Rayleigh-Ritz method

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The Rayleigh-Ritz method is an algorithm for obtaining approximate solutions to eigenvalue ODEs. It can be neatly summarized as follows:

1. Choose an approximate form for the eigenfunction with the lowest eigenvalue (the ground state wavefunction, in the language of quantum mechanics). Include one or more free parameters.

2. Find the expectation value of the eigenvalue with respect to the trial eigenfunction.

3. Minimize the resulting equation with respect to the free parameter(s), hence finding a value for the free parameter.

4. Substitute this new eigenfunction back into the expectation value.

5. The expectation value obtained is an upper bound for the actual eigenvalue of the true eigenfunction.

1 Example

Consider the Schrödinger equation for a one-dimensional harmonic oscillator potential:

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m^2\omega^2\right)\psi = E\psi$$

where m is the mass of the particle in the well, and ω is the angular velocity a classical particle would move with in the well. This equation can be solved exactly using Frobenius' method, and leads to eigenfunctions of the form of Hermite polynomials multiplied by Gaussians, and half-integer eigenvalues of the form $E_n = (n + 1/2)\hbar\omega$. Since the solutions are known, it is a good test case. We choose the ground state wavefunction of the infinite potential well as our trial eigenfunction:

$$\psi = \frac{\cos(\frac{\pi x}{2a})}{\sqrt{a}}$$

with a as our free parameter. We now find the expectation value:

$$\langle E\rangle = \langle\psi|\hat{H}|\psi\rangle = \int_{-a}^{a} \psi^* \hat{H}\psi \, dx$$

Evaluating the integral, we find

$$\langle E \rangle = \frac{\hbar^2 \pi^2}{8ma^2} + m\omega^2 a^2 \left(\frac{1}{6} - \frac{1}{pi^2} \right)$$

We now minimise this with respect to a to obtain:

$$2m\omega^2 a \left(\frac{1}{6} - \frac{1}{\pi^2} \right) = \frac{\hbar^2 \pi^2}{4ma^2}$$

Hence:

$$a = \pi \left(\frac{3}{4(\pi^2 - 6)} \right)^{\frac{1}{4}} \left(\frac{\hbar}{m\omega} \right)^{\frac{1}{2}}$$

Substituting this into the expecation value $\langle E \rangle$ we obtain

$$\langle E \rangle = \frac{1}{2} \left(\frac{\pi^2 - 6}{3} \right)^{\frac{1}{2}} \hbar\omega$$

$$\langle E \rangle \approx 0.568\hbar\omega$$

The analytical value is of course $0.5\hbar\omega$. Considering the crudeness of the approximation used, the result is impressive.