Metropolis/Variational Monte Carlo

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Metropolis Monte Carlo and Markov Chain Algorithms

Metropolis Monte Carlo is an algorithm designed to sample complicated many-variable distributions. It employs a Markov Chain Monte Carlo algorithm to achieve this.

see: *Metropolis, N., Rosenbluth, A., Rosenbluth, M., Teller, A., and Teller, E., "Equations of state calculations by fast computing machines", J. Chem. Phys. 2121(6) 1087 (1953).*

- A Markov Chain Monte Carlo Algorithm employs random walks where each step depends only upon the present position of the system (no 'history').
- The Metropolis algorithm assumes that you want to sample from a non-negative function $W(\mathbf{R})$ which may be in many dimensions: eg. $\mathbf{R} = (\mathbf{r}_i)$ for many particles i.

Metropolis Monte Carlo

- Metropolis algorithm is used to sample a multi-variable function $W(\mathbf{R})$, whose distribution is at priori unknown. But with *a priori* unknown equilibration time and unknown time between 'independent' samples.
- Detailed balance is enforced, requiring the flux from point $\mathbf{A} \rightarrow \mathbf{B}$ equals that from $\mathbf{B} \rightarrow \mathbf{A}$
- Rejection is used, we propose a move with a probability $T(\mathbf{A} \rightarrow \mathbf{B})$ and accept that move with probability $P(\mathbf{A} \rightarrow \mathbf{B})$.
- Detailed balance requires:
  $W(\mathbf{A})\ T(\mathbf{A} \rightarrow \mathbf{B})\ P(\mathbf{A} \rightarrow \mathbf{B}) \ = \ W(\mathbf{B})\ T(\mathbf{B} \rightarrow \mathbf{A})\ P(\mathbf{B} \rightarrow \mathbf{A})$

Note that detailed balance is more restrictive than strictly necessary.

Metropolis Monte Carlo

A simple Metropolis Algorithm:

1. Initialize all particles within the physical volume and calculate W(**R**)
2. Propose a move of all particles **R**′, within a box centered on the current positions: $r_i'^{\alpha} = r_i^{\alpha} + b(\xi_i^{\alpha} - 0.5)$
   where α runs over 3 dimensions and i over N particles
3. Calculate $W(\mathbf{R}')$
4. Accept this proposed move with probability P given by:
   $P = \min[W(\mathbf{R}')/W(\mathbf{R}), 1]$
5. If the move is 'accepted', set the current position to **R**′, otherwise keep the current position at **R**
6. Return to step 2, and propose a new move

After some number of steps the samples will be independent.
Averages and Errors can be calculated using these independent samples

Let's consider a many-body general Hamiltonian describing a system of N particles.

$$H = -\frac{\hbar^2}{2m}\sum_i^N \nabla_i^2 + \sum_{i<j} v(r_{ij})$$

and we want to calculate the energy:

$$E_0 \leq E = \frac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle} = \frac{\int dr_1 \dots dr_N \, \Psi_T^*(r_1 \dots r_N) H \Psi_T(r_1 \dots r_N)}{\int dr_1 \dots dr_N \, \Psi_T^*(r_1 \dots r_N) \Psi_T(r_1 \dots r_N)}$$

where $\Psi_T(r_1 \dots r_N)$ is a variational wave function that depends on the coordinates (positions) of the particles, with variational parameters $\{\alpha\}$.

For a given form of $\Psi_T(r_1 \dots r_N)$ we want to find the best value(s) of α giving the lower energy, i.e. we need to study $E[\alpha]$. How do we solve the above integral?

Some definition:

- $r_i = (x_i, y_i, z_i, ...)$ has coordinate(s) of particle i
- when used, $R = r_1 ... r_N$ (and $dR = dr_1 ... dr_N$)
- $\Psi(R) = \langle R | \Psi \rangle$

Remember:

$$\int F(x)dx = \int \frac{F(x)}{W(x)} W(x)dx = \int f(x)W(x)dx$$

So we can rewrite the integral as:

$$\begin{aligned} E &= \frac{\int dr_1 \dots dr_N \, \Psi_T^*(r_1 \dots r_N) H \Psi_T(r_1 \dots r_N)}{\int dr_1 \dots dr_N \, \Psi_T^*(r_1 \dots r_N) \Psi_T(r_1 \dots r_N)} \\ &= \int dR \, W(R) \frac{\Psi_T^*(R) H \Psi_T(R)}{\Psi_T^*(R) \Psi_T(R)} \end{aligned}$$

where

$$W(R) = \frac{\Psi_T^*(r_1 \dots r_N) \Psi_T(r_1 \dots r_N)}{\int dr_1 \dots dr_N \, \Psi_T^*(r_1 \dots r_N) \Psi_T(r_1 \dots r_N)} = \frac{|\Psi_T(R)|^2}{\int dR \, |\Psi_T(R)|^2}$$

VMC: first implementation

Easy case: 1-dimensional Harmonic oscillator ($\hbar = m = 1$).

$$H = -\frac{1}{2}\frac{d^2}{d\,x^2} + \frac{1}{2}\Omega^2 x^2$$

Let's start from the following variational wave function:

$$\Psi_T(x) = e^{-\alpha x^2/2}$$

($\Omega = \alpha$ gives the exact solution).

We will call *walker* one configuration that will be used to generate new configurations according to the Metropolis/Markov chain algorithm.

In the 1D harmonic oscillator case, *walker i* is simply

$$W_i = \{x_i\}$$

but in general (3D, multiparticles, spins, etc.) each walker will contain many more information, i.e. $\{\vec{r}_1, \ldots, \vec{r}_N, ...\}$.

VMC: first implementation

Following Metropolis, the VMC algorithm can be summarized in the following steps:

1. Generate a set of N walkers randomly distributed
2. Loop over the N walkers, and for each i-th walker:
3. Calculate $W(x_i) = |\langle \Psi_T | x_i \rangle|^2$
4. Make a "trial" step: $x_{\rm test} = x + (\xi - 0.5)\Delta$
5. Calculate $W(x_{\rm test}) = |\langle \Psi_T | x_{\rm test} \rangle|^2$
6. Calculate the ratio $W(x_{\rm test})/W(x_i)$ and do Metropolis
7. If the move is accepted, set $x_i = x_{\rm test}$.
8. Calculate averages
9. Iterate with 2) until the equilibration is reached, then reset estimators and iterate until the error is small enough

Note: in VMC, N can be even 1. But using more configurations will be very convenient when parallel machines are available.

VMC: first implementation

The calculation of observables is carried out over a total of M walkers (uncorrelated points in the Markov chain) as

$$\langle O \rangle = \frac{\sum_i^M \omega_i \frac{\langle \Psi_T | W_i \rangle \langle W_i | \hat{O} | \Psi_T \rangle}{\langle \Psi_T | W_i \rangle \langle W_i | \Psi_T \rangle}}{\sum_i^M \omega_i}$$

where ω_i is the weight of the configuration (usually 1).

For example (remember that $\Psi_T = \exp(-\alpha x^2/2)$

$$\frac{\langle \Psi_T | W_i \rangle \langle W_i | \hat{H} | \Psi_T \rangle}{\langle \Psi_T | W_i \rangle \langle W_i | \Psi_T \rangle} =$$

$$= -\frac{1}{2} \frac{\langle \Psi_T | x_i \rangle \langle x_i | \frac{d^2}{dx^2} | \Psi_T \rangle}{\langle \Psi_T | x_i \rangle \langle x_i | \Psi_T \rangle} + \frac{1}{2}\Omega^2 \frac{\langle \Psi_T | x_i \rangle \langle x_i | x^2 | \Psi_T \rangle}{\langle \Psi_T | x_i \rangle \langle x_i | \Psi_T \rangle}$$

$$= -\frac{1}{2}(\alpha^2 x_i^2 - \alpha) + \frac{1}{2}\Omega^2 x_i^2$$

Note: if Ψ_T is the exact solution, then $\frac{\Psi_T^* H \Psi_T}{\Psi_T^* \Psi_T} = E = \frac{\Omega}{2} \quad \forall x!$

VMC: the first piece of code

```
...
do j=1,nstep
  do n=1,nwalk
    psiold=exp(-0.5*alpha*xold(n)**2)
    call ran(csi,irn)
    xtest=xold(n)+sigma*(csi-0.5)
    psinew=exp(-0.5*alpha*xtest**2)
    prob=(psinew/psiold)**2
    call ran(csi,irn)
    if (csi.gt.prob) xtest=xold(n)
    eloc=-0.5*((alpha*xtest)**2-alpha)+0.5*omega**2*xtest**2
    xold(n)=xtest
  enddo
enddo
...
```

VMC: first implementation

1. Loop over the N walkers, and for each i-th walker:

```
do j=1,nstep
 do n=1,nwalk
```

2. Calculate $W(x_i) = |\langle \Psi_T | x_i \rangle|^2$

```
psiold=exp(-0.5*alpha*xold(n)**2)
```

3. Make a "trial" step: $x_{\rm test} = x + (\xi - 0.5)\Delta$

```
call ran(csi,irn)
xtest=xold(n)+sigma*(csi-0.5)
```

4. Calculate $W(x_{\rm test}) = |\langle \Psi_T | x_{\rm test} \rangle|^2$

```
psinew=exp(-0.5*alpha*xtest**2)
```

VMC: first implementation

1. Calculate the ratio $W(x_{\rm test})/W(x_i)$ and do Metropolis

```
prob=(psinew/psiold)**2
call ran(csi,irn)
```

2. If the move is accepted, set $x_i = x_{\rm test}$, otherwise reject the move

```
if (csi.gt.prob) xtest=xold(n)
xold(n)=xtest
```

3. Calculate averages

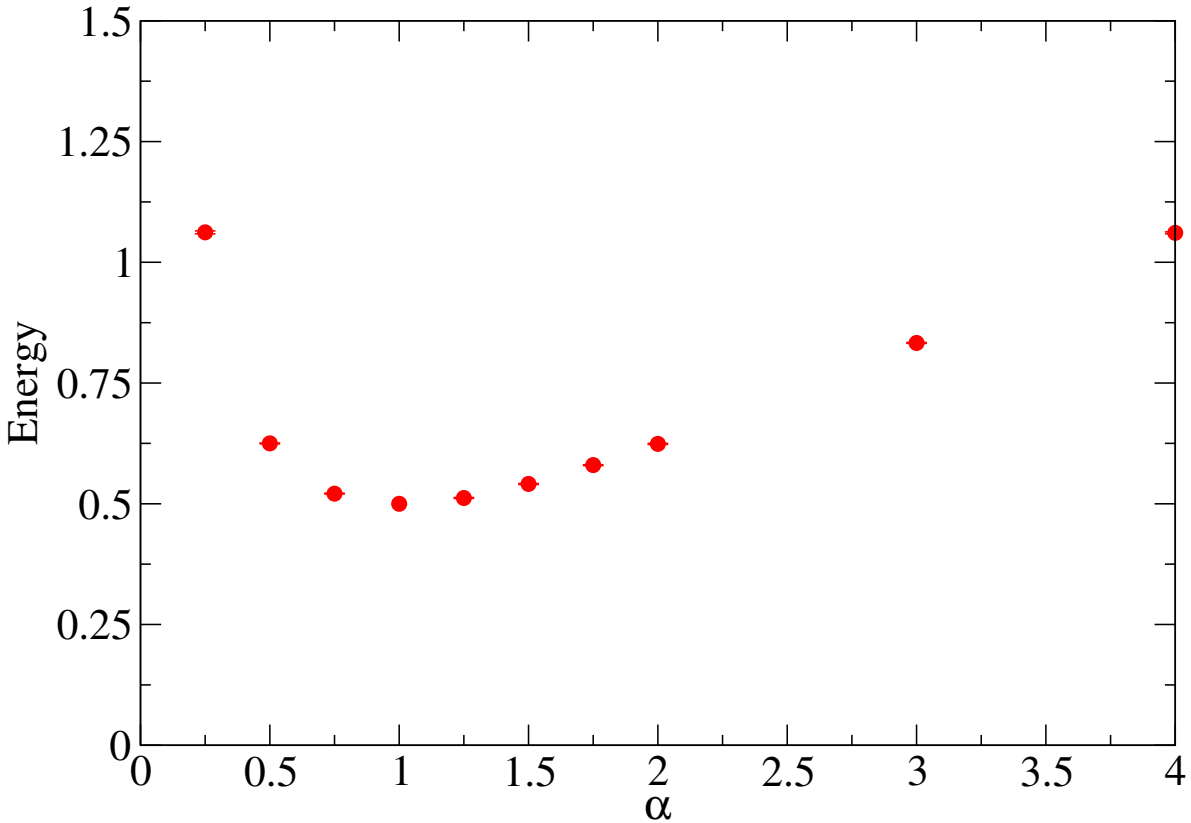
```
eloc=-0.5*((alpha*xtest)**2-alpha)+0.5*omega**2*xtest**2
```

4. Iterate with 2) until the equilibration is reached, then reset estimators and iterate until the error is small enough

Variational Monte Carlo

An example: 1D harmonic oscillator, VMC calculations.

Energy as a function of the variational parameter α:



Variational Monte Carlo

VMC is a tool to calculate the energy of a many-body system for a given wave function as a function of its variational parameters.

This requires to solve multi-dimensional integrals, that are solved using Monte Carlo integration.

Variational Monte Carlo

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... for now :-)

Backup: Harmonic Oscillator

$$\Psi_T(x) = e^{-\alpha x^2/2}$$

$$|\Psi_T|^2 = \int dx\, e^{-\alpha x^2} = \sqrt{\frac{\pi}{\alpha}}$$

$$\begin{aligned}\langle H \rangle &= \int dx\, e^{-\alpha x^2/2} \left(-\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}\Omega^2 x^2 \right) e^{-\alpha x^2/2} \\ &= \int dx\, e^{-\alpha x^2/2} \left[-\frac{1}{2}(\alpha^2 x^2 - \alpha) + \frac{1}{2}\Omega^2 x^2 \right] e^{-\alpha x^2/2} \\ &= \left[\frac{1}{4\alpha}(\Omega^2 - \alpha^2) + \frac{\alpha}{2} \right] \sqrt{\frac{\pi}{\alpha}}\end{aligned}$$

$$\frac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle} = \frac{1}{4\alpha}(\Omega^2 - \alpha^2) + \frac{\alpha}{2}$$