# 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



# The "Classic" Metropolis method

***Metropolis-Rosenbluth² -Teller² (1953) method for sampling the Boltzmann distribution is:***

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

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

- Repeat many times

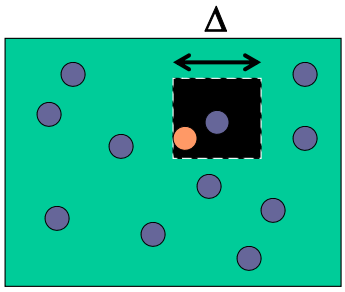
- Given ergodicity, the *distribution of s* will be the canonical distribution: $\pi(s) = \exp(-E(s)/k_BT)/Z$.

**•Convergence is guaranteed but the rate is not!**

## How to sample

S_new = S_old + Δ · (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*.**

$$A(s \to s') = \exp[-\beta(V(s') - V(s))]$$
$$= \exp[-\beta \sum_{j \neq i} (v(r_i' - r_j) - v(r_i - r_j))]$$

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



## Recall: Rejection Method

Metropolis achieves detailed balance by *rejecting* moves.
Break up transition probability into sampling and acceptance:

$$P(s \to s') = T(s \to s')A(s \to s')$$
$$T(s \to s') = \text{sampling probability}$$
$$A(s \to s') = \text{acceptance probability}$$

Optimal *acceptance probability* that gives detailed balance is:

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

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 $P(s \Rightarrow s')$ is ergodic then $\pi(s)$ is the unique steady state solution.
- Detailed balance is not compulsory.
  - Required is balance: $\Sigma_s \pi(s)\, P(s \to s') = \pi(s')$.
  - 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,…)

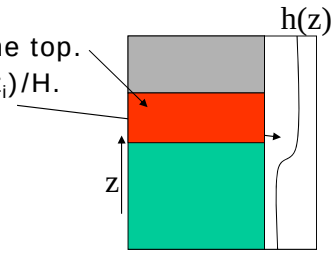
– Either will give the correct distribution even though choice 2 does not really satisfy detailed balance.
  - ✓ Theorem: If each menu item individually satisfies detailed balance, then desired state is the unique stationary state.

– *instead of randomly choosing the particle to be moved, go through them sequentially*. After one *pass*, all particles have one attempted move. 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:

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

Focus CPU time on *interesting degrees of freedom*, lowering overall acceptances but increasing 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 $T(s \to s') \approx \pi(s')/C$.

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

- 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.

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

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, e.g lattice models.
- ✓ 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.

$$V(\mathbf{r'}) = V(\mathbf{r}) - F(\mathbf{r})(\mathbf{r'} - \mathbf{r})$$

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

- 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?

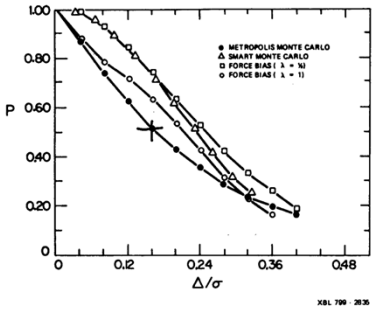



Fig. 1. Average acceptance probability.

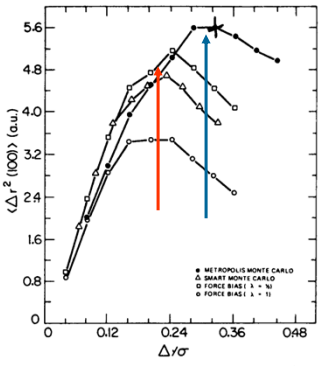



Fig. 3. $\langle(\vec{r}(i) - \vec{r}(i + 100))^2\rangle$

$\vec{r}(i)$ = 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!

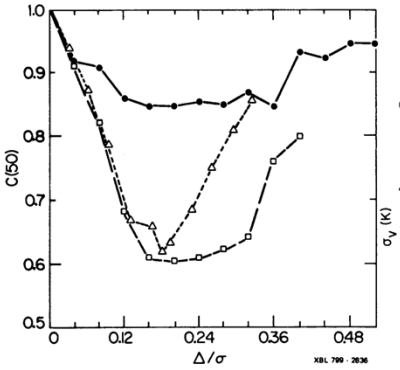



Fig. 2. $\frac{\langle \Delta V(i)\, \Delta V(i + 50)\rangle}{\langle \Delta V(i)^2 \rangle}$

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

Acceptable range of efficiency.

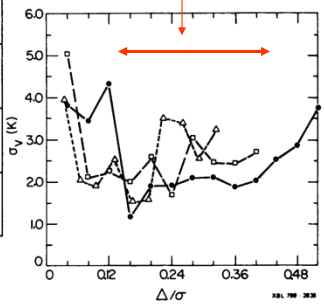



Fig. 4. The variance of the total potential energy for calculations with the same number of steps.

## Smart Monte Carlo

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

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

$$with\ trial\ displ.: \Delta r = \tau\beta F(r) + \delta \quad with < \delta >= 0 \quad and < \delta^2 >= 2\tau$$

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

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

- 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 (next lecture)



## Brownian Dynamics

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

$$\frac{\partial \rho(R,t)}{\partial t} = D\nabla^2 \rho(R,t) - \beta D \nabla[F(R)\rho(R,t)]$$

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

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

White noise
Variance ~ Dτ

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

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

Also the equation for Diffusion Quantum Monte Carlo!