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Ritz method

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The **Ritz method** is a direct method to find an approximate solution for boundary value problems. The method is named after Walter Ritz.

In quantum mechanics, a system of particles can be described in terms of an "energy functional" or Hamiltonian, which will measure the energy of any proposed configuration of said particles. It turns out that certain privileged configurations are more likely than other configurations, and this has to do with the eigenanalysis ("analysis of characteristics") of this Hamiltonian system. Because it is often impossible to analyze all of the infinite configurations of particles to find the one with the least amount of energy, it becomes essential to be able to approximate this Hamiltonian in some way for the purpose of numerical computations.

The Ritz method can be used to achieve this goal. In the language of mathematics, it is exactly the finite element method used to compute the eigenvectors and eigenvalues of a Hamiltonian system.

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As with other variational methods, a trial wave function, Ψ, is tested on the system. This trial function is selected to meet boundary conditions (and any other physical constraints). The exact function is not known; the trial function contains one or more adjustable parameters, which are varied to find a lowest energy configuration.

It can be shown that the ground state energy, E_0, satisfies an inequality:

$$E_0 \leq \frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle}.$$

That is, the ground-state energy is less than this value. The trial wave-function will always give an expectation value larger than or equal to the ground-energy.

If the trial wave function is known to be orthogonal to the ground state, then it will provide a boundary for the energy of some excited state.

The Ritz ansatz function is a linear combination of *N* known basis functions $\{\Psi_i\}$, parametrized by unknown coefficients:

$$\Psi = \sum_{i=1}^{N} c_i \Psi_i.$$

With a known Hamiltonian, we can write its expected value as

$$\varepsilon = \frac{\left\langle \sum_{i=1}^{N} c_i \Psi_i \middle| \hat{H} \middle| \sum_{i=1}^{N} c_i \Psi_i \right\rangle}{\left\langle \sum_{i=1}^{N} c_i \Psi_i \middle| \sum_{i=1}^{N} c_i \Psi_i \right\rangle} = \frac{\sum_{i=1}^{N} \sum_{j=1}^{N} c_i^* c_j H_{ij}}{\sum_{i=1}^{N} \sum_{j=1}^{N} c_i^* c_j S_{ij}} \equiv \frac{A}{B}.$$

The basis functions are usually not orthogonal, so that the overlap matrix ***S*** has nonzero nondiagonal elements. Either $\{c_i\}$ or $\{c_i^*\}$ (the conjugation of the first) can be used to minimize the expectation value. For instance, by making the partial derivatives of ε over $\{c_i^*\}$ zero, the following equality is obtained for every *k* = 1, 2, ..., *N*:

$$\frac{\partial \varepsilon}{\partial c_k^*} = \frac{\sum_{j=1}^{N} c_j (H_{kj} - \varepsilon S_{kj})}{B} = 0,$$

which leads to a set of *N* secular equations:

$$\sum_{j=1}^{N} c_j \left(H_{kj} - \varepsilon S_{kj}\right) = 0 \quad \text{for} \quad k = 1, 2, \ldots, N.$$

In the above equations, energy ε and the coefficients $\{c_j\}$ are unknown. With respect to ***c***, this is a homogeneous set of linear equations, which has a solution when the determinant of the coefficients to these unknowns is zero:

$$\det\left(H - \varepsilon S\right) = 0,$$

which in turn is true only for *N* values of ε. Furthermore, since the Hamiltonian is a hermitian operator, the ***H*** matrix is also hermitian and the values of ε_i will be real. The lowest value among ε_i (i=1,2,..,N), ε_0, will be the best approximation to the ground state for the basis functions used. The remaining *N-1* energies are estimates of excited state energies. An approximation for the wave function of state *i* can be obtained by finding the coefficients $\{c_j\}$ from the corresponding secular equation.

The relationship with the finite element method [edit]

In the language of the finite element method, the matrix H_{kj} is precisely the *stiffness matrix* of the Hamiltonian in the piecewise linear element space, and the matrix S_{kj} is the *mass matrix*. In the language of linear algebra, the value ϵ is an eigenvalue of the discretized Hamiltonian, and the vector c is a discretized eigenvector.

Papers [edit]

- Walter Ritz (1909) "Über eine neue Methode zur Lösung gewisser Variationsprobleme der mathematischen Physik" *Journal für die Reine und Angewandte Mathematik*, vol. **135**, pages 1–61. Available on-line at: http://gdz.sub.uni-goettingen.de/no_cache/dms/load/img/?IDDOC=261182 .
- J.K. MacDonald, "Successive Approximations by the Rayleigh–Ritz Variation Method", *Phys. Rev.* **43** (1933) 830

Books [edit]

- R.Courant and D.Hilbert, p.175
- G. Arfken, p.800
- E. Butkov, p.564

External links [edit]

- SpringerLink – Ritz method

See also [edit]

- Rayleigh–Ritz method
- Sturm–Liouville theory
- Hilbert space

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