Variational Monte Carlo

Variational principle

Given a hamiltonian H and a trial wave function Ψ_T, the variational principle states that the expectation value of $\langle H \rangle$, defined through

$$E[H] = \langle H \rangle = \frac{\int d\boldsymbol{R} \Psi_T^*(\boldsymbol{R}) H(\boldsymbol{R}) \Psi_T(\boldsymbol{R})}{\int d\boldsymbol{R} \Psi_T^*(\boldsymbol{R}) \Psi_T(\boldsymbol{R})},$$

is an upper bound to the ground state energy E_0 of the hamiltonian H, that is

$$E_0 \leq \langle H \rangle.$$

The trial wave function can be expanded in the eigenstates of the hamiltonian since they form a complete set, viz.,

$$\Psi_T(\boldsymbol{R}) = \sum_i a_i \Psi_i(\boldsymbol{R}),$$

and assuming the set of eigenfunctions to be normalized one obtains

$$\frac{\sum_{nm} a_m^* a_n \int d\boldsymbol{R} \Psi_m^*(\boldsymbol{R}) H(\boldsymbol{R}) \Psi_n(\boldsymbol{R})}{\sum_{nm} a_m^* a_n \int d\boldsymbol{R} \Psi_m^*(\boldsymbol{R}) \Psi_n(\boldsymbol{R})} = \frac{\sum_n a_n^2 E_n}{\sum_n a_n^2} \geq E_0,$$

The basic recipe in a VMC calculation consists of the following elements:

- Construct first a trial wave function $\psi_T(\boldsymbol{R}, \boldsymbol{\alpha})$, for a many-body system consisting of N particles located at positions $\boldsymbol{R} = (\boldsymbol{R}_1, \dots, \boldsymbol{R}_N)$. The trial wave function depends on α variational parameters $\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_M)$.
- Then we evaluate the expectation value of the hamiltonian H

$$E[H(\boldsymbol{\alpha})] = \langle H(\boldsymbol{\alpha}) \rangle = \frac{\int d\boldsymbol{R} \Psi_T^*(\boldsymbol{R}, \boldsymbol{\alpha}) H(\boldsymbol{R}) \Psi_T(\boldsymbol{R}, \boldsymbol{\alpha})}{\int d\boldsymbol{R} \Psi_T^*(\boldsymbol{R}, \boldsymbol{\alpha}) \Psi_T(\boldsymbol{R}, \boldsymbol{\alpha})}.$$

- Thereafter we vary α according to some minimization algorithm and return to the first step.

With a trial wave function $\psi_T(\boldsymbol{R})$ we can in turn construct the quantum mechanical probability distribution

$$P(\boldsymbol{R}) = \frac{|\psi_T(\boldsymbol{R})|^2}{\int |\psi_T(\boldsymbol{R})|^2 d\boldsymbol{R}}.$$

This is our new probability distribution function. We can also define a new quantity called **local energy**:

$$E_L(\boldsymbol{R}, \boldsymbol{\alpha}) = \frac{1}{\psi_T(\boldsymbol{R}, \boldsymbol{\alpha})} H\psi_T(\boldsymbol{R}, \boldsymbol{\alpha}).$$

As a consequence, we can redefine the energy as:

$$E[H(\boldsymbol{\alpha})] = \int P(\boldsymbol{R}) E_L(\boldsymbol{R}) d\boldsymbol{R} \approx \frac{1}{N} \sum_{i=1}^{N} P(\boldsymbol{R_i}, \boldsymbol{\alpha}) E_L(\boldsymbol{R_i}, \boldsymbol{\alpha})$$

with N being the number of Monte Carlo samples.

We have to keep in mind that for eigenstates (including the ground state):

$$H\psi = \text{constant} \times \psi.$$

The integral which defines various expectation values involving moments of the hamiltonian becomes then

$$\langle H^n \rangle = \frac{\int d\boldsymbol{R} \Psi_T^*(\boldsymbol{R}) H^n(\boldsymbol{R}) \Psi_T(\boldsymbol{R})}{\int d\boldsymbol{R} \Psi_T^*(\boldsymbol{R}) \Psi_T(\boldsymbol{R})} = \text{constant} \times \frac{\int d\boldsymbol{R} \Psi_T^*(\boldsymbol{R}) \Psi_T(\boldsymbol{R})}{\int d\boldsymbol{R} \Psi_T^*(\boldsymbol{R}) \Psi_T(\boldsymbol{R})} = \text{constant}.$$

This gives an important information: eigenstates lead to zero variance!

Variation is then performed by minimizing either the energy or the variance (or both).

Algorithm

The Algorithm for performing a variational Monte Carlo calculations runs thus as this

- Initialisation: Fix the number of Monte Carlo steps. Choose an initial $\boldsymbol{R}$ and variational parameters α and calculate $\left|\psi_T^{\alpha}(\boldsymbol{R})\right|^2$.
- Initialise the energy and the variance and start the Monte Carlo calculation.
  - Calculate a trial position $\boldsymbol{R}_p = \boldsymbol{R} + r * step$ where r is a random variable $r \in [0, 1]$.
  - Metropolis algorithm to accept or reject this move $w = P(\boldsymbol{R}_p)/P(\boldsymbol{R})$.
  - If the step is accepted, then we set $\boldsymbol{R} = \boldsymbol{R}_p$.
  - Update averages
- Finish and compute final averages.

Two hard-core bosons in a spherical harmonic

trap

For bosons in a harmonic oscillator-like trap we will use is a spherical (S) or an elliptical (E) harmonic trap in one, two and finally three dimensions, with the latter given by

$$V_{ext}(\mathbf{r}) = \frac{1}{2}m\omega_{ho}^2 r^2$$

and the hamiltonian is:

$$\hat{H} = \sum_i^N \left(\frac{-\hbar^2}{2m} \bigtriangledown_i^2 + V_{ext}(\mathbf{r}_i) \right) + \sum_{i<j}^N V_{int}(\mathbf{r}_i, \mathbf{r}_j),$$

We will represent the inter-boson interaction by a pairwise, repulsive potential

$$V_{int}(|\mathbf{r}_i - \mathbf{r}_j|) = \begin{cases} \infty & |\mathbf{r}_i - \mathbf{r}_j| \leq a \\ 0 & |\mathbf{r}_i - \mathbf{r}_j| > a \end{cases}$$

where a is the so-called hard-core diameter of the bosons. Clearly, $V_{int}(|\mathbf{r}_i - \mathbf{r}_j|)$ is zero if the bosons are separated by a distance $|\mathbf{r}_i - \mathbf{r}_j|$ greater than a but infinite if they attempt to come within a distance $|\mathbf{r}_i - \mathbf{r}_j| \leq a$.

Our trial wave function for the ground state with N atoms is given by

$$\Psi_T(\mathbf{R}) = \Psi_T(\mathbf{r}_1, \mathbf{r}_2, \dots \mathbf{r}_N, \alpha) = \prod_i g(\alpha, \mathbf{r}_i) \prod_{i<j} f(a, |\mathbf{r}_i - \mathbf{r}_j|),$$

where α is a variational parameter. The single-particle wave function is proportional to the harmonic oscillator function for the ground state

$$g(\alpha, \mathbf{r}_i) = \exp\left[-\alpha(x_i^2 + y_i^2 + z_i^2)\right].$$

For non-interacting bosons ($a = 0$) we have $\alpha = 1/2a_{ho}^2$. The correlation wave function is

$$f(a, |\mathbf{r}_i - \mathbf{r}_j|) = \begin{cases} 0 & |\mathbf{r}_i - \mathbf{r}_j| \leq a \\ (1 - \frac{a}{|\mathbf{r}_i - \mathbf{r}_j|}) & |\mathbf{r}_i - \mathbf{r}_j| > a. \end{cases}$$

The local energy for this trial wave function is:

$$E_L(\mathbf{r_1}, \mathbf{r_2}, \alpha) = \sum_i \frac{1}{2}m\omega_{ho}^2 r_i^2 + 2\alpha(3 - \alpha(r_1^2 + r_2^2)) + \frac{2\alpha a}{|\mathbf{r}_i - \mathbf{r}_j| - a}.$$

And now we can go to the code :)