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

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References

- 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

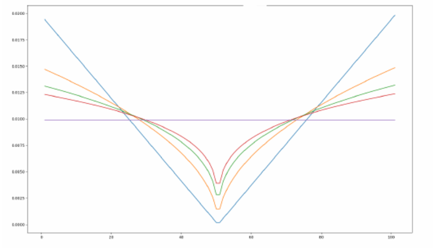
- All of MCMC: concerned with π_i/π_j, norm of π_i (usually) unknown.
  - Metropolis filter: $\mathcal{P}(i \to j) = \min(1, \pi_j/\pi_i)$.
  - NB: Flow: $\mathcal{F}_{ij} = \pi_i P_{ij}$ (usually) unknown.
- All of physics:
  - concerned with $Z = \sum_{i \in \Omega} \pi_i$ $(\pi_i = \exp(-E_i/kT))$
  - Partitition function known analytically in some limits:
    - High-temperature limit: $T \to \infty \Leftrightarrow \beta \to 0$
    - Ideal-gas limit: density $\rho \to 0$, interactions $\to 0$.
    - Ideal-solid limit: density $\rho \to \rho_{\text{max}}$, interactions $\to$ 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).

Thermodynamic integration 1/3

- 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.

Thermodynamic integration 2/3

- V-shaped: $\pi_i = \text{const}|\frac{n+1}{2} - i| \; \forall i \in \Omega = \{1, \ldots, n\}$.
- 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").
- $\alpha = 0$: $Z(\alpha = 0) = n$



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

Simulated annealing: MCMC Optimization algorithm

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

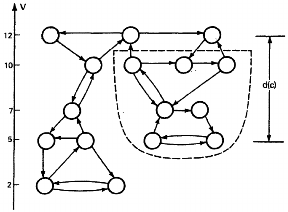
In the V-shaped probability distribution (with $\pi(n) = 0^+$), switch to temperature language.

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

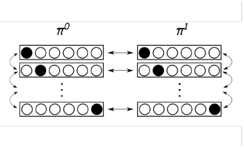
Simulated annealing 2/2

Simulated annealing: MCMC optimization algorithm

- Theorem (Hajek 1988): need $\sum_k \exp\left(-d^*/T_k\right) = \infty$ for sure convergence to lowest-energy configuration.
- Corrolary (Hajek 1988): If $T_k = c/\log\left(k+1\right)$, 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 ($\texttt{ran}(0,1) > p_{\text{copy}}$) **then**
  $\sigma_x \leftarrow \texttt{choice}\{-1, 1\}$
  if ($\texttt{ran}(0,1) < \pi^{\alpha}_{x+\sigma_x} / \pi^{\alpha}_{x}$) **then**
    $x \leftarrow x + \sigma_x$
else
  $\sigma_\alpha \leftarrow \texttt{choice}\{-1, 1\}$
  if ($\texttt{ran}(0,1) < \pi^{\alpha+\sigma_\alpha}_{x} / \pi^{\alpha}_{x}$) **then**
    $\alpha \leftarrow \alpha + \sigma_\alpha$
output $\{x, \alpha\}$

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