Smarter Monte Carlo

Today we will explore ways to change the transition probability in MCMC to allow faster convergence.

- Menus in MCMC
- Heat bath MC
- Preferential MC
- Smart MC
- Force Bias MC

Recall: The "Classic" Metropolis method

Metropolis-Rosenbluth[2] -Teller[2] (1953) method for sampling the Boltzmann distribution is:

- Move from s to s' with probability T(s→s')= constant
- Accept with move with probability:

$$\mathbf{A(s \rightarrow s') = \min [\ 1\ ,\ \exp(-\beta[E(s')-E(s)])}$$

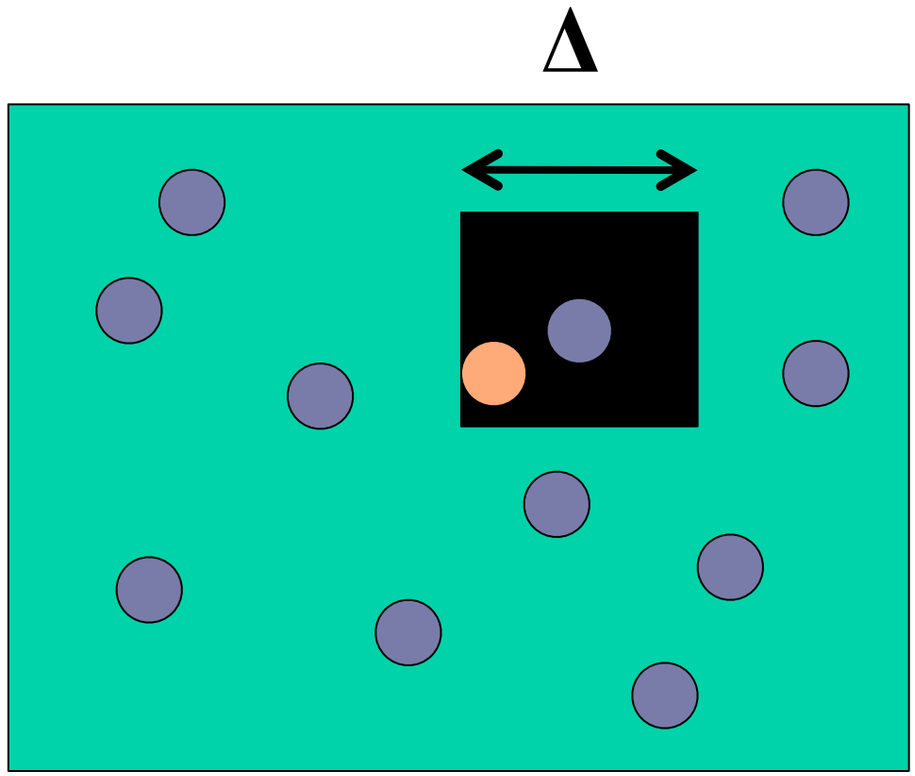
- Repeat many times

- Given ergodicity, the *distribution of s* will be the canonical distribution: $\pi(s) = \exp(-E(s)/k_B T)/Z$.

•Convergence is guaranteed but the rate is not!

Recall: How to sample

$$S\_new = S\_old + \Delta \cdot (sprng - 0.5)$$



Uniform distribution in a cube of side "Δ".

Note: It is more efficient to move one particle at a time because only the energy of that particle comes in and the acceptance ratio will be larger.

$$A(s \to s') = \exp\left[-\beta(V(s') - V(s))\right]$$

$$= \exp\left[-\beta \sum_{j \neq i} \left(v(r_i' - r_j) - v(r_i - r_j)\right)\right]$$

For V with cut-off range, difference is local.

Recall: Rejection Method

Metropolis achieves detailed balance by *rejecting* moves.

General Approach:

1. Choose distribution to sample, e.g., $\pi(s) = \exp[-\beta H(s)]/Z$
2. Impose detailed balance on transition: **$K(s \to s') = K(s' \to s)$**

   where $K(s \to s') = \pi(s)\, P(s \to s')$

   (*probability of being at s)* * (*transition probability of going to s'*).
3. Break up transition probability into sampling and acceptance:

   $P(s \to s') = T(s \to s')\, A(s \to s')$

   (*probability of generating s'* from s) * (*probability of accepting move)*

The optimal acceptance probability that gives detailed balance is:

$$A(s \to s') = \min\left\{1, \frac{T(s' \to s)\pi(s')}{T(s \to s')\pi(s)}\right\} = \min\left\{1, \frac{\pi(s')}{\pi(s)}\right\}$$

If T is constant!

IMPORTANTLY Normalization of $\pi(s)$ is not needed or used!

We want to choose T to maximize the acceptance probability.

Detailed balance

Three key concepts:

1. Sample by using an ergodic random walk.
2. Determine equilibrium state by using detailed balance.
3. Achieve detailed balance by using rejections.

Detailed balance: $\pi(s)\, P(s \to s') = \pi(s') P(s' \to s)$.

Rate balance from s to s'.

- If $P(s \to s')$ is ergodic, $\pi(s)$ is unique steady state solution.
- Detailed balance is **not** required
  - **Balance** will suffice: $\pi(s) = \sum_{s'} \pi(s') P(s' \to s)$.
  - Example: menu of moves

Menu of Moves

Suppose we have moves of type A and B, either of which satisfy detailed balance alone.

- We can either:
  1. *Randomly choose* from (A,B).
  2. *Cycle deterministically* (A,B,A,B,A,B,…)

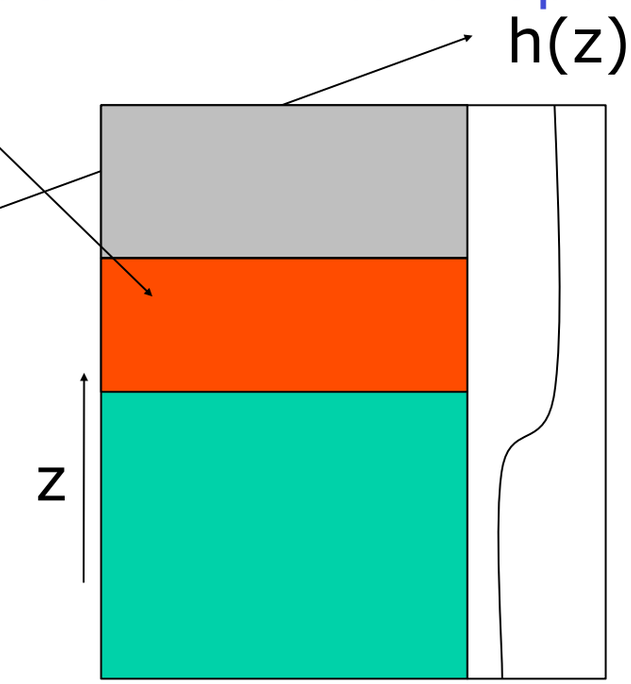
– Either will give the correct distribution even though choice 2 does not really satisfy detailed balance.
  ✓ Theorem: If each menu item individually satisfies detailed balance, then desired state is the unique stationary state.

– EX: **in classic Metropolis,** *instead of randomly choosing the particle to be moved, then one can go through them sequentially*. After one *pass*, all particles are attempted once. This is correct and might be faster.

Preferential Sampling

Sometimes it is not the overall acceptance ratio one wants to optimize.

- Consider a layered system:
- Suppose we are only interested in the top.
- Sample particles with probability $h(z_i)/H$.



$$H = \sum_{i=1}^{N} h(z_i)$$

- Then acceptance probability:

$$A(r \to r') = \frac{h(z_i)}{H} \frac{H'}{h(z_i')} \, e^{-\beta(V(r')-V(r)}$$

- We focus the CPU time on *interesting degrees of freedom* (it will lower overall acceptances but increase efficiency of what we want to calculate.)

Optimizing the moves

- (Ergodicity) Any transition rule is allowed as long as you can go anywhere in phase space with a finite number of steps.

- Try to find a T(s → s′) ≈ π(s′)/C.

$$A(s \to s') = \min\left\{1, \frac{T(s' \to s)\pi(s')}{T(s \to s')\pi(s)}\right\} = 1$$

- If you can the acceptance ratio will be 1.
- But this would be “direct sampling”. Normally very difficult.
- Heat bath corresponds to making this choice in a limited neighborhood (for lattice models).

Heat Bath

Sample a neighborhood of a given point so that it is in "local equilibrium."

$$T(s \to s') = \frac{\pi(s')}{C(s)} \quad \text{with} \quad C(s) = \sum_{s'' \in N(s)} \pi(s'')$$

Then the acceptance probability will be:

$$A(s \to s') = \min\left\{1, \frac{C(s)}{C(s')}\right\}$$

- ✓ Can be used only if it is possible to quickly compute the normalization ratio.
- ✓ Acceptance ratio=1 if C(s) is independent of s.

Force-Bias MC

We can use forces to push the walk in the right direction.

– Taylor expand about the current point.

$$V(r') = V(r) - F(r)\cdot(r'-r)$$

– Set $T(s \to s') \approx \exp[\, -\beta(V(r) - \alpha F(r)\cdot(r'-r))]$.

- We can sample this distribution using the mapping method if we assume a limited domain such as a cube.
- This is *Force-Bias Monte Carlo* (see notes and textbook for details).
- Idea is to move preferentially in direction of higher probability, thereby reducing rejections and increasing how far you can move.
- Does it work in practice?

Force bias has higher acceptance ratio than classic Metropolis. Does it lead to faster convergence?

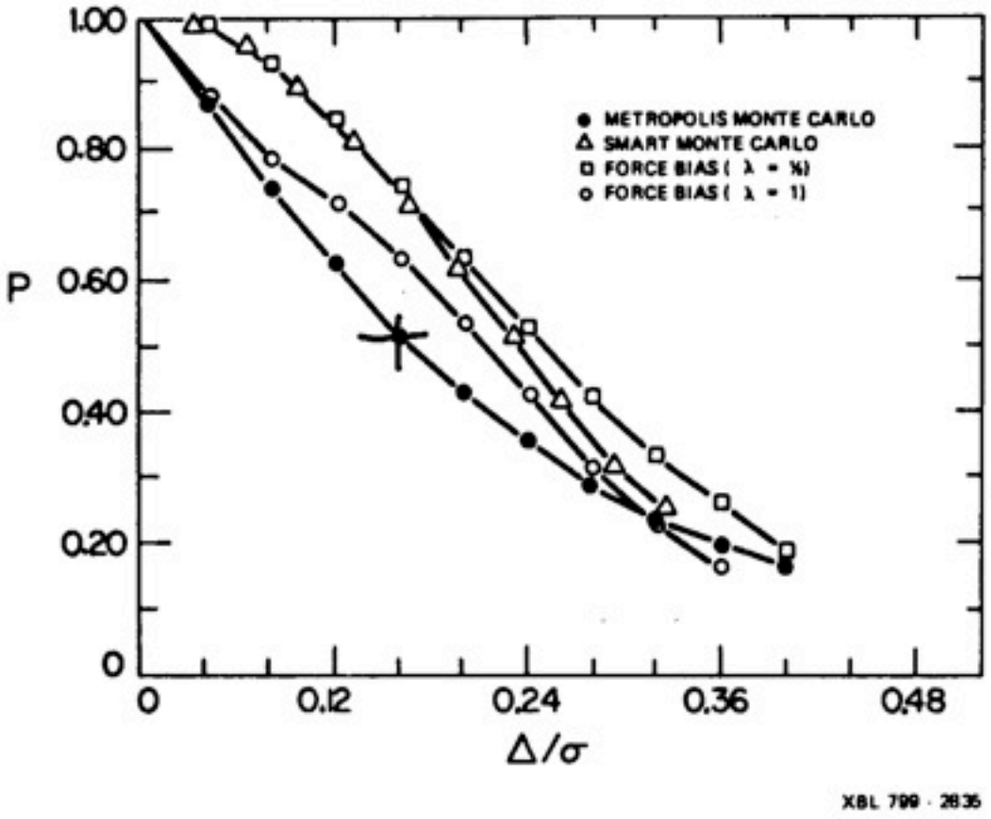


Fig. 1. Average acceptance probability.

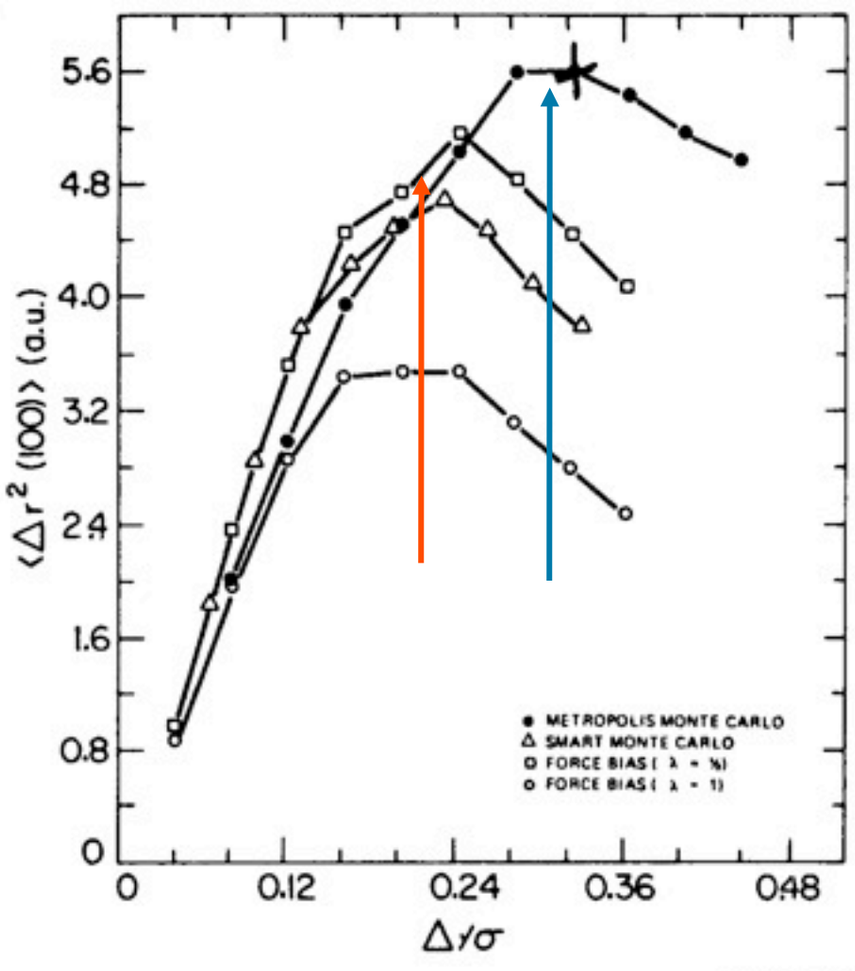


Fig. 3. $\langle(\vec{r}(i) - \vec{r}(i + 100))^2\rangle$

$\vec{r}(i)$ = 3n vector of argon positions at step i.

Variance of energy (local quantity) is not as sensitive to step size. MC is a robust method!

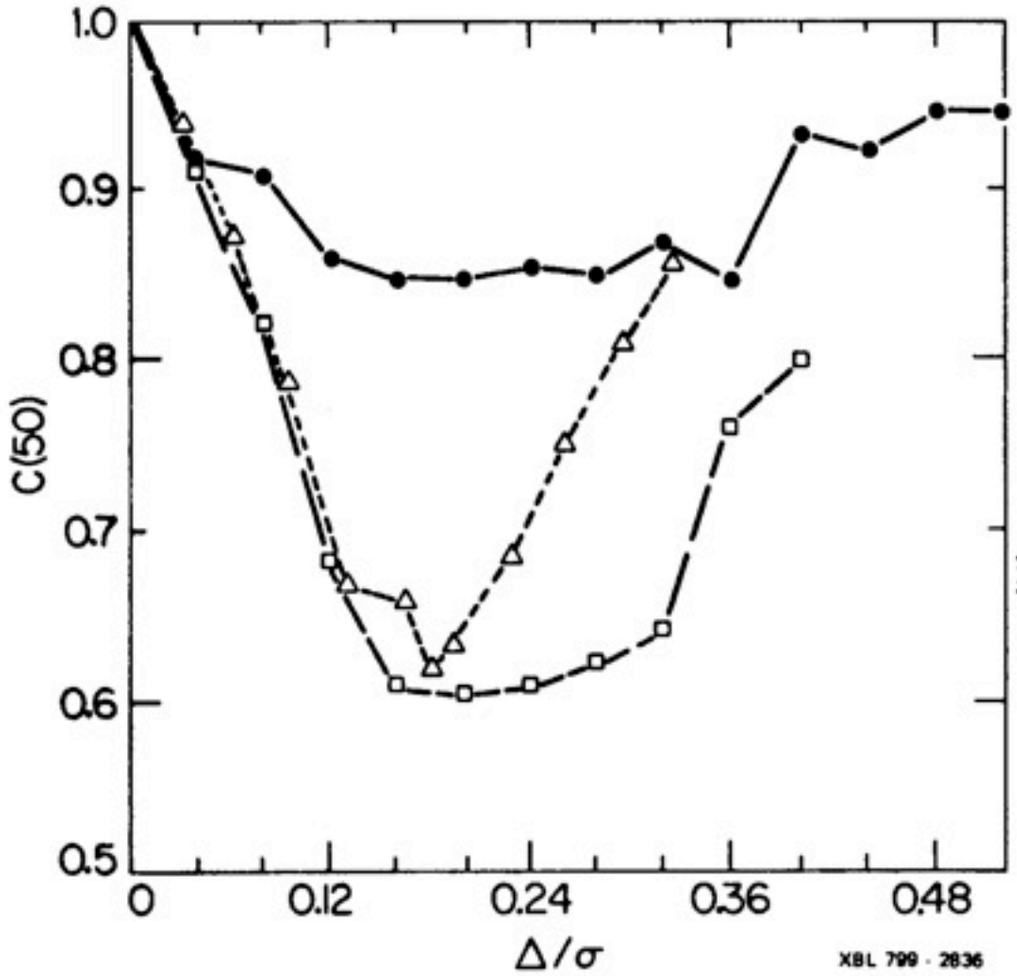


Fig. 2. $\frac{\langle \Delta V(i)\, \Delta V(i+50) \rangle}{\langle \Delta V(i)^2 \rangle}$

where i = step number and
Δ V is the deviation of potential energy from the mean.

Acceptable range of efficiency.

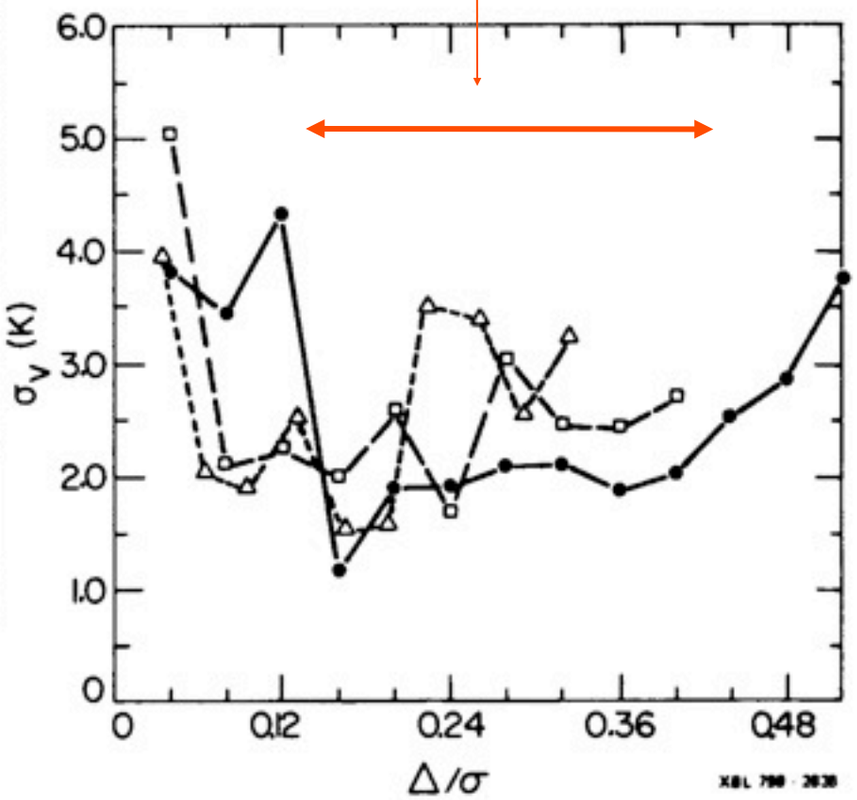


Fig. 4. The variance of the total potential energy for calculations with the same number of steps.

Smart Monte Carlo

Same idea but sample from a ***displaced Gaussian pdf***.

$$T(r \to r') = \frac{1}{(4\pi\tau)^{3/2}} \exp\left[-\frac{\left(\vec{r}' - \vec{r} - \tau\beta\vec{F}(\vec{r})\right)^2}{4\tau}\right]$$

with trial displacement: $\Delta\vec{r} = \tau\beta\vec{F}(\vec{r}) + \vec{\delta}$ where $\langle\delta\rangle = 0$ and $\langle\delta^2\rangle = 2\tau$

- Also moves in the direction of increased probability
- Acceptance rate A will be:

$$A(r \to r') = \exp\left\{-\beta\left[V(\vec{r}') - V(\vec{r}) + \frac{\vec{F}(\vec{r}') + \vec{F}(\vec{r})}{2} \cdot \left(\vec{r}' - \vec{r} + \tau\beta\frac{\vec{F}(\vec{r}') - \vec{F}(\vec{r}))}{2}\right)\right]\right\}$$

- A=1 in case the potential is linear in region sampled $O(\tau^{1/2})$.
- Note that sampling domain is infinite, in principle.
- There is a nice way of deriving this -- related to Brownian dynamics and quantum Monte Carlo.

Brownian Dynamics

Consider a big molecule in a solvent. In the high-viscosity limit the "master equation" is:

$$\frac{\partial \rho(R,t)}{\partial t} = D\nabla^2 \rho(R,t) - \beta D \nabla \cdot \left(\vec{F}(R)\rho(R,t) \right)$$

$$R(t+\tau) = R(t) + \tau \beta D \vec{F}(R(t)) + \vec{\eta}(t)$$

$$\langle \vec{\eta}(t) \rangle = 0 \qquad \langle \eta^2(t) \rangle = 2\tau D$$

White noise
Variance ~ Dτ

Enforce *detailed balance by rejections*! (hybrid method)

$$T(R \to R') \propto \exp\left[-\frac{(R' - R - \beta D \tau F(R))^2}{2D\tau} \right]$$

Also the equation for Diffusion Quantum Monte Carlo!