

Advanced topics in Markov-chain Monte Carlo

Lecture 6:

Sampling π (stationary distributions), computing π (Free energies)

Part 2/2: Thermodynamic Integration / Simulated annealing
/ Simulated tempering

Werner Krauth

ICFP -Master Course Ecole Normale Supérieure, Paris, France

22 February 2023

- D. Frenkel, B Smit, **Understanding Molecular Simulation: From Algorithms to Applications**, (Elsevier, 2001)
- B. Hajek, **Cooling Schedule for optimal annealing**, Mathematics of Operations Research (1988)

Thermodynamic integration

- All of MCMC: concerned with π_i/π_j , norm of π_i (usually) unknown.
 - Metropolis filter: $\mathcal{P}(i \rightarrow j) = \min(1, \pi_j/\pi_i)$.
 - NB: Flow: $\mathcal{F}_{ij} = \pi_i P_{ij}$ (usually) unknown.
- All of physics:
 - concerned with $Z = \sum_{i \in \Omega} \pi_i$ ($\pi_i = \exp(-E_i/kT)$)
 - Partition function known analytically in some limits:
 - High-temperature limit: $T \rightarrow \infty \Leftrightarrow \beta \rightarrow 0$
 - Ideal-gas limit: density $\rho \rightarrow 0$, interactions $\rightarrow 0$.
 - Ideal-solid limit: density $\rho \rightarrow \rho_{\max}$, interactions \rightarrow harmonic.
 - Keep Ω , change π .
- Creating a path from a known limit to the relevant $\{\Omega, \pi\}$ is called “Thermodynamic integration”.
- Path must (normally) be smooth (avoid phase transitions).

- Partition function $Z(\alpha) = \sum_{i \in \Omega} \tilde{\pi}_i^\alpha$ (“ $\tilde{\pi}_i$ to the power α ”)
(NB: π : normalized, $\tilde{\pi}$: non-normalized).

- $$Z(\alpha') = \sum_{i \in \Omega} \tilde{\pi}_i^{\alpha'} = \sum_{i \in \Omega} \tilde{\pi}_i^\alpha \frac{\tilde{\pi}_i^{\alpha'}}{\tilde{\pi}_i^\alpha}$$

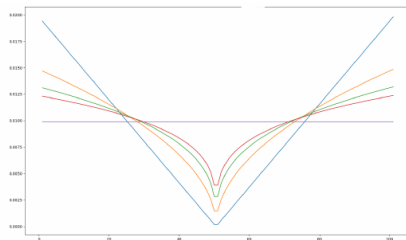
- $$\frac{Z(\alpha')}{Z(\alpha)} = \frac{1}{Z(\alpha)} \sum_{i \in \Omega} \tilde{\pi}_i^{\alpha'} = \sum_{i \in \Omega} \pi_i^\alpha \frac{\tilde{\pi}_i^{\alpha'}}{\tilde{\pi}_i^\alpha} = \mathbb{E} \left(\frac{\tilde{\pi}_i^{\alpha'}}{\tilde{\pi}_i^\alpha} \right)_\alpha$$

- $$Z(1) = \left[\frac{Z(1)}{Z(0.75)} \right] \left[\frac{Z(0.75)}{Z(0.5)} \right] \left[\frac{Z(0.5)}{Z(0.25)} \right] \left[\frac{Z(0.25)}{Z(0)} \right] Z(0)$$

- Only $Z(0)$ is known.

- V-shaped: $\pi_i = \text{const} |\frac{n+1}{2} - i| \forall i \in \Omega = \{1, \dots, n\}$.
- Suppose that $\text{const} = \frac{4}{n^2}$ is unknown.
- \tilde{V} -shaped: $\tilde{\pi}_i = |\frac{n+1}{2} - i| \forall i \in \Omega$.
- Partition function $Z = \sum_{i \in \Omega} \tilde{\pi}_i$.
- Consider $\tilde{\pi}^\alpha$ (“pi to the power alpha”).
- $\alpha = 0$: $Z(\alpha = 0) = n$

Thermodynamic integration 3/3



- This is Problem 1 of today's TD.
- Relation to Simulated annealing.
- Relation to Simulated tempering.

Simulated annealing 1/2

Simulated annealing: MCMC Optimization algorithm

- Start at very small values of α ,
- At each step, slowly increase α by a tiny amount.

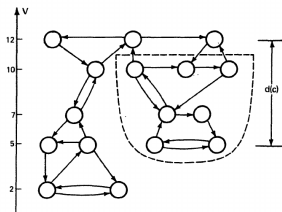
In the V-shaped probability distribution (with $\pi(n) = 0^+$), switch to temperature language.

- $U_i = -\log(\pi_i)$
- Set up temperature schedule $T_k \rightarrow 0$ for $k \rightarrow \infty$
- Accept / reject move ΔU with Metropolis filter
 $\min[1, \exp(-\Delta U/T_k)]$

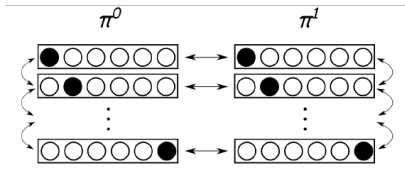
Simulated annealing 2/2

Simulated annealing: MCMC optimization algorithm

- Theorem (Hajek 1988): need $\sum_k \exp(-d^*/T_k) = \infty$ for sure convergence to lowest-energy configuration.
- Corrolary (Hajek 1988): If $T_k = c/\log(k+1)$, then need $c \geq d^*$
- Easy to check in V-shaped distribution on the path graph.



Simulated tempering 1/2



```
procedure temp-rev
input  $\mathcal{P}^{\text{padded}}, \{x, \alpha\}, p_{\text{copy}}$ 
if ( $\text{ran}(0, 1) > p_{\text{copy}}$ ) then
    {
         $\sigma_x \leftarrow \text{choice}\{-1, 1\}$ 
        if ( $\text{ran}(0, 1) < \pi_x^\alpha / \pi_{x+\sigma_x}^\alpha$ ) then
            {
                 $x \leftarrow x + \sigma_x$ 
            }
    }
else
    {
         $\sigma_\alpha \leftarrow \text{choice}\{-1, 1\}$ 
        if ( $\text{ran}(0, 1) < \pi_x^{\alpha+\sigma_\alpha} / \pi_x^\alpha$ ) then
            {
                 $\alpha \leftarrow \alpha + \sigma_\alpha$ 
            }
    }
output  $\{x, \alpha\}$ 
```

- Let the system evolve at several temperatures.
- Move between temperatures, move between positions.