Note III.612 22 April 2008

Eigenfunctions and Eigenfunction Expansions

There is a strong analogy between solving some of the named ODEs and finding the eigenvectors and eigenvalues of a matrix.

Hermite’s equation

\[ y'' - 2xy' + 2\alpha y = 0 \]  \hspace{1cm} (1)

can be written

\[ Ly = \lambda y \]  \hspace{1cm} (2)

where \( L \) is the differential operator

\[ L = -\frac{d^2}{dx^2} + 2x \]  \hspace{1cm} (3)

and \( \lambda = 2\alpha \).

Legendre’s equation can be written in the same way, with

\[ L = -(1 - x^2)\frac{d^2}{dx^2} + 2x \frac{d}{dx} \]  \hspace{1cm} (4)

with \( \lambda = \alpha \).

We can think of the differential operator \( L \) as a matrix, albeit an infinite dimensional one, and the function it acts on, \( y \), as a vector.

To make this more precise it is useful to recall some properties of certain finite, say \( n \times n \), matrices.

- A symmetric matrix \( S \) satisfies

\[ S^T = S \]  \hspace{1cm} (5)

where the superscript \( T \) denotes the transpose \([A^T]_{ij} = [A]_{ji}\).

- A Hermitian matrix is an \( n \times n \) matrix with complex entries satisfying

\[ H^\dagger = H \]  \hspace{1cm} (6)

where the superscript dagger is the adjoint, the complex conjugate of the transpose

\[ [A^\dagger]_{ij} = [A]_{ji}^\ast \]. \hspace{1cm} (7)

\(^1\)Conor Houghton, houghton@maths.tcd.ie, see also http://www.maths.tcd.ie/~houghton/231
\(^2\)Based on notes I got from Chris Ford
Clearly a real symmetric matrix is Hermitian.

Let $v$ be an $n$-component column vector with complex entries. $v$ is an **eigenvector** of $H$ if

$$ Hv = \lambda v $$

(8)

for some complex number $\lambda$, the **eigenvalue**.

Now, an important theorem is that the eigenvalues of a Hermitian matrix are real. To prove this, let $v$ be an eigenvector of $H$ with eigenvalue $\lambda$

$$ v^\dagger Hv = \lambda v^\dagger v. $$

(9)

Since $v^\dagger v$ is real it suffices to prove that $v^\dagger Hv$ is real:

$$ (v^\dagger H v)^\dagger = v^\dagger H^\dagger v = v^\dagger Hv $$

(10)

since $v^\dagger H v$ is a $1 \times 1$ matrix

$$ (v^\dagger H v)^\dagger = (v^\dagger H v)^\dagger = v^\dagger H^\dagger v = v^\dagger Hv $$

(11)

if $H$ is Hermitian. Note that $(AB)^\dagger = B^\dagger A^\dagger$.

Another important property is that the eigenvectors of a Hermitian matrix corresponding to distinct eigenvalues are orthogonal, that is if $Hv_1 = \lambda_1 v_1$ $Hv_2 = \lambda_2 v_2$ with $\lambda_1 \neq \lambda_2$ then $v_1^\dagger v_2 = 0$ or, in the inner product notation, $(v_1, v_2) = 0$. To prove this we take the eigenvector equations and multiply them on the left to give

$$ v_1^\dagger H v_1 = \lambda_1 v_1^\dagger v_1 $$

$$ v_1^\dagger H v_2 = \lambda_1 v_1^\dagger v_2 $$

(12)

Take the complex conjugate of the second

$$ v_2^\dagger H v_1 = \lambda_2 v_2^\dagger v_1 $$

(13)

using $H^\dagger = H$ and $\bar{\lambda}_2 = \lambda_2$. Subtracting the first gives

$$ 0 = (\lambda_2 - \lambda_1) v_2^\dagger v_1 $$

(14)

so that $(v_2, v_1) = 0$ if $\lambda_1 \neq \lambda_2$. If the eigenvalues are degenerate we can choose eigenvectors to be orthogonal using Gram-Schmidt orthogonalization.

Thus, we can choose the $n$ eigenvectors $v_i$, $i = 1, 2, ..., n$, of an Hermitian matrix $H$ to be **orthonormal**

$$ v_i^\dagger v_j = \delta_{ij} $$

(15)

or

$$ (v_i, v_j) = \delta_{ij} $$

(16)

Any $n$-component vector $v$ can be written as a linear combination of the $v_i$s

$$ v = c_1 v_1 + c_2 v_2 + ... + c_n v_n $$

(17)
where $c_1, c_2, \ldots, c_n$ are complex numbers. Using the orthonormal property

$$(v_i, v) = c_i$$

(18)

Also

$$|v|^2 = (v, v) = |c_1|^2 + |c_2|^2 + \ldots + |c_n|^2,$$

(19)

which can be thought of as an $n$-dimensional version of Pythagoras or a finite dimensional version of Parseval.

Furthermore, the eigenvector basis can be used to rewrite the matrix

$$H = \sum_{i=1}^{n} \lambda_i v_i v_i^\dagger,$$

(20)

since we know by definition

$$Hv = H(c_1v_1 + c_2v_2 + \ldots + c_nv_n) = c_1\lambda_1v_1 + c_2\lambda_2v_2 + \ldots + c_n\lambda_nv_n$$

(21)

and

$$\sum_{i=1}^{n} \lambda_i v_i v_i^\dagger v_j = \lambda_j v_j$$

(22)

so this will have the same effect on $v$. The resolution of unity is a similar formula for the identity matrix, it can be written as

$$I = \sum_{i=1}^{n} v_i v_i^\dagger,$$

(23)

since acting on any vector, $v = c_1v_1 + c_2v_2 + \ldots + c_nv_n$, will reproduce $v$. The inverse of an Hermitian matrix can be written as

$$H^{-1} = \sum_{i=1}^{n} \frac{1}{\lambda_i} v_i v_i^\dagger,$$

since left or right multiplication by $H$ reproduces the identity matrix.

Now, back to differential operators. A differential operator $L$ acts on some vector space of functions. It is normal to require functions to be such that

$$\int dx \overset{*}{u}(x)(Lu)(x) < \infty.$$  

(24)

and, in practice, it is usual to impose further restrictions on the functions such as

1. square integrability $\int_{-\infty}^{\infty} dx \overset{*}{u}(x)u(x) < \infty.$

2. periodicity
3. vanishing at the end points of an interval \([a, b] \subset \mathbb{R}; u(a) = u(b) = 0\).

In each of these cases an inner product can be defined
1. \((u, v) = \int_{-\infty}^{\infty} dx \bar{u}(x)v(x)\)
2. \((u, v) = \int_{-\pi}^{\pi} dx \bar{u}(x)u(x) \quad (l = 2\pi)\)
3. \((u, v) = \int_{a}^{b} dx \bar{u}(x)v(x)\).

Once an inner product is defined, we can look for an analogue of a Hermitian matrix. Suppose
\[(u, Lv) = (Lu, v)\] (25)
for any \(u, v\) in the chosen space of functions then \(L\) is called symmetric. If some further technical requirements are met it is called self-adjoint or Hermitian. We will be sloppy and call any symmetric operator Hermitian. An example is
\[L = -\frac{d^2}{dx^2}\] (26)
for any of the three conditions above. Here the symmetric condition is just
\[- \int dx \bar{u}(x)v''(x) = - \int dx \bar{v}''v(x).\] (27)

To establish this integrate by parts twice, for example, for the periodic case
\[\int_{-\pi}^{\pi} dx \bar{u}(x)v''(x) = \bar{u}(x)v'(x)|_{-\pi}^{\pi} - \int_{-\pi}^{\pi} dx \bar{u}'(x)v'(x)\] (28)
\[\bar{u}(x)v'(x)|_{-\pi}^{\pi}\] is zero since \(u\) and \(v\) are periodic. Integrating by parts once more gives the result.

\(L = -d^2/dx^2\) can be viewed as an Hermitian matrix acting on the space of periodic functions \((l = 2\pi)\). The eigenvectors, or eigenfunctions, are the functions
\[v_n(x) = e^{inx}\] (29)
with \(n \in \mathbb{Z}\) with corresponding eigenvalues
\[\lambda_n = n^2\] (30)

These are orthogonal, as expected since \(L\) is Hermitian,
\[(v_m, v_n) = \int_{-\pi}^{\pi} dx \bar{v}_m(x)v_n(x) = \int_{-\pi}^{\pi} dx e^{-imx}e^{inx} = 0\] (31)
for \(n \neq m\). Can make them orthonormal
\[v_n(x) = \frac{1}{\sqrt{2\pi}}e^{inx}\] (32)
gives

\[(v_m, v_n) = \delta_{mn}.\]  
\hspace{1cm} (33)

A periodic function, \(f\), can be thought of as a vector in the space acted on by \(L\). Expanding \(f\) in eigenvectors of \(L\)

\[f(x) = \sum_{n \in \mathbb{Z}} c_n v_n(x)\]  
\hspace{1cm} (34)

just gives Fourier analysis

\[c_m = (v_m, f) = \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} dx \, e^{-imx} f(x).\]  
\hspace{1cm} (35)

Fourier analysis is thus equivalent to expanding in eigenvectors of the Hermitian operator \(L = -\frac{d^2}{dx^2}\). We can choose a different Hermitian operator and this leads to alternative expansions: we expect to able to get Legendre series, Hermite series and so on, instead of the Fourier series.

**Legendre Series**

Consider Legendre’s equation

\[(1 - x^2)y''(x) - 2xy'(x) + \alpha y(x) = 0\]  
\hspace{1cm} (36)

This ODE has, regular, singularities at \(x = \pm 1\). If \(\alpha\) is of the form \(\alpha = n(n + 1)\) where \(n\) is a non-negative integer then the ODE has a polynomial solution, see problem sheet 17, which is well defined at \(x = \pm 1\), the other solutions all blow up at \(x = 1\) or \(x = -1\).

We can rewrite the the ODE as an eigenvalue problem:

\[Ly(x) = \lambda y(x),\]

\[L = -(1 - x^2) \frac{d^2}{dx^2} + 2x \frac{d}{dx}.\]  
\hspace{1cm} (37)

Let us consider in \(L\) in the space of functions which are finite throughout \([-1, 1]\); this will include the polynomial solutions, but will exclude the other solutions since they blow up at the end points. The inner product is taken as

\[(u, v) = \int_{-1}^{1} dx \, \bar{u}(x)v(x).\]  
\hspace{1cm} (38)

It is straightforward to prove that with these boundary conditions \(L\) is Hermitian; it helps to write \(L\) in the form

\[L = -\frac{d}{dx} (1 - x^2) \frac{d}{dx}.\]  
\hspace{1cm} (39)

The eigenfunctions are the polynomial solutions of Legendre’s equation \(P_n(x)\) with \(n = 0, 1, 2, \ldots\) with corresponding eigenvalues \(\lambda_n = n(n + 1)\). The first few Legendre polynomials are \(P_0(x) = 1\), \(P_1(x) = x\) and \(P_2(x) = \frac{1}{2}(3x^2 - 1)\).
For $n$ even or odd $P_n$ is even or odd, like the Hermite polynomials. There are various formulae for the Legendre polynomials, for example they can be combined into a generating function

$$\Phi(x, h) = (1 - 2xh + h^2)^{-\frac{1}{2}} = \sum_{n=0}^{\infty} h^n P_n(x).$$

(40)

The polynomials are orthogonal, they can be made orthonormal, but the following convention is standard

$$\int_{-1}^{1} dx \ (P_n(x))^2 = \frac{2}{2n+1}. \quad (41)$$

Let $f$ be a function defined on $[-1, 1]$. Can expand in Legendre polynomials (i.e. in the eigenfunctions of the Hermitian operator $L$)

$$f(x) = \sum_{n=0}^{\infty} c_n P_n(x). \quad (42)$$

Much as in Fourier analysis

$$(P_m, f) = \sum_{n=0}^{\infty} c_n (P_m, P_n) = \sum_{n=0}^{\infty} c_n \frac{2\delta_{mn}}{2m+1} = \frac{2c_m}{2m+1}, \quad (43)$$

so that

$$c_m = \left(m + \frac{1}{2}\right) (P_m, f) = \left(m + \frac{1}{2}\right) \int_{-1}^{1} dx \ P_m(x) f(x). \quad (44)$$

Hermite’s equation

$$y''(x) - 2xy'(x) + 2\alpha y(x) = 0 \quad (45)$$

can be written as $Ly(x) = \lambda y(x)$, where

$$L = -\frac{d^2}{dx^2} + 2x \frac{d}{dx} \quad (46)$$

with $\lambda = 2\alpha$. the problem is $L$ is not Hermitian! $(u, Lv) \neq (Lu, v)$ regardless of boundary conditions. However if we change the definition of the inner product

$$(u, v)_{\text{new}} = \int dx \ e^{-x^2} \ \bar{u}(x)v(x). \quad (47)$$

the operator is Hermitian and similar results as to the Legendre case can be derived using the new inner product.