Variational Monte Carlo: practical session

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Also thanks to:
Lucas Wagner
Yubo (Paul) Yang

Preparing for Monte Carlo intergration

$\mathbf{R}$ positions
$\mathbf{P}$ parameters

Compute an expectation value:

$$\langle E \rangle = \int d^{3N}\mathbf{R}\ \Psi^*(\mathbf{R},\mathbf{P})\hat{H}\Psi(\mathbf{R},\mathbf{P})$$

$$= \int d^{3N}\mathbf{R}\frac{\hat{H}\Psi(\mathbf{R},\mathbf{P})}{\Psi(\mathbf{R},\mathbf{P})}|\Psi(\mathbf{R},\mathbf{P})|^2$$

Some function of $\mathbf{R}$
$E(\mathbf{R})$ "local energy"

Probability distribution

Basic concept of Monte Carlo integration

Expectation value of a probability distribution:

$$\langle f(R) \rangle = \int dr \; f(r) p(R = r)$$

Sample mean:

$$\langle f(R) \rangle = \lim_{M \to \infty} \frac{1}{M} \sum_{r_i} f(r_i)$$

M samples
r_i drawn with probability $p(r_i)$

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Applying Monte Carlo to the expectation value

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$$\langle E \rangle = \int d^{3N}\mathbf{R} \frac{\hat{H}\Psi(\mathbf{R},\mathbf{P})}{\Psi(\mathbf{R},\mathbf{P})} |\Psi(\mathbf{R},\mathbf{P})|^2$$

$$\langle E \rangle = \lim_{M \to \infty} \frac{1}{M} \sum_{\mathbf{R}_i} \frac{\hat{H}\Psi(\mathbf{R}_i,\mathbf{P})}{\Psi(\mathbf{R}_i,\mathbf{P})}$$

M samples
$\mathbf{R}_i$ drawn with probability $|\Psi(\mathbf{R}_i,\mathbf{P})|^2$

Overview of VMC algorithm

$$\langle E \rangle = \lim_{M \to \infty} \frac{1}{M} \sum_{\mathbf{R}_i} \frac{\hat{H}\Psi(\mathbf{R}_i, \mathbf{P})}{\Psi(\mathbf{R}_i, \mathbf{P})}$$

1. Need to evaluate

$\mathbf{R}_i$ drawn with probability $|\Psi(\mathbf{R}_i, \mathbf{P})|^2$

2. Need to be able to sample

3. Once we can evaluate $\langle E \rangle$, explore $\mathbf{P}$ or change wave function to minimize

Goals for today

For a He atom:

1. Implement pieces (evaluation and sample)
2. Explore parameters.
3. Explore effect of including correlations in wave function.

Details are provided in "instructions.pdf"

Make sure you have the most recent version!

Tips to avoid getting stuck

- Test early and often.
- Do simplest implemention first.
- Avoid solutions until you've struggled for at least 30 minutes. Ask questions first.

Discuss interpretation questions with group.

Classes in python:

`class Hamiltonian:`

Member data:	Member functions:
`self.Z`	`def compute_energy(self,pos)`
(ion charge)	(compute an energy)

How to use:

1. Create instance: calls `__init__(self,...)`

   `ham=Hamiltonian(Z=2)`

2. Use functions:

   `ham.compute_energy(pos1)`

   `ham.compute_energy(pos2)`