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

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

but the boundary conditions often immensely simplifies the expression. For example, k_x and k_y may be quantised to integer multiples 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 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 homogeneous $\boxed{G = 0 \text{ on } S}$ 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 and $\mathbf{r}'$ can be any point inside V. 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.

Since the proposed PDE is radially symmetric, we would expect G to only have radial dependence, giving

$$\nabla^2 G = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial G}{\partial r} \right) = 0 \qquad \Longrightarrow \; G = \frac{C}{r} + A \quad (r \neq 0),$$

where A, C are arbitrary constants. The constant offset A must be 0 for a Dirichlet problem but can be left undetermined for a Neumann problem. The strength C can be determined by the flux out from the origin:

$$\int_{r<\epsilon} \nabla^2 G \mathrm{d}V = \oint_{r=\epsilon} \frac{\partial G}{\partial r} \mathrm{d}S = 1,$$

giving (shifting the origin)

$$\boxed{G = -\frac{1}{4\pi \left| \mathbf{r} - \mathbf{r}' \right|}.}$$

2.3.2 2D fundamental solution

Similarly, the fundamental solution to the 2D Poisson's equation

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

is

$$\boxed{G(\mathbf{r}, \mathbf{r}') = \frac{1}{2\pi} \ln \left| \mathbf{r} - \mathbf{r}' \right| + \text{const.}}$$

Note that in two dimensions we can no longer require $G \to 0$ at infinity, so the Dirichlet boundary conditions are usually specified in other ways.

2.3.3 The method of image for complicated geometry

We can seek Green's function over a infinite domain using the fundamental solution. However, we often want to find Green's functions in some more complicated domains, like a half-plane or a circle. This calls for the method of image which relies on uniqueness of solution to Poisson's equation. If we can cleverly introduce point sources **outside** the domain V such that the fundamental solution over the whole space also *happens* to satisfy the homogeneous boundary condition on the finite domain V, we can claim to find the **unique** solution.

For example, for a infinite plane/line boundary, we could simply reflect the source, as shown in Fig.1 to give the Green's function as a superposition of fundamental solutions:

$$G = -\frac{1}{4\pi} \left(\frac{1}{|\mathbf{r} - \mathbf{r_0}|} \pm \frac{1}{|\mathbf{r} - \mathbf{r_1}|} \right),$$

where $\mathbf{r_1}$ is the position of the image charge. With Dirichlet boundary conditions, an image source of opposite sign is introduced and we essentially have a dipole field with all flux through the wall (none to infinity). With Neumann boundary conditions, on the other hand, all the flux spreads out to infinity.

For a spherical or circular boundary with Dirichlet boundary condition, we could put an image charge at the inverse point $\mathbf{x_1} = (a^2 / |\mathbf{r_0}|) \mathbf{r_0}$ (so that a is the geometric mean of r_0 and r_1). For a 2D circle, the strength of the image charge is just $q = -Q$ while for a 3D sphere the image charge must have a weaker strength $q = -a/r_0$.

If the boundary is in more complicated geometry, some numerical methods are probably needed to find the Green's function. However, an inhomogeneous forcing or an inhomogeneous boundary condition with a simple geometry could be resolved by the following integral solution.

(a) Dirichlet boundary condition (b) Neumann boundary condition

Figure 1: Image charges (red) for an infinite plane boundary conditions.

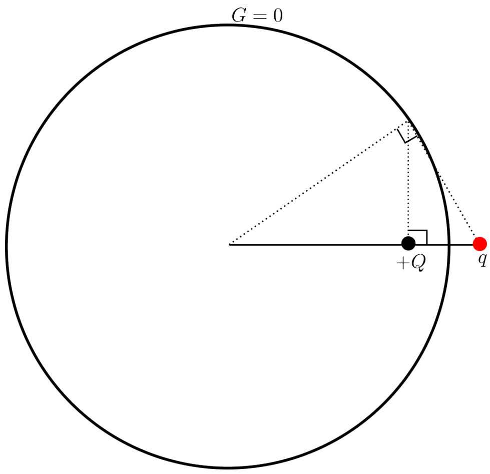

Figure 2: Inverse point for a spherical or circular Dirichlet boundary.

2.4 Integral solution to Poisson's equation

With the Green's function in hand, we could solve the inhomogeneous Poisson's equation $\nabla^2\Phi = \rho(\mathbf{r})$ with inhomogeneous boundary condition $\Phi = f(\mathbf{r})$ on S or $\nabla\Phi \cdot \hat{\mathbf{n}} = f(\mathbf{r})$ on S. From the same vector calculus identity we used in proving uniqueness of Poisson's equation, we could prove Green's second identity ($\Psi = G$)

$$\boxed{\int_V = (\Phi\nabla^2\Psi - \Psi\nabla^2\Phi)\mathrm{d}V = \oint_S \left(\Phi\frac{\partial\Psi}{\partial n} - \Psi\frac{\partial\Phi}{\partial n}\right).}$$

For a Dirichlet boundary condition, this simplifies to

$$\boxed{\Phi(\mathbf{r}') = \int_V \rho(\mathbf{r})G(\mathbf{r},\mathbf{r}')\mathrm{d}V + \oint f(\mathbf{r})\nabla G \cdot \mathrm{d}\mathbf{S},}$$

where the first term comes from superposition of different sources and the second term comes from inhomogeneous boundary conditions. Similarly, the solution from Neumann boundary condition is

$$\boxed{\Phi(\mathbf{r}') = \int_V \rho(\mathbf{r})G(\mathbf{r},\mathbf{r}')\mathrm{d}V - \oint f(\mathbf{r})G(\mathbf{r},\mathbf{r}')\mathrm{d}S + C.}$$