Rayleigh-Ritz Method

The Sturm-Liouville equation

Note: sign convention different from (MW) and (AW)

$$\mathcal{L}[u] = (p(x)u'(x))' + q(x)u(x) = \lambda w(x)u(x), \quad a<x<b$$

is an Euler-Lagrange equation for the functional

$$I[u] = \int_a^b [p(u')^2 - (q-\lambda w)u^2]dx \qquad (\text{we assume } p(x) \geq 0)$$

Indeed, $\frac{\delta I}{\delta u} = -\frac{d}{dx}\frac{\partial I}{\partial u'} + \frac{\partial I}{\partial u} = -(2pu')' - (q-\lambda w)\cdot 2u = 0$

Lagrange multiplier!

Rewriting: $I[u] = \int_a^b [p(u')^2 - qu^2]dx + \lambda \int_a^b u^2 w\, dx$

we see that stationary values of I coincide with stationary values of

$$I'[u] = \int_a^b [p(u')^2 - qu^2]dx$$

subject to the constraint $N[u] = \int_a^b u^2 w\, dx = \text{const}$ ← normalization!

In other words, stationary values (minima) of the functional $I[u]$ are reached when λ is an eigenvalue of the S-L problem.

Note: minimizing $I[u]$ is equivalent to maximizing

$$K[u] = -\frac{I'[u]}{N[u]}$$

Note! We can rewrite $I'[u]$ in an alternative form:

$$I'[u] = \int_a^b [p(u')^2 - qu^2]dx = \int_a^b pu'u'dx - \int_a^b qu^2 dx =$$

$$= \cancel{(puu')\Big|_a^b} - \int_a^b (pu')'u\, dx - \int_a^b (qu)u\, dx = -\int_a^b u\mathcal{L}u\, dx$$

When $u = \psi_n$:

$$K[\psi_n] = \frac{\int_a^b \psi_n \mathcal{L}\psi_n dx}{\int_a^b \psi_n^2 w\, dx} = \frac{\int_a^b \psi_n \lambda_n \psi_n w\, dx}{\int_a^b \psi_n^2 w\, dx} = \lambda_n$$

Using this relation it is possible to show that (for $p(x) \geq 0$):

1) There is a largest eigenvalue λ_0: $\lambda_n \leq \lambda_0$, $n \neq 0$.
2) $\lambda_n \to -\infty$, $n \to \infty$
3) more precisely $\lambda_n \sim \text{const} \cdot n^2$, $n \to \infty$

Let us find the absolute maximum of $K[u] = \lambda_0$:

This can be done approximately by making a good guess at ψ_0:

$u = \psi_0 + c_1\psi_1 + c_2\psi_2 + \dots$ (assume ψ_n are normalized)

$$I'[u] = -\int_a^b u \mathcal{L} u \, dx = -\int_a^b (\psi_0 + c_1\psi_1 + \dots) \mathcal{L} (\psi_0 + c_1\psi_1 + \dots) w \, dx =$$
$$= -\int_a^b (\psi_0 + c_1\psi_1 + \dots)(\lambda_0\psi_0 + c_1\lambda_1\psi_1 + \dots) w \, dx = -\lambda_0 \int_a^b \psi_0^2 w \, dx -$$
$$- c_1(\lambda_0 + \lambda_1) \int_a^b \psi_0 \psi_1 w \, dx - c_1^2 \lambda_1 \int_a^b \psi_1^2 w \, dx - \dots = -\lambda_0 - c_1^2\lambda_1 - c_2^2\lambda_2 - \dots$$

$$N[u] = \int_a^b (\psi_0 + c_1\psi_1 + \dots)^2 w \, dx = 1 + c_1^2 + c_2^2 + \dots$$

$$\Rightarrow K[u] = \frac{\lambda_0 + c_1^2\lambda_1 + c_2^2\lambda_2 + \dots}{1 + c_1^2 + c_2^2 + \dots} = \lambda_0 + O(c_1^2, c_2^2, \dots)$$

Note: 1^{st} order accurate guess for ψ_0 gives 2^{nd} order accurate estimate of λ_0!

Example:

Find the largest eigenvalue of $\begin{cases} u'' = \lambda u \\ u(0) = u(1) = 0 \end{cases}$

The exact answer is $\lambda_0 = -\pi^2$, $\psi_0 = \sqrt{2}\sin(\pi x)$

take trial function $u_0(x) = x(1-x)$: (it has to satisfy b.c.!)

$$\lambda_0 \approx \frac{\int_0^1 x(1-x)[x(1-x)]'' dx}{\int_0^1 [x(1-x)]^2 dx} = -\frac{2\int_0^1 x(1-x) dx}{\int_0^1 x^2(1-x^2)^2 dx} = -\frac{\frac{1}{3}}{\frac{1}{30}} = -10$$

Exact result, $\lambda_0 = -\pi^2 = -9.8696$ (Less than 2% error)

How do we find the other eigenvalues (at least approximately)?

$\lambda_n = K[\varphi_n] \approx K[u]$, where $u \approx \varphi_n$

$\mathcal{L}$ is self-adjoint $\Rightarrow \varphi_n \perp \varphi_m$, $n \neq m$

So, for instance, λ_1 is an absolute maximum of $K[u]$ restricted to $u \perp \varphi_0$:

$$\lambda_1 = \max_u \left[K[u] + \mu \int_a^b u\varphi_0 w\,dx \right], \quad \int_a^b u\varphi_0 w\,dx = 0$$

and so on.

Example:

Find λ_1 for $x'' = \lambda x$, $x(0) = x(1) = 0$.

Both $\varphi_0 = \sqrt{2}\sin(\pi x)$ and $u_0 = x(1-x)$ are even w.r.t $x = \frac{1}{2}$

Take $u_1 = x(1-x)(x-\frac{1}{2})$ which is odd w.r.t. $x = \frac{1}{2}$, such that u_1 is orthogonal to both u_0 and φ_0

$$\lambda_1 \approx \frac{\int_0^1 u_1(u_1'')\,dx}{\int_0^1 u_1^2\,dx} = \frac{\int_0^1 x(1-x)(x-\frac{1}{2})[x(1-x)(x-\frac{1}{2})]''dx}{\int_0^1 [x(1-x)(x-\frac{1}{2})]^2 dx} = \frac{-\frac{1}{20}}{\frac{1}{840}} = -42$$

Exact answer is $\lambda_1 = -(2\pi)^2 = -39.438$ (6% accuracy)

Example: (Quantum Harmonic Oscillator)

$H\psi = E\psi$, $H = -\frac{d^2}{dx^2} + x^2$: What is the ground state energy E_0?

Trial wavefunction: $\psi = (1+\alpha x^2)e^{-x^2}$

$$E_0 \leq \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\int_{-\infty}^{\infty}\psi^*(-\psi'' + x^2\psi)\,dx}{\int_{-\infty}^{\infty}|\psi|^2 dx} = \frac{\frac{5}{4} - \frac{\alpha}{8} + \frac{43}{64}\alpha^2}{1 + \frac{\alpha}{2} + \frac{3}{16}\alpha^2} \equiv E(\alpha)$$

Find α for which $E(\alpha)$ reaches the minimal value:

$$\frac{\partial E}{\partial \alpha} = \frac{23\alpha^2 + 56\alpha - 48}{(\ \ldots\ )} = 0 \Rightarrow \alpha = 0.67 \Rightarrow E_0 \leq E(0.67) \approx 1.034$$

Exact answer $E_0 = 1$ (3% accuracy)