Tutorial 5: Variational Monte Carlo on the Harmonic oscillator

May 31, 2019

The objective of this tutorial is to find the ground state properties of the Harmonic oscillator using the Variational Monte Carlo (VMC) method.

VMC is usually implemented to estimate the ground state energy E_0 of an Hamiltonian $\hat{H}$ by using a were crafted state $|\Psi_{\boldsymbol{\alpha}}\rangle$ which has to be representative enough of the ground state $|\phi_0\rangle$. $\boldsymbol{\alpha}$ stands for a set of variational parameters that needs to be optimized.

The ground state energy is then approximated through the variational energy which is given by:

$$E_{var} = \frac{\langle\Psi_{\boldsymbol{\alpha}}|\hat{H}|\Psi_{\boldsymbol{\alpha}}\rangle}{\langle\Psi_{\boldsymbol{\alpha}}|\Psi_{\boldsymbol{\alpha}}\rangle}, \tag{1}$$

The *variational principle* guarantees that E_{var} acts as an upper bound to the ground state energy of the Hamiltonian $\hat{H}$. The essence of VMC would therefore be to find the optimal set of variational parameters $\boldsymbol{\alpha}_{opt}$ for which the variational energy is minimum. This is usually achieved through some minimization procedure.

Recall that the Hamiltonian of the harmonic oscillator in one dimension is given by:

$$\hat{H} = \frac{\hat{p}}{2} + x^2 \tag{2}$$

where the energy is in units of $\hbar\omega$. The ground state wave-function can be computed exactly and is given by:

$$\phi_0(x) = (\frac{1}{\pi})^{1/4} e^{-x^2/2} \tag{3}$$

In this tutorial, we will consider the variational wave-function $\Psi_\alpha(x) = e^{-\alpha x^2/2}$ where α is the variational parameter to determine.

a) Run the code `tutorial5_vmc_ho.py` with `num_walkers = 400`, `num_MC_steps = 30000`, `num_equil_steps = 3000`, and convince yourself that the variational energy is indeed an upper bound to the exact ground state energy.

b) Plot the standard deviation of E_{var} with respect to different values of α. What can you interpret from the result? How does the standard deviation varies with respect to the number of walkers?

c) Use the code `tutorial5_training_vmc_ho.py` to optimize the parameter α using stochastic gradient descend. Check how the hyper-parameters such as the learning rate and the number of samples affect the training.

d) Compute the exact derivative of variational energy with respect to α and compare it with its stochastic estimate given by:

$$\partial_\alpha E_{var} = 2\big[\langle E_{loc}(x) F_\alpha(x)\rangle - \langle E_{loc}(x)\rangle\langle F_\alpha(x)\rangle\big] \tag{4}$$

e) Check that the optimization still work when implemented with the exact derivative of the variational energy. Comment on whether or not it is advisable to use it during the training.

f) Comment on the difference between in the SGD method implemented here and the one routinely implement in the training of neural networks.

g) Change the initialization of the walkers to be distributed between $[-4.5 : 5.5]$. Run the stochastic gradient descent algorithm. What do you notice? Could the problem be fixed by any form of smart proposal move?

For further information, check the modern machine learning software for energy minimization of variational wave functions [1].

References

[1] NetKet, `https://www.netket.org/getstarted/home/`.