

Statement of Rayleigh-Ritz method -

for approximating the (whole) discrete spectrum

The problem of finding stationary points
of

$$(4.65) \quad I(u) = \int_0^1 \rho u'^2 + q u^2 dx - p(1)u(1)u'(1) + \\ + p(0)u(0)u'(0)$$

subject to $N+1$ constraints

$$\int_0^1 w u^2 dx = 1, \quad \int_0^1 w u u_i dx = 0, \quad i=1, \dots, N$$

has a unique solution which is $N+1^{th}$
e'function u_{N+1} of the problem

$$L u_{N+1} = \lambda_{N+1} w u_{N+1} \quad B_i(u_{N+1}) = 0$$

and

$\lambda_{N+1} = I(u_{N+1})$. Approximate solutions of
the variational problem yield approximate
solutions of the eigenvalue problem.

Procedure

To solve S.-L. e'value problem

$$-(pu')' + qu + zwu = 0 \quad x \in (0, 1)$$

$$B_1(u) = u(0) + c_1 u'(0) = 0$$

$$B_2(u) = u(1) + c_2 u'(1) = 0$$

with $p(x) > 0$, $w(x) > 0$, $q(x) \geq 0$, $c_1 \leq 0$, $c_2 \geq 0$

Take an infinite sequence of lin. independent functions $\psi_1(x), \psi_2(x), \dots$ in D_B and seek an approximate solution to the e'value problem, for the first N e'values and e'functions by substituting

$$g_N = \sum_{j=1}^N \alpha_j \psi_j(x)$$

in the variational problem (4.65) and solving for $\{\alpha_j\}$.

(4.64) and (4.65) \Rightarrow

$$\vec{\alpha} = \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_N \end{pmatrix} \quad I(g_N) \equiv \bar{\Phi}(\vec{\alpha}) = \sum_{i,j} A_{ij} \alpha_i \alpha_j$$

where

$$A_{ij} = \int_0^l \rho \psi_i' \psi_j' + g \psi_i' \psi_j dx + c_2 \rho(1) \psi_i'(1) \psi_j'(1) - c_1 \rho(0) \psi_i'(0) \psi_j'(0)$$

$A = (A_{ij})$: matrix, real symmetric
and positive definite

Use the constraint $\Omega = 1 \Rightarrow$

$$Q(g_N) \equiv \Psi(\vec{\alpha}) = \sum_i B_{ij} \alpha_j = 1 \quad \text{sum over } i \text{ and } j$$

$B = (B_{ij})$: also real symmetric and positive definite

$$B_{ij} = \int_0^l \omega \psi_i' \psi_j dx$$

$$\begin{aligned} \text{Let } \mathcal{F} &= \bar{\Phi}(\vec{\alpha}) - \lambda (\Psi(\vec{\alpha}) - 1) = \\ &= \sum_i A_{ij} \alpha_j - \lambda (\sum_i B_{ij} \alpha_j - 1) \end{aligned}$$

where λ is the Lagrange multiplier and
find $\vec{\alpha}$ s.t. \mathcal{F} is stationary with
 $\Psi(\vec{\alpha}) = 1$. Now a finite (N) dimensional
problem is

$$\frac{\partial \mathcal{F}}{\partial \alpha_i} = 0 \Rightarrow A_{ij}\alpha_j - \gamma B_{ij}\alpha_j = 0 \quad i=1, \dots, N$$

sum over j

ii.

$$(A - \gamma B) \vec{\alpha} = \vec{0}$$

$$\Rightarrow \det(A - \gamma B) = 0 \quad (4.66)$$

Note: (4.66) is a generalized eigenvalue problem since $B \neq I$ in general. The polynomial $\det(A - \gamma B) = 0$ is of degree N and has N roots

$$\hat{\gamma}_1, \hat{\gamma}_2, \dots, \hat{\gamma}_N \quad (\text{ordered})$$

Result: The $\hat{\gamma}_i$, $i=1, \dots, N$, approximate the first N eigenvalues, i.e. $\hat{\gamma}_i \approx \gamma_i$. The corresponding eigenvectors of (4.66) are $\vec{\alpha}^{(i)}$ and they approximate the first N eigenfunctions via

$$g_N^{(i)} = \sum_{j=1}^N \alpha_j^{(i)} \psi_j(x) \approx u_i(x) \quad i=1, \dots, N$$

(A and B are positive definite, i.e. in matrix notation, $\vec{\alpha}^T A \vec{\alpha} > 0$ and $\vec{\alpha}^T B \vec{\alpha} > 0$ for $\vec{\alpha} \neq \vec{0}$)

Indeed,

$$\begin{aligned}\vec{\alpha}^T B \vec{\alpha} &= \sum_i \sum_j \alpha_i B_{ij} \alpha_j = \sum_i \sum_j \alpha_i \alpha_j \int_0^1 \omega \psi_i \psi_j dx \\ \text{swap } &= \sum_i \sum_j \int_0^1 \omega \left(\sum_i \alpha_i \psi_i \right) \left(\sum_j \alpha_j \psi_j \right) dx = \\ &= \int_0^1 \omega \left(\sum_i \alpha_i \psi_i \right)^2 dx > 0 \quad \Rightarrow \quad B \text{ is positive definite}\end{aligned}$$

(unless $\sum_i \alpha_i \psi_i = 0$ but then $\vec{\alpha} = \vec{0}$ \Downarrow
so $\{\psi_i\}$ are lin. indep.)

Similarly

$$\begin{aligned}\vec{\alpha}^T A \vec{\alpha} &= \sum_i \sum_j \alpha_i \alpha_j \left(\int_0^1 p \psi_i' \psi_j' + g \psi_i \psi_j dx - \right. \\ &\quad \left. + c_2 p(1) \psi_i'(1) \psi_j'(1) - c_1 p(0) \psi_i'(0) \psi_j'(0) \right) = \\ &= \int_0^1 p \left(\sum_i \alpha_i \psi_i' \right)^2 + g \left(\sum_i \alpha_i \psi_i \right)^2 dx + \\ &\quad + c_2 p(1) \left(\sum_i \alpha_i \psi_i' \right)^2 - c_1 p(0) \left(\sum_i \alpha_i \psi_i \right)^2 > 0\end{aligned}$$

Since ψ_i are lin. independent, $p, q > 0$, $c_2 \geq 0$,
 $G \leq 0$

Positive definite $\Rightarrow \det A \neq 0$, $\det B \neq 0$.

Claim Show that $\hat{\gamma}_i > 0$.

From (4.66)

$$\vec{\alpha}^T \cdot | A \vec{\alpha}^{(i)} = \hat{\gamma}_i B \vec{\alpha}^{(i)}$$

$$\Rightarrow \underbrace{\vec{\alpha}^{(i)T} A \vec{\alpha}^{(i)}}_{>0} = \hat{\gamma}_i \cdot \underbrace{\vec{\alpha}^{(i)T} B \vec{\alpha}^{(i)}}_{>0} \quad (4.67)$$

$$\Rightarrow \hat{\gamma}_i > 0$$

Claim $\hat{\gamma}_i = \Phi(\vec{\alpha}^{(i)})$

We have

$$\Phi(\vec{\alpha}^{(i)}) = \vec{\alpha}^{(i)T} A \vec{\alpha}^{(i)}$$

and

$$\Phi(\vec{\alpha}^{(i)}) = \vec{\alpha}^{(i)T} B \vec{\alpha}^{(i)} = 1 \quad (\text{constraint})$$

so, (4.67) gives

$$\underbrace{\vec{\alpha}^{(i)\top} A \vec{\alpha}^{(i)}}_{\Phi(\vec{\alpha}^{(i)})} = \hat{\gamma}_i \underbrace{\vec{\alpha}^{(i)\top} B \vec{\alpha}^{(i)}}_{\Psi(\vec{\alpha}^{(i)})} = 1$$

$$\therefore \hat{\gamma}_i = \Phi(\vec{\alpha}^{(i)})$$

Claim: $\vec{\alpha}^{(j)\top} B \vec{\alpha}^{(i)} = \delta_{ij}$

This corresponds to the e 'functions being orthogonal, i.e. to

$$\int w u_i u_j dx = \delta_{ij}$$

a result we would expect or hope for even though it was not imposed directly as a constraint.

Proof

$$\underline{i=j} : \vec{\alpha}^{(i)\top} B \vec{\alpha}^{(i)} = 1 \quad \text{is the applied constraint } \Psi(\vec{\alpha}^{(i)}) = 1$$

$i \neq j$:

$$\vec{\alpha}^{(j)\top} A \vec{\alpha}^{(i)} = \hat{\gamma}_i B \vec{\alpha}^{(i)}$$

$$\vec{\alpha}^{(j)\top} A \vec{\alpha}^{(i)} = \hat{\gamma}_i \vec{\alpha}^{(j)\top} B \vec{\alpha}^{(i)}$$

$$\text{LHS} = \underset{A \text{ is symmetric}}{\left(A \vec{\alpha}^{(j)} \right)^T \vec{\alpha}^{(i)}} = \hat{\pi}_j \cdot (B \vec{\alpha}^{(j)})^T \vec{\alpha}^{(i)} =$$

$$= \hat{\pi}_j \vec{\alpha}^{(j)T} B \vec{\alpha}^{(i)} \quad \text{since } B \text{ is symmetric}$$

$\therefore (\hat{\pi}_i - \hat{\pi}_j) \vec{\alpha}^{(j)T} B \vec{\alpha}^{(i)} = 0 \Rightarrow \text{obtain the result}$
since $\hat{\pi}_i \neq \hat{\pi}_j$

Example

Approximate the first two eigenpairs of

$$u'' + \lambda u = 0 \quad u(0) = u(1) = 0$$

using $\psi_1 = x(1-x)$, $\psi_2 = x^2(1-x)$. We know

$$\lambda_1 = \pi^2, \quad u_1 = \sqrt{2} \sin \pi x$$

$$\lambda_2 = 4\pi^2, \quad u_2 = \sqrt{2} \sin 2\pi x$$

$$I(u) = \int_0^1 u'^2 dx \quad Q(u) = \int_0^1 u^2 dx$$

$$g_2 = \alpha_1 \psi_1(x) + \alpha_2 \psi_2(x)$$

$$A_{11} = \int_0^1 \psi_1'^2 dx = \frac{1}{3}, \quad A_{12} = A_{21} = \int_0^1 \psi_1' \psi_2' dx = \frac{1}{6}$$

$$A_{22} = \int_0^1 \psi_2'^2 dx = \frac{2}{15}$$

$$B_{11} = \int_0^1 \psi_1^2 dx = \frac{1}{30} \quad B_{12} = B_{21} = \int_0^1 \psi_1 \psi_2 dx = \frac{1}{60}$$

$$B_{22} = \int_0^1 \psi_2^2 dx = \frac{1}{105}$$

The variation method is to make

$$\mathcal{F} = \alpha^T A \alpha - 2(\alpha^T B \alpha - 1)$$

stationary subject to constraint

$$\alpha^T B \alpha = 1$$

\Rightarrow

$$(A - 2B) \vec{\alpha} = 0$$

i.e

$$\left\{ \begin{array}{l} \left(\frac{1}{3} - \frac{2}{30} \right) \alpha_1 + \left(\frac{1}{6} - \frac{2}{60} \right) \alpha_2 = 0 \\ \left(\frac{1}{6} - \frac{2}{60} \right) \alpha_1 + \left(\frac{2}{15} - \frac{2}{105} \right) \alpha_2 = 0 \end{array} \right. (*)$$

Charact. eq $\Rightarrow \det(A - 2B) = 0 \Rightarrow$

$$z^2 - 52z + 420 = 0 \Rightarrow (z-10)(z-42) = 0$$

$$\hat{z}_1 = 10 \quad \text{and} \quad \hat{z}_2 = 42$$

$$(z_1 = \bar{v}^2 \Rightarrow 1.3\% \text{ error})$$

$$z_2 = 4\bar{v}^2 \Rightarrow 6\% \text{ error})$$

$\vec{\alpha}^{(1)}$: substitute $\hat{a}_1 = 10$ in (*) and find

$$\text{e}'\text{vector } \vec{\alpha}^{(1)} \Rightarrow \alpha_2 = 0 \Rightarrow \vec{\alpha}^{(1)} = \alpha_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

Apply constraint

α_1 is arbitrary
 $\alpha_1 \neq 0$

$$\Psi(\vec{\alpha}) = 1$$

$$\sum_{i,j} \alpha_i B_{ij} \alpha_j = \alpha_1^2 B_{11} = 1$$

$$\Rightarrow \alpha_1^2 \int_0^1 \psi_1^2 dx = 1 \Rightarrow \alpha_1 = \sqrt{30}$$

Hence, with $\hat{a}_1 = 0$,

$$g_2^{(1)} = \alpha_1^{(1)} \psi_1(x) + \alpha_2^{(1)} \psi_2(x) = \sqrt{30} x (1-x)$$

Similarly,

$\vec{\alpha}^{(2)}$: substitute $\hat{a}_2 = 42$ into (*)

$$\begin{aligned} \Rightarrow -32 \alpha_1 - 16 \alpha_2 &= 0 \\ -16 \alpha_1 - 8 \alpha_2 &= 0 \end{aligned} \quad \left\{ \Rightarrow 2 \alpha_1 + \alpha_2 = 0 \Rightarrow \alpha_2 = -2 \alpha_1 \right.$$

$$\Rightarrow \vec{\alpha}^{(2)} = \alpha_1 \begin{pmatrix} 1 \\ -2 \end{pmatrix} \text{ and } g_2^{(2)} = \alpha_1 (4_1 - 2_2)$$

Applying the constraint $\Phi(\vec{\alpha}) = 1$

$$\Rightarrow \sum_i \sum_j \alpha_i B_{ij} \alpha_j = 1$$

$$\Rightarrow \underbrace{\alpha_1^2}_{\alpha_2 = -2\alpha_1} B_{11} + \underbrace{\alpha_1 \alpha_2}_{-2\alpha_1} B_{12} + \underbrace{\alpha_2 \alpha_1}_{-2\alpha_1} B_{21} + \underbrace{\alpha_2^2}_{(-2\alpha_1)^2} B_{22} = 1$$

$$\alpha_1^2 [B_{11} - 2B_{12} - 2B_{21} + 4B_{22}] = 1$$

$$\alpha_1^2 [B_{11} - 4B_{12} + 4B_{22}] = 1$$

$$\alpha_1^2 \left[\frac{1}{30} - \frac{4}{60} + \frac{4}{105} \right] = 1 \Rightarrow \alpha_1 = \sqrt{210}$$

Hence,

with $\hat{\alpha}_2 = 42$,

$$g_2^{(2)} = \sqrt{210} (x(1-x) - 2x^2(1-x))$$

or

$$g_2^{(2)} = \sqrt{210} x(1-x)(1-\alpha x)$$

We can verify the "approximate orthogonality condition"

$$\vec{\alpha}^{(i)\top} B \vec{\alpha}^{(j)} = \delta_{ij}$$