Note III.6[1,2] 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

$$y'' - 2xy' + 2\alpha y = 0 \tag{1}$$

can be written

$$Ly = \lambda y \tag{2}$$

where L is the differential operator

$$L = -\frac{d^2}{dx^2} + 2x \tag{3}$$

and $\lambda = 2\alpha$.

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

$$L = -(1-x^2)\frac{d^2}{dx^2} + 2x\frac{d}{dx} \tag{4}$$

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

  $$S^T = S \tag{5}$$

  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

  $$H^\dagger = H \tag{6}$$

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

  $$[A^\dagger]_{ij} = \overline{[A]_{ji}}. \tag{7}$$

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[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

$$Hv = \lambda v \tag{8}$$

for some complex number λ, 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 λ

$$v^\dagger H v = \lambda v^\dagger v. \tag{9}$$

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

$$\overline{v^\dagger H v} = \overline{(v^\dagger H v)^T} \tag{10}$$

since $v^\dagger H v$ is a 1×1 matrix

$$\overline{(v^\dagger H v)^T} = (v^\dagger H v)^\dagger = v^\dagger H^\dagger v = v^\dagger H v \tag{11}$$

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 $Hv_1 = \lambda_1 v_1 \quad Hv_2 = \lambda_2 v_2$ 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

$$\begin{aligned} v_2^\dagger H v_1 &= \lambda_1 v_2^\dagger v_1 \\ v_1^\dagger H v_2 &= \lambda_1 v_1^\dagger v_2 \end{aligned} \tag{12}$$

Take the complex conjugate of the second

$$v_2^\dagger H v_1 = \lambda_2 v_2^\dagger v_1 \tag{13}$$

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

$$0 = (\lambda_2 - \lambda_1) v_2^\dagger v_1 \tag{14}$$

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**

$$v_i^\dagger v_j = \delta_{ij} \tag{15}$$

or

$$(v_i, v_j) = \delta_{ij} \tag{16}$$

Any n-component vector v can be written as a linear combination of the v_is

$$v = c_1 v_1 + c_2 v_2 + ... + c_n v_n \tag{17}$$

where c_1, c_2,... c_n are complex numbers. Using the orthonormal property

$$(v_i, v) = c_i \tag{18}$$

Also

$$|v|^2 = (v, v) = |c_1|^2 + |c_2|^2 + ... + |c_n|^2, \tag{19}$$

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

$$H = \sum_{i=1}^{n} \lambda_i v_i \; v_i^\dagger, \tag{20}$$

since we know by definition

$$Hv = H(c_1 v_1 + c_2 v_2 + ... + c_n v_n) = c_1 \lambda_1 v_1 + c_2 \lambda_2 v_2 + \ldots + c_n \lambda_n v_n \tag{21}$$

and

$$\sum_{i=1}^{n} \lambda_i v_i \; v_i^\dagger v_j = \lambda_j v_j \tag{22}$$

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

$$I = \sum_{i=1}^{n} v_i \; v_i^\dagger, \tag{23}$$

since acting on any vector, $v = c_1 v_1 + c_2 v_2 + ... + c_n v_n$, 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

$$\int dx \; \bar{u}(x)(Lu)(x) < \infty. \tag{24}$$

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

1. square integrability $\int_{-\infty}^{\infty} dx \; \bar{u}(x)u(x) < \infty$.
2. periodicity

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

In each of these cases an inner product can be defined

1. $(u, v) = \int_{-\infty}^{\infty} dx \; \bar{u}(x)v(x)$
2. $(u, v) = \int_{-\pi}^{\pi} dx \; \bar{u}(x)u(x) \qquad (l = 2\pi)$
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

$$(u, Lv) = (Lu, v) \tag{25}$$

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

$$L = -\frac{d^2}{dx^2} \tag{26}$$

for any of the three conditions above. Here the symmetric condition is just

$$-\int dx \; \bar{u}(x)v''(x) = -\int dx \; \bar{u}''v(x). \tag{27}$$

To establish this integrate by parts twice, for example, for the periodic case

$$\int_{-\pi}^{\pi} dx \; \bar{u}(x)v''(x) = \bar{u}(x)v'(x)|_{-\pi}^{\pi} - \int_{-\pi}^{\pi} dx \; \bar{u}'(x)v'(x) \tag{28}$$

$\bar{u}(x)v'(x)|_{-\pi}^{\pi}$ 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

$$v_n(x) = e^{inx} \tag{29}$$

with $n \in \mathbf{Z}$) with corresponding eigenvalues

$$\lambda_n = n^2 \tag{30}$$

These are orthogonal, as expected since L is Hermitian,

$$(v_m, v_n) = \int_{-\pi}^{\pi} dx \; \bar{v}_m(x)v_n(x) = \int_{-\pi}^{\pi} dx \; e^{-imx}e^{inx} = 0 \tag{31}$$

for $n \neq m$. Can make them orthonormal

$$v_n(x) = \frac{1}{\sqrt{2\pi}} e^{inx} \tag{32}$$

gives

$$(v_m, v_n) = \delta_{mn}. \tag{33}$$

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

$$f(x) = \sum_{n \in Z} c_n v_n(x) \tag{34}$$

just gives Fourier analysis

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

Fourier analysis is thus equivalent to expanding in eigenvectors of the Hermitian operator $L = -d^2/dx^2$. 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

$$(1 - x^2)y''(x) - 2xy'(x) + \alpha y(x) = 0 \tag{36}$$

This ODE has, regular, singularities at $x = \pm 1$. If α 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:

$$\begin{aligned} Ly(x) &= \lambda y(x), \\ L &= -(1 - x^2)\frac{d^2}{dx^2} + 2x\frac{d}{dx}. \end{aligned} \tag{37}$$

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

$$(u, v) = \int_{-1}^{1} dx\ \bar{u}(x)v(x). \tag{38}$$

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

$$L = -\frac{d}{dx}(1 - x^2)\frac{d}{dx}. \tag{39}$$

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

$$\Phi(x, h) = (1 - 2xh + h^2)^{-\frac{1}{2}} = \sum_{n=0}^{\infty} h^n P_n(x). \tag{40}$$

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

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

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

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

Much as in Fourier analysis

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

so that

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

Hermite's equation

$$y''(x) - 2xy'(x) + 2\alpha y(x) = 0 \tag{45}$$

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

$$L = -\frac{d^2}{dx^2} + 2x\frac{d}{dx}, \tag{46}$$

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

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

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