Variational Approximation

Consider the Sturm-Liouville type eigenvalue equation

\[ \frac{d^2 A(z)}{dz^2} - q(z)A(z) = -\lambda A(z) \quad (1) \]

or equivalently,

\[ \tilde{L}A(z) = \lambda A(z), \quad \tilde{L} = -\frac{d^2}{dz^2} + q(z) \]

and impose the boundary conditions that

\[ A(z) \quad \text{or} \quad \frac{dA}{dz} \]

vanish at the boundaries \( z = a \) and \( z = b \).

If the eigenvalue problem were exactly solvable, the solution would consist of a sequence of eigenfunctions and eigenvalues, given by

\[ A_0(z), \; A_1(z), \; A_2(z), \; \cdots \quad \text{and} \quad \lambda_0 < \lambda_1 < \lambda_2 < \cdots, \]

all of which satisfy Eqn.(1) and the boundary conditions, i.e.,

\[ \frac{dA'_n(z)}{dz} - q(z)A_n(z) = -\lambda_n A(z) \quad (2) \]

Multiplying the above equation by \( A_m(z) \) and integrating, we obtain

\[ \int_a^b A_m \frac{dA'_n}{dz} \, dz - \int_a^b qA_m A_n \, dz = -\lambda_n \int_a^b A_m A_n \, dz \quad (3) \]

Evaluating the first integral by parts, we have

\[ \int_a^b A_m \frac{dA'_n}{dz} \, dz = A_m A'_n |^b_a - \int_a^b A'_m A'_n \, dz \]

Using this together with the orthonormality condition:

\[ \int_a^b A_m A_n \, dz = \delta_{m,n} \]

we achieve the following two integrals which we shall use in the foregoing approximate theory

\[ \int (A'_n)^2 + qA_n^2 \, dz = \lambda_n \quad (4) \]

and

\[ \int (A'_n A'_m + qA_n A_m) \, dz = 0 \quad \text{for} \quad m \neq n \quad (5) \]
**Trial eigenfunction:**

Without solving the eigenvalue equation exactly, one can obtain an approximate value for the lowest eigenvalue $\lambda_0$. The basic essential in the method is the introduction of a suitable “trial” function: $A_{tr}(z)$ capable of imitating the lowest mode eigenfunction $A_0(z)$. A reasonably good trial function must

- satisfy the boundary conditions,
- look qualitatively like the exact solution,
- lead to simple calculations.

If, either by a keen insight into the problem or by chance, $A_{tr}(z)$ turns out to be really a perfect guess, i.e.,

$$A_{tr}(z) \simeq A_0(z),$$

one should naturally expect the approximate value for $\lambda_0$ to come out as extremely close to the exact value.

In general, the trial function may contain one or more free adjustable parameters: $\alpha, \beta, \ldots$; and by tuning these parameters one can make the approximation to approach the exact eigenvalue. It is interesting that a trial function which is a relatively poor approximation to $A_0(z)$ may still give a fairly good approximation for $\lambda_0$.

To see how this comes about, we note that if $A_{tr}(z | \alpha, \beta, \ldots)$ is proposed so as to mimic $A_0(z)$, it has to satisfy the eigenvalue equation (1) and the boundary conditions at the end points. We therefore write

$$\frac{dA_{tr}'}{dz} - q(z)A_{tr} = -\lambda A_{tr} \quad (6)$$

Multiplying the above equation by $A_{tr}$ and integrating,

$$A_{tr}A_{tr}'|_a^b - \int_a^b [A_{tr}']^2dz - \int_a^b qA_{tr}^2dz + \lambda \int_a^b A_{tr}^2dz = 0,$$

one obtains an approximation for the lowest eigenvalue

$$\lambda = \frac{\int_a^b dz \{[A_{tr}'(z | \alpha, \beta, \ldots)]^2 + q(z)[A_{tr}(z | \alpha, \beta, \ldots)]^2\}}{\int_a^b dz [A_{tr}(z | \alpha, \beta, \ldots)]^2} = I(\alpha, \beta, \ldots)$$

where, to stress on once again, $\alpha, \beta, \ldots$ are the tunable parameters (called the “variational” parameters). The absolute minimum of the functional $I$ proves to be a reasonable approximation for $\lambda_0$. Thus, minimizing $I$ with respect to the variational parameters $\alpha, \beta, \ldots$, one can obtain an upper bound for $\lambda_0$, i.e.,

$$\lambda_0 \leq I_{\text{min}}$$

To verify this assertion, assume that the trial function is expanded in terms the actual eigenfunctions $\{A_n(z) \mid n = 0, 1, 2, \ldots\}$:

$$A_{tr}(z | \alpha, \beta, \ldots) = \sum_{n=0}^{\infty} c_n A_n(z)$$
If $A_{tr}(z | \alpha, \beta, \ldots)$ is indeed a good guess, one must have
\[ c_0 \approx 1, \quad \text{and} \quad c_n \approx 0 \quad \text{for} \quad n \geq 1 \]

One therefore writes
\[ A_{tr} \approx A_0 + c_1 A_1 + c_2 A_2 + \cdots \]

If the true eigenfunctions are normalised, so is $A_{tr}$ except for terms of order 1 and higher.

The estimate for $\lambda_0$ is therefore
\[
I = \frac{\int \left\{ (A_0' + c_1 A_1' + c_2 A_2' + \ldots)^2 + q(A_0 + c_1 A_1 + c_2 A_2 + \ldots)^2 \right\} dz}{1 + c_1^2 + c_2^2 + \ldots}
\]

Using Eqns.(4) and (5), i.e.,
\[
\int (A_n' A_m' + q A_n A_m) dz = \lambda_n \delta_{m,n}
\]

we obtain
\[
I = \frac{\lambda_0 + c_1^2 \lambda_1 + c_2^2 \lambda_2 + \ldots}{1 + c_1^2 + c_2^2 + \ldots} \approx \lambda_0 + c_1^2 (\lambda_1 - \lambda_0) + c_2^2 (\lambda_2 - \lambda_0) + \cdots \geq \lambda_0
\]

We therefore note that $I$ cannot be smaller than $\lambda_0$, and is equal to $\lambda_0$ only if $c_0 = 1$, and $c_1 = c_2 = c_3 = \cdots = 0$; that is, if
\[ A_{tr}(z) = A_0(z) \]