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In quantum mechanics, the variational method is one way of finding approximations to the lowest energy eigenstate or ground state, and some excited states. This allows calculating approximate wavefunctions such as molecular orbitals. The basis for this method is the variational principle. The method consists of choosing a "trial wavefunction" depending on one or more parameters, and finding the values of these parameters for which the expectation value of the energy is the lowest possible. The w

[Variational method \(quantum mechanics\) - Wikipedia](#)

We can cast this solution in a form that resembles the variational method: $E^-_n = \langle \psi_n | H | \psi_n \rangle = \langle \psi_n | H^0 + V | \psi_n \rangle$ Now since $H^0 | \psi_n \rangle = E^0_n | \psi_n \rangle$ we have $\langle \psi_n | H^0 | \psi_n \rangle = E^0_n$ we can write Eq. (7) in the form: $E^-_n = \langle \psi_n | H^0 + V | \psi_n \rangle = E^0_n + \langle \psi_n | V | \psi_n \rangle$ where $\langle \psi_n | V | \psi_n \rangle$ (8) The interpretation of Eq. (8) is that 1st order perturbation theory is equivalent

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Variational Methods for Inference Dexiong Chen Chia-Man Hung Baoyang Song January 20, 2017 Abstract Probabilistic inference problem is a major problem in graphical models. Such problem of computing marginal probabilities and conditional probabilities can be computationally intractable when the structure of the graphical models gets com-plex.

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This variational characterization of eigenvalues leads to the Rayleigh–Ritz method: choose an approximating u as a linear combination of basis functions (for example trigonometric functions) and carry out a finite-dimensional minimization among such linear combinations. This method is often surprisingly accurate.

[Calculus of variations - Wikipedia](#)

The Variational Method. The variational method is the other main approximate method used in quantum mechanics. Compared to perturbation theory, the variational method can be more robust in situations where it's hard to determine a good unperturbed Hamiltonian (i.e., one which makes the perturbation small but is still solvable).

[The Variational Method](#)

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