

2.2 Transform Techniques

The separation of variable technique works very well when the differential operator is of fairly simple form, and discrete separation constants are accessible. This is not always the case, and in particular, the initial/boundary conditions may not be periodic. Discrete sums over separation constants may be infinite, and moreover, continuous sampling of them may prove necessary. This domain is optimal for employing transform techniques, and we illustrate the approach using two examples.

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Example 1: Consider the 1D wave equation

$$\frac{\partial^2 y}{\partial x^2} - \frac{1}{c^2} \frac{\partial^2 y}{\partial t^2} = 0 \quad , \quad (34)$$

with the initial conditions

$$y(x, 0) = \phi(x) \quad , \quad \dot{y}(x, 0) = 0 \quad . \quad (35)$$

Note that these are Cauchy conditions on the temporal boundary curve. Taking the Fourier transform with respect to x ,

$$Y(k, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} y(x, t) e^{ikx} dx \quad , \quad (36)$$

so that the Fourier transform of $\partial^2 y / \partial x^2$ is $-k^2 Y(k, t)$. The wave equation then becomes an ODE in time when thus transformed:

$$-k^2 Y - \frac{1}{c^2} \frac{\partial^2 Y}{\partial t^2} = 0 \quad . \quad (37)$$

This is then simply solved:

$$Y(k, t) = Y_1(k) e^{ikct} + Y_2(k) e^{-ikct} \quad , \quad (38)$$

where the $Y_i(k)$ are the constants of integration. These are constrained by the two initial conditions in Fourier space:

$$\begin{aligned} Y(k, 0) &= Y_1(k) + Y_2(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(x) e^{ikx} dx \quad , \\ \dot{Y}(k, 0) &= ikc [Y_1(k) - Y_2(k)] = 0 \quad , \end{aligned} \quad (39)$$

from which it follows that

$$Y_1(k) = Y_2(k) = \frac{1}{2\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(x) e^{ikx} dx \quad . \quad (40)$$

Inverting the transform in k space leads to the complete solution

$$y(x, t) = \frac{1}{4\pi} \int_{-\infty}^{\infty} e^{-ikx} \left(e^{ikct} + e^{-ikct} \right) dk \int_{-\infty}^{\infty} \phi(x') e^{ikx'} dx' \quad . \quad (41)$$

This can be simplified by reversing the order of the integrations:

$$\begin{aligned} y(x, t) &= \frac{1}{4\pi} \int_{-\infty}^{\infty} dx' \phi(x') \int_{-\infty}^{\infty} dk \left(e^{-ik(x-x'-ct)} + e^{-ik(x-x'+ct)} \right) \\ &= \frac{1}{2} \int_{-\infty}^{\infty} dx' \phi(x') \left\{ \delta[x - x' - ct] + \delta[x - x' + ct] \right\} \quad , \end{aligned} \quad (42)$$

using the complex exponential integral definition of the Dirac δ function. This then trivially reduces to the final compact form for the solution:

$$y(x, t) = \frac{1}{2} \left[\phi(x - ct) + \phi(x + ct) \right] \quad , \quad (43)$$

which is easily demonstrated to satisfy the Cauchy conditions in Eq. (35), as well as the original wave equation.

- N. B. We could equally well take the Fourier transform with respect to time, however the implementation of the initial conditions would have been more complicated, although the answer would have been the same.

Example 2: Now we look at a slightly more interesting example. Consider the 1D diffusion equation

$$\frac{\partial^2 \rho}{\partial x^2} = \frac{1}{\kappa} \frac{\partial \rho}{\partial t} \quad . \quad (44)$$

Here $\rho(x, t)$ represents some quantity such as the concentration of an impurity in a background fluid, or the excess temperature of a fluid element.

Suppose that we introduce a finite amount of ρ at $t = 0$ so that $\rho = 0$ for $t < 0$. Our boundary condition is therefore

$$\rho(x, 0) = \sigma_0 \delta(x) \quad . \quad (45)$$

Let us add the condition that the total amount of the impurity is conserved at all times:

$$\int_{-\infty}^{\infty} \rho(x, t) dx = \int_{-\infty}^{\infty} \rho(x, 0) dx = \sigma_0 \quad . \quad (46)$$

Now take the Fourier transform in space of ρ , defining

$$R(k, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \rho(x, t) e^{ikx} dx \quad . \quad (47)$$

The Fourier transform of the diffusion equation is

$$\frac{\partial R}{\partial t} = -\kappa k^2 R(k, t) \quad \Rightarrow \quad R(k, t) = R(k, 0) e^{-\kappa k^2 t} \quad , \quad (48)$$

solving this as a first-order ODE. We can determine the initial value of $R(k, 0)$ via

$$R(k, 0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \sigma_0 \delta(x) e^{ikx} dx = \frac{\sigma_0}{\sqrt{2\pi}} \quad , \quad (49)$$

so that $R(k, t)$ is completely defined. We now take the inverse Fourier transform

$$\rho(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} R(k, t) e^{-ikx} dk = \frac{\sigma_0}{2\pi} \int_{-\infty}^{\infty} e^{-\kappa k^2 t - ikx} dk \quad . \quad (50)$$

Now complete the squares in the argument of the exponential, expressing it as

$$-\kappa t \left(k + \frac{ix}{2\kappa t} \right)^2 - \frac{x^2}{4\kappa t} \quad (51)$$

The resulting Gaussian integral is simply evaluated, and the final solution is

$$\rho(x, t) = \frac{\sigma_0}{\sqrt{4\pi \kappa t}} e^{-x^2/4\kappa t} \quad . \quad (52)$$

This Gaussian clearly satisfies Eq. (46), and also realizes $\rho(x, 0) = \sigma_0 \delta(x)$. The mean free path for spatial diffusion is $\lambda \sim \sqrt{2\kappa t}$.

13. EIGENFUNCTIONS

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1 Eigenfunctions and Eigenvalues for Linear Differential Equations

As an extension of our vector and matrix considerations, observe that linear operators can be differential in nature, for example

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$$L_x \equiv \frac{d^2}{dx^2} + k^2 \quad \text{with} \quad L_x y = 0 \quad (1)$$

as an ODE. Add to this our knowledge that the solution of PDEs via the technique of separation of variables suggests eigenvalues similar to those in the matrix context. Specifically, separation of variables is a sequence of eigenvalue problems,

$$L y(\vec{x}) = \lambda y(\vec{x}) \quad . \quad (2)$$

We will now draw upon our vector space tools to develop pedagogy for eigenvalue problems involving differential operators. This method is known as **Sturm-Liouville theory**.

* This is very valuable in studies of quantum mechanics.

- A linear differential operator L is said to be **Hermitian** (self-adjoint) if

$$\int_{\Omega} y_1^*(\vec{x}) L y_2(\vec{x}) d^3x = \left[\int_{\Omega} y_2^*(\vec{x}) L y_1(\vec{x}) d^3x \right]^* \quad , \quad (3)$$

where y_1 and y_2 are *arbitrary* functions that satisfy a given set of conditions on the region boundary Ω .

- Suppose that L is Hermitian. Then *its eigenvalues λ_i are real, and its distinct eigenvectors $y_i(\vec{x})$ are orthogonal.* For a proof, use

$$L y_i(\vec{x}) = \lambda_i y_i(\vec{x}) \quad , \quad L y_j(\vec{x}) = \lambda_j y_j(\vec{x}) \quad (4)$$

to define two eigenvectors and corresponding eigenvalues, both of which must satisfy specified conditions on the boundary Ω . Then

$$I_1 \equiv \int_{\Omega} y_j^*(\vec{x}) L y_i(\vec{x}) d^3x = \lambda_i \int_{\Omega} y_j^*(\vec{x}) y_i(\vec{x}) d^3x \quad (5)$$

and

$$I_2 \equiv \left[\int_{\Omega} y_i^*(\vec{x}) L y_j(\vec{x}) d^3x \right]^* = \left[\lambda_j \int_{\Omega} y_i^*(\vec{x}) y_j(\vec{x}) d^3x \right]^* \quad , \quad (6)$$

which becomes

$$I_2 = \lambda_j^* \int_{\Omega} y_j^*(\vec{x}) y_i(\vec{x}) d^3x \quad . \quad (7)$$

Since L is Hermitian, $I_2 = I_1$, from which it immediately follows that

$$I_1 - I_2 \equiv (\lambda_i - \lambda_j^*) \int_{\Omega} y_j^*(\vec{x}) y_i(\vec{x}) d^3x = 0 \quad . \quad (8)$$

The claims then follow: the real nature of the eigenvalues results for $i = j$, and orthogonality is obtained for $i \neq j$, since $\lambda_j^* \neq \lambda_i$.

* Note that this Hermitian result is totally analogous with the matrix case.

* Observe that the integrals that appear in these manipulations are effectively **dot products** for integrals in measure theory:

$$y_j \cdot y_i \equiv \int_{\Omega} y_j^*(\vec{x}) y_i(\vec{x}) d^3x \quad . \quad (9)$$

The complex conjugation leads to real results for complex functions when the dot product involves a function and itself: it therefore becomes a measure of the square of the real length of the functional vector.

- Now we see the context for why Hermite's ODE is described as not being self-adjoint, where as the modified ODE for the functions $\exp\{-x^2/2\}H_n(x)$ is Hermitian, and these functions are mutually orthogonal.

Example 1: Let us consider a familiar set of orthonormal functions, namely trigonometric functions that satisfy periodic boundary conditions.

$$\frac{d^2 y}{dx^2} + \lambda y = 0 \quad , \quad 0 \leq x \leq 2\pi \quad . \quad (10)$$

We have $y(2\pi) = y(0)$ and $y'(2\pi) = y'(0)$ on the boundaries (Cauchy conditions). The question we pose is whether or not the operator $L_x = d^2/dx^2$ is Hermitian? Form the integral

$$\begin{aligned} \int_0^{2\pi} y_1^* L_x y_2 dx &= \left[\cancel{y_1^* \frac{dy_2}{dx}} \right]_0^{2\pi} - \int_0^{2\pi} \frac{dy_1^*}{dx} \frac{dy_2}{dx} dx \\ &= \left[\cancel{-\frac{dy_1^*}{dx} y_2} \right]_0^{2\pi} + \int_0^{2\pi} y_2 \frac{d^2 y_1^*}{dx^2} dx \\ &= \left[\int_0^{2\pi} y_2^* L_x y_1 dx \right]^* \quad , \end{aligned} \quad (11)$$

where successive integration by parts has been employed, and periodic solutions presumed. Therefore $L_x = d^2/dx^2$ is Hermitian for this set of Cauchy boundary conditions. However, observe that *it would not necessarily be Hermitian* if non-periodic boundary conditions were adopted.

Example 2: To elucidate further, we look again at the separation of variables technique for PDEs, using the 2D wave equation in cylindrical geometry as our basis. This could correspond to the problem of drumskin vibrations.

$$\begin{aligned} \nabla^2 u - \frac{1}{c^2} \frac{\partial^2 u}{\partial t^2} &= 0 \\ \Rightarrow \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial u}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 u}{\partial \theta^2} - \frac{1}{c^2} \frac{\partial^2 u}{\partial t^2} &= 0 \quad . \end{aligned} \quad (12)$$

One can, and should, require period boundary conditions for this in the azimuthal angle dimension: $u(\theta = 2\pi) = u(\theta = 0)$. Write

$$u(\vec{x}) = R(r) \Theta(\theta) T(t) \quad \text{and define} \quad L_\theta = \frac{d^2}{d\theta^2} \quad . \quad (13)$$

Then, if $\Theta(\theta) = e^{\pm i n \theta}$,

$$L_\theta u(\vec{x}) = R(r) T(t) \left\{ L_\theta \Theta \right\} = -n^2 R(r) T(t) \Theta(\theta) = -n^2 u(\vec{x}) \quad . \quad (14)$$

Here, n is an integer, and $-n^2$ is the eigenvalue for L_θ . We can now form

$$u(\vec{x}) = \sum_{n=0}^{\infty} R(r) T(t) \left\{ a_n e^{in\theta} + b_n e^{-in\theta} \right\} . \quad (15)$$

If we define the radial differential operator

$$L_r \equiv \frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} - \frac{n^2}{r^2} , \quad (16)$$

then the wave equation now becomes

$$\frac{1}{R(r)} L_r [R(r)] = \frac{1}{c^2 T(t)} \frac{d^2 T(t)}{dt^2} \rightarrow -k^2 . \quad (17)$$

To proceed further, one needs radial boundary conditions. Let these be that $u(r=0)$ is finite, and that $u(r=r_d) = 0$, a common set-up for cylindrical BVPs that is suited to the drumskin acoustic problem. Then not only do we have $L_r R = \text{const. } R$, so that the $R(r)$ satisfy a form of Bessel's ODE, but that R is related to the zeros $k_{jn} r_d$ of the J_n Bessel function:

$$R(r) = J_n(k_{jn} r) \quad \text{with} \quad J_n(k_{jn} r_d) = 0 . \quad (18)$$

While the k_{jn} afford a new type of character for the eigenvalues, the $J_n(k_{jn} r)$ do obey orthogonality relations. Specifically, if the α_{ni} are the zeroes of $J_n(x)$ (an infinite set), then

$$\int_0^1 x J_n(\alpha_{ni} x) J_n(\alpha_{nj} x) dx = 0 \quad , \quad i \neq j . \quad (19)$$

There is also a normalization relation

$$\int_0^1 x \left[J_n(\alpha_{ni} x) \right]^2 dx = \frac{1}{2} \left[J_{n+1}(\alpha_{ni}) \right]^2 . \quad (20)$$

The two combine to be of use not just for this Sturm-Liouville problem, but also for Fourier-Bessel series.

The wave function is now of the form

$$u(\vec{x}) = \sum_{n=0}^{\infty} \sum_{j=1}^{\infty} g_{jn}(t) J_n(k_{jn}r) \left\{ a_n e^{in\theta} + b_n e^{-in\theta} \right\} , \quad (21)$$

and the remaining ODE for the time dependence is

$$k_{jn}^2 g_{jn}(t) + \frac{1}{c^2} L_t g_{jn}(t) = 0 \quad , \quad L_t \equiv \frac{d^2}{dt^2} . \quad (22)$$

This possesses a solution

$$g_{jn}(t) = e^{\pm i\omega_{jn}t} \quad , \quad \omega_{jn} = ck_{jn} . \quad (23)$$

Here the third differential operator is L_t , which possesses eigenvalues ω_{jn} .

The complete solution for this eigenvalue/eigenvector problem can be written in real form as

$$u(r, \theta, t) = \sum_{n=1}^{\infty} \sum_{j=1}^{\infty} J_n(k_{jn}r) \cdot \left\{ a_n \sin n\theta + b_n \cos n\theta \right\} \\ \times \left\{ \alpha_{jn} \sin \omega_{jn}t + \beta_{jn} \cos \omega_{jn}t \right\} . \quad (24)$$

Observe that we have three Hermitian differential operators, and hence three sets of eigenvectors, *but only two independent sets of eigenvalues*.

* Observe that the appearance of the Bessel functions is not happenstance: this 2D problem is akin to cylindrical geometry in 3D, and so one would naturally expect the $J_n(k_{jn}r)$ functions to appear.

* The general decline of $|J_n(k_{jn}r)|^2$ as r gets large connects physically to energy conservation in the plane for centrally-located initial perturbations.

* If one combines the angular and temporal portions, one can characterize $n\theta \pm \omega_{jn}t = \text{const.}$ at a fixed radius. These define non-radial modes of oscillation, with a fundamental ($n = 0$) and higher frequency harmonics: these are akin to surface seismic modes on Earth. One can also discern these when dropping two stones into a pond.