Separation of variables & Sturm-Liouville theory

In physics, we often have problems that depend on several variables. Consider for example the case of a wave in a medium, in 1D, with vanishing boundary conditions:

$$\hat{\mathcal{D}}\, U(x,t) - \frac{1}{c^2}\frac{\partial^2}{\partial t^2} U(x,t) = 0$$

where c is the wave's speed, and $\hat{\mathcal{D}}$ is a (second order) differential operator e.g. $\hat{\mathcal{D}} = \frac{\partial^2}{\partial x^2} + p(x)\frac{\partial}{\partial x} + q(x)$.

with $U(x_1,t) = U(x_2,t) = 0$ BC

$U(x,0) = U_0(x), \frac{\partial U}{\partial t}(x_0,0) = U_0'(x)$. IC.

The standard way of solving this problem is through separation of variables. That is, assume:

$$U(x,t) = y(x)\,T(t).$$

Substituting this in the D.E. gives

$$T\hat{\mathcal{D}}y - \frac{1}{c^2} y T'' = 0$$

or $$\frac{\hat{\mathcal{D}}y(x)}{y(x)} = \frac{T''(t)}{c^2 T(t)}.$$

The LHS depends only on x, the RHS on t. Yet, they must be equal $\forall x,t$.

Therefore, both sides must be <u>constant</u>

Let this constant be called λ. Then

$$\hat{\mathcal{D}} y = \lambda y \qquad (1)$$

$$T''(t) = c^2 \lambda T \qquad (2)$$

(2) Has a simple solution

$$T(t) = A_1 e^{c\sqrt{\lambda} t} + A_2 e^{-c\sqrt{\lambda} t},$$

while (1) gives the so-called "Sturm-Liouville" problem

$$\boxed{\begin{array}{ll} \hat{\mathcal{D}} y - \lambda y = 0 & \text{DE} \\ x_1 \le x \le x_2 . & \text{ROI} \\ y(x_1) = y(x_2) = 0 & \text{BC.} \end{array}}$$

As discussed in the notes about selfadjoint operators, we can make the operator selfadjoint by writing $y(x) = \alpha(x)\, u(x)$, where $\alpha(x)$ is the Wronskian. Then

$$\hat{\mathcal{D}} y = \hat{\mathcal{L}} u = (\alpha u')' + \beta u, \quad \alpha = W_0 e^{-P(x)}, \ \beta = (q - p')\alpha$$

The equation for u is then

$$\boxed{\begin{array}{ll} \mathcal{L} u = \lambda w u, & \text{D. E.} \\ x_1 \le x \le x_2 & \text{R. O. I.} \\ u(x_1) = u(x_2) = 0 & \end{array}}$$

where the "weight function" $w(x)$ is the Wronskian $\alpha(x)$.

This problem is analogous to the eigenvalue problems for Matrices:

$$\mathbb{M}\vec{u} = \lambda \vec{u}$$

which have a discrete set of solutions (eigenvectors) $\vec{u}_i$ with corresponding eigenvalues λ

The same is true for the functional problem:

$$\hat{\mathcal{L}} u_i = \lambda_i w u_i$$

i.e. there are a discrete set of solutions $u_i(x)$ (eigenfunction) with eigenvalues λ_i.

Note that, if we define the inner product:

$$\langle u, v\rangle = \int_{x_1}^{x_2} u^*(x) w(x) v(x) dx$$

weight function, which happens to be equal to the ~~Jacobian~~, Wronskian

Then

$$\int_{x_1}^{x_2} u_i^* \hat{\mathcal{L}} u_j dx = \lambda_j \int_{x_1} u_i^* w u_j dx = \lambda_j \langle u_i, u_j\rangle$$

but, because $\hat{\mathcal{L}}$ is self adjoint and $u_i(x_1) = u(x_2) = 0$,

$$\int_{x_1}^{x_2} u_i^* \hat{\mathcal{L}} u_j dx = \left[\int_{x_1}^{x_2} u_j^* \hat{\mathcal{L}} u_i dx\right]^* \quad \text{so}$$

$$\lambda_j \langle u_i, u_j\rangle = \lambda_i^* \underbrace{\langle u_j, u_i\rangle^*}_{\langle u_i, u_j\rangle}$$

or

$$(\lambda_j - \lambda_i^*)\langle u_i, u_j\rangle = 0$$

- If $i=j$, this means that

$$\lambda_i^* = \lambda_i \Rightarrow \lambda_i = \text{real}.$$

The eigenvalues of self-adjoint operators are always real.

- If $i \neq j$ and $\lambda_i \neq \lambda_j$, then

$$\langle u_i, u_j\rangle = 0$$

The eigenfunctions (with different eigenvalues) of a self-adjoint operator are orthogonal.

- If $i \neq j$ and $\lambda_i = \lambda_j$ then u_i & u_j are said to be degenerate. u_i & u_j are not necessarily orthogonal, but can be recombined into orthogonal eigenfunctions using a Gram-Schmidt procedure.

Notice that the Sturm-Liouville equation can be written as

$$\hat{\mathcal{L}}u - \lambda w u = (\alpha u')' + (\beta - \lambda w)u = 0$$

$$= (\alpha u')' + \bar{\beta} u \quad , \text{ where } \bar{\beta} = \beta - \lambda w.$$
$$= \beta - \lambda \alpha$$

Also, recall that $u(x_1) = u(x_2) = 0$.

Therefore, we are looking for MODES of the modified self-adjoint operator

$$\hat{\bar{\mathcal{L}}} u = (\alpha u')' + \bar{\beta} u$$

We know (from the notes on self-adjoint operators) that there are no modes if

$$\alpha \bar{\beta} \leq 0 \quad \text{for all } x \in [x_1, x_2] \text{, i.e.}$$

$$\alpha \beta - \lambda \alpha^2 \leq 0, \text{ that is:}$$

No modes with $\lambda \geq \beta / \alpha \quad \forall x \in [x_1, x_2]$

That is, <u>there is an upper bound on the possible value of the eigenvalue</u>

The ~~eigenvalue~~ eigenfunction with the largest eigenvalue is called the "ground state". (In some applications we let $\lambda = -k$, where k then has a lower bound.)