear PDEs, including separation of variables and finite fourier transforms and which needs full understanding to properly apply them. You can read about Finite fourier transform methods in Deen chapters 4.1 to 4.2. after reading this tutorial.

Summary of the Linear Operator Theory

Here, we present the mathematical basis of the eigenfunction expansion method of solving PDEs. This might not make sense to you at first; but with the introduction of the Sturm-Liouville operators, you will see why the following properties are important for solving PDEs.

1. <u>Linear Vector Spaces and Linear Operators</u>

   Vector spaces are defined as a space in which a set of vectors exist and in which the following operations are allowed:

   - Vector addition $\vec{u} + \vec{v} = \vec{w}$
   - Scalar multiplication of vectors $A\vec{u} = \vec{z}$

   Linear operators, L, define and describe such linear vector spaces. For example, a linear operator can be

   $$L = \frac{d^2}{dx^2},$$

   then the vector, $\vec{u}$ in the vector space is described by

   $$L\vec{u} = \frac{d^2\vec{u}}{dx^2}$$

   The linear operator has the following linearity property:

$$L\left(A\vec{u}+B\vec{v}\right)=AL\vec{u}+BL\vec{v}=A\frac{d^2\vec{u}}{dx^2}+B\frac{d^2\vec{v}}{dx^2}$$

Why do we care? We are going to think of vectors as functions or variables from now on, so *u* and *v* are functions in the following discussion. We will use vector space and function space interchangeably. We will therefore drop the vector notation.

2. Inner Products

Another linear operator is the inner product (also called dot product for vectors). In a linear vector space, an inner product exists such that

$\langle u, v\rangle=\alpha$ (inner product of *u* with respect to *v*)

where α is a scalar, and

$$\langle Au+Bv, z\rangle=A\langle u, z\rangle+B\langle v, z\rangle$$

The inner product of a vector or function with itself is defined as the square of the magnitude of the function or vector:

$$\langle z, z\rangle=\|z\|^2 \qquad (2)$$

In the continuous function (or vector) space bounded by *a* and *b*, the inner product is defined as

$$\langle u, v\rangle=\int_a^b w(x)u(x)v(x)dx \qquad (3)$$

where *w*(*x*) is a weighing factor, whose importance will be discussed later.

A linear vector space is called **Hilbert space** if all vectors have a finite magnitude, i.e. for all vectors or functions *z*,

$$\langle z, z\rangle=\|z\|^2<\infty$$

3. Self –Adjoint Linear Operators

Linear operators in Hilbert spaces are self-adjoint if

$\langle Lu, v\rangle=\langle u, Lv\rangle$ for all *u*, *v* in space. (4)

4. Eigenvalue Problem

For self-adjoint linear operators, there exists a set of functions, ϕ, such that

$$L\phi=\lambda\phi \qquad (5)$$

where λ is are constants. These functions, ϕ, are called eigenfunctions and λ their corresponding eigenvalues. These functions are linearly independent and satisfy the boundary conditions of the function space.

5. Orthogonality of Eigenfunctions

The eigenfunctions defined by the linear operator L are orthogonal to each other. So for all n, m

$$\begin{aligned} \langle \phi_n, \phi_m \rangle &= 0 \qquad \text{if } n \neq m \\ &= \|\phi_m\|^2 \quad \text{if } n = m \end{aligned} \tag{6}$$

The inner product with respect to itself ($n = m$) is the squared magnitude of the function, according to (2).

6. Linear combination of eigenfunctions – the solution

Any function in the function space can be written as a linear combination of the eigenvectors of the linear operator defining space.

$$u = \sum_{n=1}^{\infty} A_n \phi_n \tag{7}$$

where A_n are a set of constants (not eigenvalues!).

Let's take the inner product of this equation with respect to ϕ_m. Then,

$$\langle u, \phi_m \rangle = \sum_{n=1}^{\infty} A_n \langle \phi_n, \phi_m \rangle$$

The summation sign can be taken out of the inner product since the inner product operation is linear. With equation (6)

$$\begin{aligned} \langle u, \phi_m \rangle &= \sum_{n=1}^{\infty} A_n \langle \phi_n, \phi_m \rangle \\ &= A_m \langle \phi_m, \phi_m \rangle \\ &= A_m \|\phi_m\|^2 \end{aligned}$$

Then,

$$A_n = \frac{\langle u, \phi_n \rangle}{\|\phi_n\|}$$

(we switched m with n here)

7. Solution to the linear operator

The solution to the linear operator problem is then given by

$$u = \sum_{n=1}^{\infty} \langle u, \phi_n \rangle \frac{\phi_n}{\|\phi_n\|^2} \tag{8}$$

If $\|\phi_n\|^2 = 1$, then we call ϕ_n orthonormal eigenfunctions. So, if ϕ_n are orthonormal, then

$$u = \sum_{n=1}^{\infty} \langle u, \phi_n \rangle \phi_n \tag{9}$$

This solution is a powerful tool as it doesn't only provide the solution to the partial differential equation set by the linear operator, it also provides solutions to

- Algebraic (matrix) equations
- Ordinary differential equations
- Integral equations

Sturm-Liouville Operators

Now, why was the linear operator theory so important, i.e. what does that have to do with PDEs? Many problems in engineering systems can be described by a set of operators called Sturm-Liouville operators.

$$L = \frac{1}{w(x)}\left[\frac{d}{dx}\left(p(x)\frac{d}{dx}\right) + q(x)\right] \text{ defined in the space bounded by } a \le x \le b$$

Our motivating problem given by equation (1) is described by the Sturm-Liouville operator:

$$\frac{\partial c}{\partial t} = Lc$$

where

$$w(x) = r^2 \qquad a = 0$$
$$p(x) = r^2 \qquad b = 1$$
$$q(x) = \alpha^2 r^2$$

The inner product is defined as

$$\langle u, v \rangle = \int_a^b w(x) u(x) v(x) dx$$

It turns out that the linear function space described by the Sturm-Liouville operator lies in the Hilbert space. Also, the Sturm-Liouville operator is self-adjoint with Dirichlet, Neumann or Robin boundary conditions, i.e.

$$c = 0 \; ; \; \frac{dc}{dx} = 0 \; ; \; \frac{dc}{dx} + Ac = 0$$

where A is a constant. So, the Sturm-Liouville operator is self-adjoint only with boundary conditions (you can prove it yourself with equation (4)). Another property of this operator is that all of its eigenvalues are real and negative, so

$$\lambda = -\alpha^2$$

Since the linear operator describing our motivating problem lies in the Hilbert space, is self-adjoint, there exist eigenvalues and eigenfunctions, such that the solution is given by

$$c = \sum_{n=1}^{\infty} \langle c, \phi_n \rangle \phi_n$$

if the boundary conditions are homogeneous.

Examples: Making the Boundary Conditions Homogeneous

Example 1

Recall that the boundary conditions to our motivating problem was given by

$$\left.\frac{\partial c}{\partial r}\right|_{r=0} = 0 \text{ ; } c(r=1) = 1$$

The second boundary condition is non-homogeneous. At this stage, we cannot take advantage of the linear operator theory for a solution of this problem. To get around this problem, we define

$$c'(r,t) = c(r,t) - 1$$

so that the boundary condtions become

$$\left.\frac{\partial c'}{\partial r}\right|_{r=0} = 0 \text{ ; } c'(r=1) = 0$$

Where did the non-homogeneity in the boundary condition disappear to? Let’s change our governing equation accordingly:

$$\frac{\partial c'}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial c'}{\partial r}\right) - \alpha^2 c' - \alpha^2$$

The non-homogeneity appears in the governing equation as $-\alpha^2$. The governing equation with the Sturm-Liouville operator becomes

$$\frac{\partial c'}{\partial t} = Lc' - \alpha^2$$

Example 2

Let’s turn to a simpler example, similar to the problem discussed in class:

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} \text{ with I.C. } c(x,0) = 0 \text{ and B.C.s } c(0,t) = c_0 \text{ and } c(L,t) = 0$$

To avoid confusion with units, it is wise to non-dimensionalize the variables before attempting to solve the equation. Let

$$\eta = \frac{x}{L} \qquad \gamma = \frac{c}{c_0} \qquad \tau = \frac{D}{L^2}t$$

Then the problem is rewritten to

$$\frac{\partial \gamma}{\partial \tau} = \frac{\partial^2 \gamma}{\partial \eta^2} \text{ with I.C. } \gamma(\eta,0) = 0 \text{ and B.C.s } \gamma(0,\tau) = 1 \text{ and } \gamma(1,\tau) = 0$$

The boundary conditions are non-homogeneous. This can be fixed by dividing the solution into a steady-state solution and a transient solution:

$$\gamma(\eta,\tau) = \gamma_{ss}(\eta) + \gamma_t(\eta,\tau)$$

The steady-state solution of the problem is obtained by solving

$$\frac{\partial^2 \gamma_{ss}}{\partial \eta^2} = 0$$

with the boundary conditions given above; this gives

$$\gamma_{ss} = 1 - \eta$$

The transient solution of the problem is obtained by solving

$$\frac{\partial \gamma_t}{\partial \tau} = \frac{\partial^2 \gamma_t}{\partial \eta^2} \tag{10}$$

With the help of the steady-state solution, we can rewrite our boundary and initial conditions of the transient part of the problem to

$$\gamma_t(0,\tau) = 0 \;\; ; \;\; \gamma_t(1,\tau) = 0 \text{ and } \gamma_t(\eta,0) = \eta - 1$$

In this case, the non-homogeneity now appears in the initial condition. The boundary conditions are now homogeneous, and the problem can be solved by equation (8).

Example: Solving PDEs Using Eigenfunction Expansion Method

We'll take the simpler problem (the problem discussed in class) for our example. Our problem now is

$$\frac{\partial \gamma_t}{\partial \tau} = Lc_t \quad \text{where} \quad L = \frac{\partial^2}{\partial \eta^2} \text{ with } w(\eta) = 1;\; p(\eta) = 1;\; q(\eta) = 0$$

The inner product is defined in this space as

$$\langle u,v\rangle = \int_0^1 u(\eta)v(\eta)d\eta$$

Therefore, the linear operator L is self-adjoint. There exists an eigenvalue problem, such that

$$L\phi = \lambda\phi \quad \text{with} \quad \phi(0)=0 \quad \text{and} \quad \phi(1)=0$$

Since all eigenvalues are real and negative, we can write $\lambda_n = -\alpha_n^{\ 2}$ with j = 1,2,3…. We are to solve

$$\frac{d^2\phi_j}{d\eta^2} = -\alpha_n^{\ 2}\phi_n$$

The solution to this eigenvalue problem (ordinary differential equation) is

$$\phi_n(\eta) = A_n \sin(\alpha_n\eta) + B_n \cos(\alpha_n\eta)$$

Applying boundary conditions, we obtain $B_n = 0$ and $\alpha_n = n\pi$

$$\Rightarrow \phi_n(\eta) = A_n \sin(n\pi\eta)$$

A_n can be determined by the fact that ϕ_n should be orthonormal according to (9). Therefore, by the definition of the inner product,

$$\begin{aligned}
\|\phi_n\|^2 &= \langle\phi_n,\phi_n\rangle = 1 \\
&= \int_0^1 A_n^{\ 2}\sin^2(n\pi\eta)\,d\eta \\
&\Rightarrow \frac{A_n^{\ 2}}{2} = 1 \\
&\Rightarrow A_n = \sqrt{2}
\end{aligned}$$

$$\Rightarrow \phi_n(x) = \sqrt{2}\sin(n\pi\eta)$$

The solution so far according to equation (9) is

$$\gamma_t = \sum_{n=1}^{\infty}\langle\gamma_t,\phi_n\rangle\sqrt{2}\sin(n\pi\eta) \qquad (11)$$

What is $\langle\gamma_t,\phi_n\rangle$? Following is a crucial step, which makes this eigenfunction expansion method possible for solving PDEs. Let's plug in equation (11) into the PDE governing γ_t (10) (leaving ϕ_n as is)

$$\frac{\partial}{\partial\tau}\left(\sum_{n=1}^{\infty}\langle\gamma_t,\phi_n\rangle\phi_n\right) = \sum_{n=1}^{\infty}\langle L\gamma_t,\phi_n\rangle\phi_n$$

Since L is self-adjoint,

$$\frac{\partial}{\partial \tau}\left(\sum_{n=1}^{\infty}\left\langle \gamma_t,\phi_n\right\rangle \phi_n\right)=\sum_{n=1}^{\infty}\left\langle \gamma_t, L\phi_n\right\rangle \phi_n$$

$$=\sum_{n=1}^{\infty}\left\langle \gamma_t,\lambda_n\phi_n\right\rangle \phi_n$$

$$=\sum_{n=1}^{\infty}\lambda_n\left\langle \gamma_t,\phi_n\right\rangle \phi_n$$

The second equality is derived from the properties of the eigenvalue problem. The last equality is valid since λ_n is a constant and the inner product is a linear operation. If we now take the inner product of both sides with respect to ϕ_m, summation signs are eliminated due to orthogonality properties of eigenfunctions:

$$\frac{\partial}{\partial \tau}\left\langle \gamma_t,\phi_m\right\rangle = \lambda_m\left\langle \gamma_t,\phi_m\right\rangle$$

which is a linear first-order ordinary differential equation with $\left\langle \gamma_t,\phi_m\right\rangle$ as the dependent variable and η as the only independent variable. Solving the equation,

$$\left\langle \gamma_t,\phi_m\right\rangle = c_1 e^{\lambda_m \tau} \quad \text{where } c_1 \text{ is a constant}$$

The initial condition is given by

$$\left\langle \gamma_t\left(\eta,0\right),\phi_m\right\rangle = \int_0^1\left(\eta-1\right)\sqrt{2}\sin\left(n\pi\eta\right) = -\frac{\sqrt{2}}{n\pi}$$

Applying the initial condition,

$$\left\langle \gamma_t,\phi_m\right\rangle = \frac{\sqrt{2}}{n\pi}e^{\lambda_m \tau}$$

The eigenvalues were found above as $\lambda_n = -\alpha^2 = -n^2\pi^2$

$$\left\langle \gamma_t,\phi_m\right\rangle = \frac{\sqrt{2}}{n\pi}e^{-n^2\pi^2\tau}$$

The final solution of γ_t is then

$$\gamma_t\left(\eta,\tau\right)=\sum_{n=1}^{\infty}\left\langle \gamma_t,\phi_n\right\rangle\phi_n = \sum_{n=1}^{\infty}-\frac{2}{n\pi}\sin\left(n\pi\eta\right)e^{-n^2\pi^2\tau}$$

The final, final solution of γ is then

$$\gamma(\eta,\tau) = 1 - \eta - \sum_{n=1}^{\infty} \frac{2}{n\pi} \sin(n\pi\eta)\, e^{-n^2\pi^2\tau}$$