NST IB Mathematical Methods II

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1 Sturm-Liouville Theory

1.1 The operator

A Sturm-Liouville operator

$$\boxed{\mathcal{L} = -\frac{\mathrm{d}}{\mathrm{d}x}\left(\rho(x)\frac{\mathrm{d}}{\mathrm{d}x}\right) + \sigma(x), \qquad \rho(x) > 0,\, \sigma(x) \in \mathbb{R}}$$

can be shown to be self-adjoint under appropriate boundary conditions

$$\rho\left(vu^{*\prime} - u^* v'\right)\Big|_\alpha^\beta = 0,$$

meaning $\langle u|\mathcal{L}v\rangle = \langle \mathcal{L}u|v\rangle$ (equivalently, $\mathcal{L}^\dagger = \mathcal{L}$).

Such self-adjointness provides many convenient features. Just like Hermitian matrices, for example, in the eigenvalue equation for a self-adjoint operator $\mathcal{L}y_n = \lambda_n y_n$, the eigenvalues λ_n are real and **non-degenerate** eigenfunctions y_n are mutually orthogonal. Moreover, the eigenfunctions commonly form a complete basis, from which we could solve inhomogeneous linear differential equations.

1.2 A generalisation to any 2nd order linear ODE

Despite being seemingly restrictive, the Sturm-Liouville operator could express any second order linear differential operator ($a = -p, b = p' - q$)

$$\tilde{\mathcal{L}} = p(x)\frac{\mathrm{d}^2}{\mathrm{d}x^2} + q(x)\frac{\mathrm{d}}{\mathrm{d}x} + r(x) = -\frac{\mathrm{d}}{\mathrm{d}x}\left(a(x)\frac{\mathrm{d}}{\mathrm{d}x}\right) - b(x)\frac{\mathrm{d}}{\mathrm{d}x} + r(x)$$

could be converted into a Sturm-Liouville form by choosing $w(x)$ such that

$$w\tilde{\mathcal{L}} = -\frac{\mathrm{d}}{\mathrm{d}x}\left(aw\frac{\mathrm{d}}{\mathrm{d}x}\right) + (aw' - bw)\frac{\mathrm{d}}{\mathrm{d}x} + rw$$

has a vanishing coefficient for the first derivative term:

$$\boxed{w(x) = C\exp\left[\int^x \frac{b(x')}{a(x')}\mathrm{d}x'\right] > 0.}$$

This way, a Sturm-Liouville operator

$$\mathcal{L} = w(x)\tilde{\mathcal{L}} = -\frac{\mathrm{d}}{\mathrm{d}x}\left(\rho(x)\frac{\mathrm{d}}{\mathrm{d}x}\right) + \sigma(x), \qquad \rho = aw,\, \sigma = rw$$

could be constructed. From this, an eigenvalue problem $\tilde{\mathcal{L}}y_n = \lambda y_n$ involving $\tilde{\mathcal{L}}$ could be converted to a generalised eigenvalue problem $\mathcal{L}y_n = \lambda w(x) y_n$ of the Sturm-Liouville operator $\mathcal{L}$. Alternatively, we could stick with the original operator $\tilde{\mathcal{L}}$ and introduce the weight in the definition of inner product such that

$$\langle u|v\rangle_w = \int_\alpha^\beta w^* uv\,\mathrm{d}x \implies \|v\|_m^2 = \int_\alpha^\beta w^* |v|^2\,\mathrm{d}x,$$

and the self-adjoint condition becomes $\langle u|\mathcal{L}v\rangle_w = \langle \mathcal{L}u|v\rangle_w$. Under this convention, $\tilde{\mathcal{L}}$ satisfying the original eigenvalue equation is self-adjoint with weight $w(x)$ while $\mathcal{L}$ satisfying the generalised eigenvalue equation is self-adjoint with weight 1.

2 Laplace's and Poisson's equation

Many physical systems, including incompressible irrotational fluids, heat conduction, and electrostatics, can be described by Poisson's equation

$$\nabla^2\Phi(\mathbf{r}) = \rho(\mathbf{r}), \tag{1}$$

where $\Phi(\mathbf{r})$ is defined in some region V with **Dirichlet** boundary conditions $\Phi(\mathbf{r}) = \Psi(\mathbf{r})$ or **Neumann** boundary conditions $\nabla\Phi\cdot\hat{n} = \Psi(\mathbf{r})$ on ∂V. Sometimes Φ is itself an observable, like temperature, while sometimes it is only $\nabla\Phi$ that is physical, like in electrostatics. The distinction sometimes brings about a difference in boundary conditions. We are sometimes (like in heat conduction) also interested in the flux $\mathbf{F} = \kappa\nabla\Phi$, where κ is (piecewise) constant.

2.1 Laplace's equation

When $\rho(\mathbf{r}) = 0$ in Eq.(1), it simplifies into Laplace's equation

$$\nabla^2\Phi(\mathbf{r}) = 0,$$

where $\Phi(\mathbf{r})$ satisfies the same types of boundary conditions as described above. We could express $\Phi(\mathbf{r})$ as a superposition of separable solutions in cartesian coordinates, planar polar, or spherical polar coordinates.

2.1.1 Cartesian coordinates

Separation into cartesian coordinates gives $\Phi(x,y,z) = X(x)Y(y)Z(z)$ and the Laplace's equation reads

$$\frac{X''(x)}{X} + \frac{Y''(y)}{Y} + \frac{Z''(z)}{Z} = 0,$$

$$\implies \frac{\mathrm{d}^2X}{\mathrm{d}x} = -k_x^2X, \quad \frac{\mathrm{d}^2Y}{\mathrm{d}y} = -k_y^2Y, \quad \frac{\mathrm{d}^2Z}{\mathrm{d}z} = (k_x^2+k_y^2)Z.$$

Therefore, one part of the solution must be qualitatively different from the other two. The most general solution is

$$X = A\cos(k_xx+B) \quad Y = C\cos(k_yy+D), \quad Z = E\exp\left(\sqrt{k_x^2+k_y^2}z\right) + F\exp\left(-\sqrt{k_x^2+k_y^2}z\right),$$

but the boundary conditions often immensely simplifies the expression. For example, k_x and k_y may be quantised to integer multiplies of some quantities and $B = D = 0$ if oscillatory boundary conditions are given in X and Y. Furthermore, the exponential growth solution in Z are often killed due to regularity constraint at infinity.

2.1.2 Planar polar coordinates

In planar polar coordinates, the solution can be separated as $\Phi(r,\phi) = P(\phi)R(r)$ and the Laplace's equation reads

$$\nabla^2\Phi = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial\Phi}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2\Phi}{\partial\phi^2} = 0,$$

giving the separated ODE as

$$\frac{\mathrm{d}^2P}{\mathrm{d}\phi} + n^2P = 0, \quad r^2\frac{\mathrm{d}^2R}{\mathrm{d}r^2} + r\frac{\mathrm{d}R}{\mathrm{d}r} - n^2R = 0,$$

where $n = 0,1,2,\ldots$ from the physical requirement on periodicity of P or P': if Φ is physically meaningful, then we require $P(\phi+2\pi) = P(\phi)$ and if only $\nabla\Phi$ is physical, only P' needs to be periodic. The ODE on P gives oscillatory solution while that on R is of Euler's type and gives a power function solution $R = r^{\pm n}$ or $R = \ln r$. Thus, the general solution is

$$\boxed{\Phi(r,\phi) = A_0 + B_0\phi + C_0\ln r + \sum_{\substack{n=-\infty\\ n\neq 0}}^{\infty} r^n(A_n\cos(n\phi) + B_n\sin(n\phi)).}$$

The $B_0\phi$ term is only present when the physical quantity is $\nabla\Phi$. Regularity condition at $r=0$ kills $\ln r$ and all the r^{-n} while regularity at infinity kills all the r^{-n} dependence (and $\ln r$ if it is posted on Φ itself). Specifying one more boundary condition then gives A_n and B_n in terms of Fourier coefficients.

The only solution to the Laplace's equation in all space is a constant function, which is consistent with Liouville's theorem in complex analysis (though this is true in 3D as well). Therefore, we usually study the behaviour parts of the space (e.g. a circular disc). Alternatively, we could allow $\hat{n}\cdot\nabla\Phi$ to have a jump discontinuity across some boundaries and split the solution into two piecewise parts. This may correspond to a point source or a discontinuity in the conductivity κ (conserving flux $\mathbf{F}$).

2.1.3 Spherical polar coordinates

Laplace's equation in axisymmetric spherical polar coordinates (no ϕ dependence) is

$$\nabla^2\Phi = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\Phi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Phi}{\partial\theta}\right) = 0,$$

where $\Phi(r,\theta) = \Theta(u)R(r)$ and $u=\cos\theta$. The equation can then be separated as

$$\frac{\mathrm{d}}{\mathrm{d}u}\left[(1-u^2)\frac{\mathrm{d}\Theta}{\mathrm{d}u}\right] + l(l+1)T = 0, \quad r^2\frac{\mathrm{d}^2R}{\mathrm{d}r} + 2r\frac{\mathrm{d}R}{\mathrm{d}r} - l(l+1)r = 0.$$

The ODE on Θ is of the Legendre type and is only regular at $u=\pm1$ when $l=0,1,\ldots$ The second ODE is of Euler's type and admits power function solutions $R=r^l, r^{-l-1}$. Thus, the general solution is

$$\boxed{\Phi(r,\theta) = \sum_{l=0}^{\infty}\left(A_l r^l + B_l r^{-l-1}\right)P_l(\cos\theta),}$$

where $P_l(x)$ is the Legendre polynomial with normalisation $P_l(1)=1$.

(*) When the system is not axisymmetric, the Laplace's equation becomes

$$\nabla^2\Phi = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\Phi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Phi}{\partial\theta}\right) + \frac{1}{r^2\sin\theta}\frac{\partial^2\Phi}{\partial\phi^2} = 0.$$

It needs to be separated into $\Phi(r,\theta,\phi) = R(r)\Theta(\theta)P(\phi)$ with two separation constants, as shown below:

$$\begin{cases} \dfrac{\sin^2\theta}{R}\dfrac{\mathrm{d}}{\mathrm{d}r}\left(r^2\dfrac{\mathrm{d}R}{\mathrm{d}r}\right) + \dfrac{\sin\theta}{\Theta}\dfrac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\dfrac{\mathrm{d}\Theta}{\mathrm{d}\theta}\right) = -\dfrac{1}{P}\dfrac{\mathrm{d}^2P}{\mathrm{d}\phi^2} & = \lambda_1, \\ \dfrac{1}{R}\dfrac{\mathrm{d}}{\mathrm{d}r}\left(r^2\dfrac{\mathrm{d}R}{\mathrm{d}r}\right) = -\dfrac{1}{\Theta\sin\theta}\dfrac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\dfrac{\mathrm{d}\Theta}{\mathrm{d}\theta}\right) + \dfrac{\lambda_1}{\sin^2\theta} & = \lambda_2. \end{cases}$$

2.2 Uniqueness of solutions to Poisson's equation

The uniqueness theorem states that if $\nabla^2\Phi = \rho(\mathbf{r})$ in V and Dirichlet or Neumann boundary conditions are satisfied on ∂V, then the solution must be unique, or unique up to a constant for Neumann conditions. This can be proved by showing that $\Psi = \Phi_2 - \Phi_1$ satisfies

$$\int_V |\nabla\Psi|^2\,\mathrm{d}V = \oint_{\partial V}\Psi\nabla\Psi\cdot\mathrm{d}\mathbf{S} = 0$$

using the vector identity $\boxed{\nabla\cdot(\Psi\nabla\Psi) = |\nabla\Psi|^2 + \Psi\nabla^2\Psi}$.

This allows us to use the method of image to convert a Poisson's equation in a confined space to a Poisson's equation over all space.

2.3 Green's function to a point source

Green's function to the Poisson's equation in V bounded by S is

$$\boxed{\nabla_r^2 G(\mathbf{r},\mathbf{r}') = \delta^{(3)}(\mathbf{r}-\mathbf{r}')}$$

satisfying $\boxed{G = 0 \text{ on } S}$ for a Dirichlet problem or $\boxed{\nabla \cdot G = 1/A \text{ on } S}$ for a Neumann problem, where A is surface area of S. It is not hard to verify that $G(\mathbf{r}, \mathbf{r}')$ is symmetric under $\mathbf{r} \Leftrightarrow \mathbf{r}'$. The condition on Neumann problem comes from conserving the flux

$$\oint_S \nabla G \cdot \mathrm{d}\mathbf{S} = \int_V \nabla^2 G \, \mathrm{d}V = \int_V \delta^{(3)}(\mathbf{r} - \mathbf{r}') \, \mathrm{d}V = 1.$$

2.3.1 3D fundamental solution

A fundamental solution $G(\mathbf{r}, \mathbf{r}')$ is the Green's function satisfying the boundary conditions in the whole space. Just as what we did in finding the Green's function of an ODE, G can be obtained by solving the Laplace's equation but allowing for discontinuity with determined strength at the origin.

2.3.2 2D fundamental solution

2.3.3 The method of image for complicated geometry

2.4 Integral solution to Poisson's equation