Variational Monte Carlo methods for nuclear physics

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Abstract

Solving the quantum-mechanical many-body problem is a computationally intensive task due to the high-dimensionality of the position space, as well as the number of spin and isospin degrees of freedom. Variational Monte Carlo is a technique for evaluating the high-dimension integrals required by the variational principle. A simple example implementation of variational Monte Carlo is presented.

INTRODUCTION

Ab Initio Nuclear Theory

Atomic nuclei are complex many-body systems showing a wide variety of phenomena and behaviors. *Ab inito* theory methods attempt to predict these phenomena from the underlying interactions between nucleons. In principle, one would like to begin with the fundamental quark degrees of freedom described by quantum chromodynamics (QCD); however, low energy QCD is extremely non-perturbative and is computationally infeasible for all but the smallest composite systems. Instead, one begins with realistic nucleon-nucleon (NN) and three-nucleon (3N) interactions which capture the essential physics necessary for describing nuclei. These interactions can be constructed in a variety of ways, often guided by the underlying symmetries of QCD such as with chiral effective field theory χEFT [1]. Usually such potentials are fitted to a combination of nucleon-nucleon scattering data as well as selected nuclear binding energies. Phenomenological potentials such as the Argonne $v18'$ potential are able to describe the structure of light nuclei with great precision.

Variational Principle

The quantum mechanical variational principle states that for any trial wave function $|\Psi_T\rangle$, the expectation value

$$\langle H \rangle = \frac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle} \geq E_0$$

where E_0 is the ground-state energy of the Hamiltonian H. The best approximation to the lowest energy eigenvalue E_0 and ground state wave function $|\Psi_0\rangle$ is determined by taking the variation of $\langle H \rangle$ and setting it equal to zero

$$\delta \langle H \rangle = \delta \left(\frac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle} \right) = 0$$

Approximating the wave function and its ground state energy then consists of varying some parameters in $|\Psi_T\rangle$ and finding the minimum.

For many-body systems, calculating the expectation value $\langle H \rangle$ involves integrating over $3A$ spatial dimensions (where A is the number of particles) as well as summing over all spin and isospin degrees of freedom. For traditional methods such as Simpson's rule or Gaussian quadrature, the error goes as $O(N^{-k/(3A)})$ [2]. This exponential growth means

that numerical integration with such techniques rapidly becomes computationally infeasible as the number of particles grows. In order to evaluate these integrals, one usually turns to Monte Carlo techniques; this class of methods samples an integrand at a large number of random points in space and relates the average of the integrand to the value of the integral via the mean value theorem

$$\int_a^b f(x)g(x)dx = \langle f \rangle \int_a^b g(x)dx$$

This can be rewritten in a more useful form for Monte Carlo integration

$$\int_a^b f(x)g(x)dx \approx \frac{1}{N}\sum_{i=1}^{N} f(X_i), \quad X_i \in \{g(x)\}$$

where the function $f(x)$ is sampled at points X_i drawn from the probability distribution $g(x)$. This converges as $O^{-1/2}$ regardless of dimensionality [2]; thus, Monte Carlo integration is the ideal choice for integrals over high-dimension spaces.

To evaluate the expectation value $\langle H \rangle$, we define the *local energy operator*

$$\hat{\mathbf{E}}_L(\mathbf{r}) = \frac{1}{\Psi_T(\mathbf{r})}\hat{\mathbf{H}}\Psi_T(\mathbf{r})$$

and probability distribution function

$$P(\mathbf{r}) = \frac{|\Psi_T(\mathbf{r})|^2}{\int |\Psi_T(\mathbf{r})|^2 d\mathbf{r}}$$

giving us

$$\langle H \rangle = \int P(\mathbf{r})\hat{\mathbf{E}}_L(\mathbf{r})d\mathbf{r} \approx \frac{1}{N}\sum_{i=1}^{N} \hat{\mathbf{E}}_L(\mathbf{r}_i), \quad \mathbf{r}_i \in \{P(\mathbf{r})\}$$

Thus, to calculate the estimate of the energy for the state $|\Psi_T\rangle$, we average the value of the local energy at points selected from a probability distribution proportional to $\langle \Psi_T | \Psi_T \rangle$.

Metropolis Algorithm

In general, $P(\mathbf{r})$ is not readilty available because the value of the normalization constant would require doing an integral over the whole space. The Metropolis algorithm gives a way of sampling random values from an unknown probability distribution $P(\mathbf{r})$ as long as some function $G(\mathbf{r}) \sim P(\mathbf{r})$ is known.

To generate the sequence of points at which we sample the local energy, we follow a random walk through the space:

Generating random numbers from a random walk

1. Begin with a point $\mathbf{r}_i$. Propose $\mathbf{r}_{i+1} = \mathbf{r}_i + \delta\xi$ where $\xi_k \in [0, 1)$.
2. Calculate $R = \frac{G(\mathbf{r}_{i+1})}{G(\mathbf{r}_i)}$;
   - if $R \geq 1$, accept the proposal for $\mathbf{r}_{i+1}$,
   - if $r < 1$, generate another random number $\zeta \in [0, 1)$ and accept proposal if $\zeta < R$, otherwise set $\mathbf{r}_{i+1} = \mathbf{r}_i$.
3. Use X_i to calculate the value of the integrand $f(X_i)$.

In effect, the sequence $\mathbf{r}_i$ takes a random walk, always accepting moves to areas with greater probability density, but always having some chance of moving to areas with lower probability density. It can be shown [3] that as $N \to \infty$, the sequence $\{\mathbf{r}_1, \ldots, \mathbf{r}_N\}$ will be be randomly sampled from $P(\mathbf{r})$.

NUCLEAR WAVE FUNCTIONS

The most important task when performing a VMC calculation is selection of an appropriate trial wave function. For nuclear physics one usually chooses a wave function factored into a short-range correlation and long-range structure form [1, 2]

$$|\Psi_T\rangle = \left(\prod_{i<j} f(r_{ij})\right) |\Phi\rangle$$

where r_{ij} is the distance between the ith and jth particle. Since the behavior of two nucleons close together is dominated by the NN-interaction between them, the functions $f(r_{ij})$ satisfy the one-dimensional Schrödinger equation

$$\left(-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}r_{ij}^2} + qV(r_{ij})\right) f(r_{ij}) = \epsilon f(r_{ij})$$

where q is a variational parameter adjusting the strength of the short-range interaction, and a boundary condition is imposed such that $f(r_{ij})$ is constant beyond $r_{ij} > h$ where h is another variational parameter controlling the range of the correlation.

The long-range structure $|\Phi\rangle$ is an antisymmetric function which captures the behavior of the nucleons when separated at larger distances. Often $|\Phi\rangle$ is chosen to be a single Slater determinant or sum of Slater determinants.

An additional simplification can be made for nuclear Hamiltonians which are spin-independent: we may additionally factor the Slater determinants into [4]

$$\Phi = \det[\phi_{p_i\uparrow}] \det[\phi_{p_i\downarrow}] \det[\phi_{n_i\uparrow}] \det[\phi_{n_i\downarrow}]$$

COMPUTATIONAL IMPLEMENTATION AND PRELIMINARY RESULTS

The algorithms above were implemented in C++11. Random numbers are generated the Intel Math Kernel Library with the Mersenne-Twister pseudorandom number generator algorithm. The Metropolis algorithm has an adaptive step size, and attempts to hit a particular acceptance rate target; if the acceptance rate is too high, it is likely that the step size is too small, leading to correlations between nearby sample points, while an acceptance rate too low implies that the step often tries to move to areas of very small probability density. Wave functions are implemented as subclasses of `wf::WaveFunction`. Each wave function class is expected to provide `value(r)`, `local_grad(r)`, `local_laplacian(r)` and can optionally override `norm(r)`, `grad(r)`, and `laplacian(r)`.

For the simplest test case, a ground-state harmonic oscillator wave function is provided by `wf::SphericalOscillatorWF`, representing

$$\phi(\mathbf{r}) = e^{-r^2/2b^2}$$

Potentials are defined by the `potential::Potential` class and are expected to override `operator()` to accept the state and return a potential energy. `potential::HarmonicOscillator` represents

$$V(\mathbf{r}) = \frac{\hbar^2}{2m}\frac{r^2}{b^4}$$

This object-oriented structure allows for having a general framework in which VMC calculations can be done, both for one-body and many-body systems. Shown in the figures are energies as a function of wave function length parameter for a harmonic oscillator and an anharmonic oscillator ($V(r) \sim r^4$).

[1] J. Carlson, S. Gandolfi, F. Pederiva, S. C. Pieper, R. Schiavilla, K. E. Schmidt, and R. B. Wiringa, Rev. Mod. Phys. **87**, 1067 (2015).

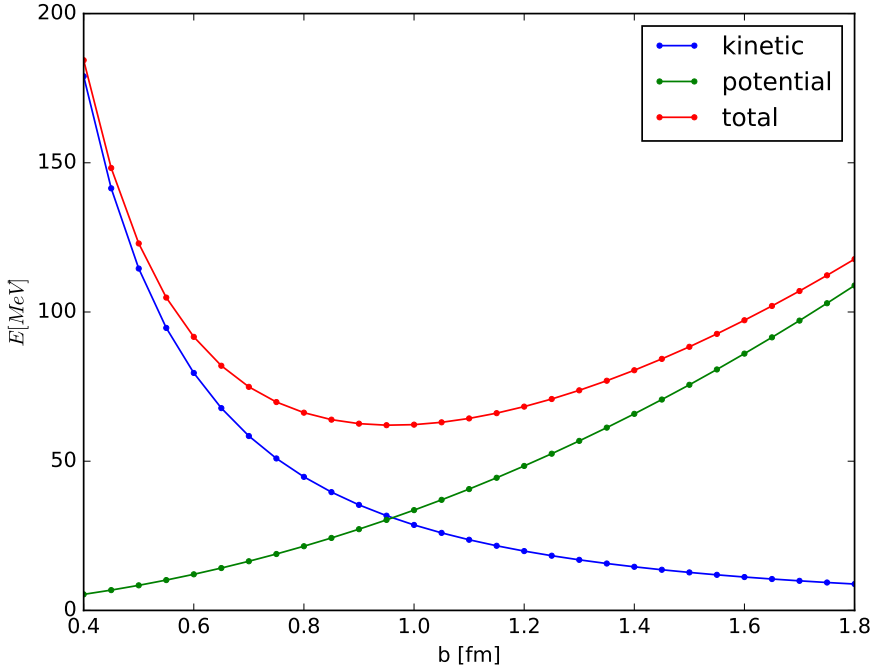

FIG. 1. Variational energy as a function of oscillator length for the harmonic oscillator.

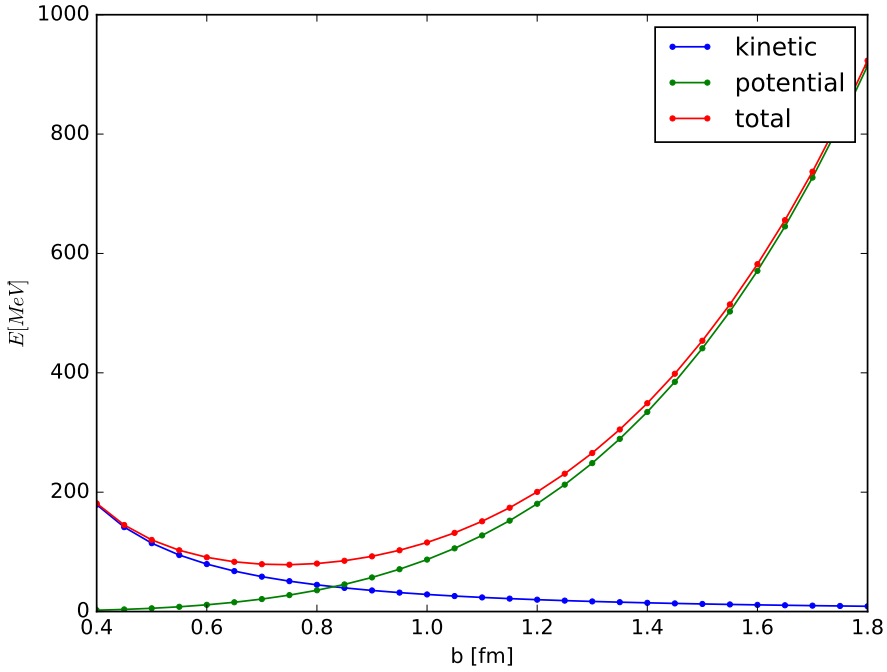

FIG. 2. Variational energy as a function of oscillator length for the anharmonic oscillator.

[2] M. Hjorth-Jensen, *Computational Physics* (University of Oslo, 2013).

[3] M. H. Kalos and P. A. Whitlock, *Monte Carlo Methods*, 2nd ed. (Wiley-VCH Verlag, 2008).

[4] F. Pederiva, A. Roggero, and K. E. Schmidt, "Variational and diffusion monte carlo approaches to the nuclear few- and many-body problem," in *An advanced course in computational nuclear physics*, edited by M. Hjorth-Jensen, M. P. Lombardo, and U. E. van Kolck (Springer, 2016) pp. 311–368.