The Monte Carlo Method

1 The Monte Carlo Method

Consider state space $\mathcal{X} \triangleq \mathcal{Z}^N$ for N interacting particles.

Definition 1.1. For a finite state space $\mathcal{X}$, we denote the set of probability measures over $\mathcal{X}$ as $\mathcal{M}(\mathcal{X}) \triangleq \{\nu \in [0,1]^{\mathcal{X}} : \sum_{x\in\mathcal{X}} \nu_x = 1\}$.

Many optimization problems are of the form $\min\{E(x) : x \in \mathcal{X}\}$ for some feasible set of states $\mathcal{X}$ and the optimization function $E \in \mathbb{R}^{\mathcal{X}}$. For classical reasons, we will call E as an energy function, and solving this minimization problem is equivalent to finding the set of minimum energy states defined as

$$\mathcal{X}_0 \triangleq \left\{ x \in \mathcal{X} : E(x) \leqslant \min_y E(y) \right\}.$$

We will show in Section 3 that finding the configurations that minimize the energy while being regularized for highest randomness with Lagrange multiplier β for the regularization term, is equivalent to finding the support of Boltzmann distribution $\mu_\beta \in \mathcal{M}(\mathcal{Z}^N)$ for inverse temperature β. Computing Boltzmann distribution is vey hard for large N since the computation of partition function $Z(N,\beta) \triangleq \sum_{x\in\mathcal{Z}^N} e^{-\beta E(x)}$ is infeasible for large N. The goal of Monte Carlo methods is to simulate a Markov process that converges to a stationary distribution μ_β of interest.

1.1 Motivation

Markov Chain Monte Carlo (MCMC) is a technique which can be used to solve hard optimization problems. We'll design MCMC algorithms to solve the following three problems, and one can solve many more.

- *Graph coloring problem:* Given a graph $G = (V, E)$ and a set of colors $\{1, 2, \ldots, q\}$, a proper q-coloring of G is an assignment of colors to the vertices V such that neighboring vertices do not receive the same color, *i.e*, the set of proper q-colorings of G is defined as $\mathcal{A} \triangleq \{x \in [q]^V : x_v \neq x_w, (v,w) \in E\}$. Find the set $\mathcal{A}$ of proper q-colorings of G.

- *The knapsack problem:* Suppose you have a knapsack which has some maximum weight capacity W. There are n items with weights $w_1, \ldots, w_n > 0$ and values $v_1, \ldots, v_n > 0$, and we want to choose the subset of them that maximizes the total value subject to the weight constraint of the knapsack. Let $\mathcal{S} \triangleq \{S \subseteq [n] : \sum_{i\in S} w_i \leqslant W\}$ be the set of feasible knapsack packings, then find $S^* \triangleq \arg\max\{\sum_{i\in S} v_i : S \in \mathcal{S}\}$.

- *The travelling salesman problem (TSP):* Suppose you want to find the best route (minimizing total distance travelled) between the 28 Indian state capitals that we want to visit! A valid route starts and ends in the same state capital, and visits each capital exactly once (this is known as the TSP, and is known to be NP-Hard).

As the name suggests, this technique depends a bit on the idea of Markov Chains. Most of this section then will actually be building up the foundations of Markov Chains, and MCMC will follow soon after.

2 Markov chains

Definition 2.1. A random process $X : \Omega \to \mathcal{X}^{\mathbb{Z}_+}$ for finite state space $\mathcal{X}$ is called a *Markov chain* if for each time $n \in \mathbb{Z}_+$ and states $x_0, \dots, x_n, y \in \mathcal{X}$

$$P(\{X_{n+1} = y\} \mid \cap_{k=0}^{n} \{X_k = x_k\}) = P(\{X_{n+1} = y\} \mid \{X_n = x_n\}).$$

That is, the future is independent of the past conditioned on the present.

Definition 2.2. For a Markov chain $X : \Omega \to \mathcal{X}^{\mathbb{Z}_+}$, we can define a *probability transition matrix* $P(n) \in [0,1]^{(\mathcal{X}) \times \mathcal{X}}$ for each initial state x at each time $n \in \mathbb{Z}_+$, and all next state $y \in \mathcal{X}$ as

$$p_{xy}(n) \triangleq P(\{X_{n+1} = y\} \mid \{X_n = x\}).$$

Remark 1. We observe that each row $p_x(n) \triangleq \{p_{xy}(n) : y \in \mathcal{X}\}$ of probability transition matrix is the conditional probability of X_{n+1} conditioned on the event $\{X_n = x\}$, and hence $P \in \mathcal{M}(\mathcal{X})^{\mathcal{X}}$.

Definition 2.3. A Markov chain $X : \Omega \to \mathcal{X}^{\mathbb{Z}_+}$ is called *time homogeneous* if the associated transition probability matrix $P(n)$ is identical for all times $n \in \mathbb{Z}_+$, and is denoted by $P \in \mathcal{M}(\mathcal{X})^{\mathcal{X}}$. Let $\nu(n) \in \mathcal{M}(\mathcal{X})$ be the marginal probability distribution of Markov chain X at time $n \in \mathbb{Z}_+$.

Remark 2. For a time homogeneous Markov chain $X : \Omega \to \mathcal{X}^{\mathbb{Z}_+}$ with probability transition matrix $P \in \mathcal{M}(\mathcal{X})^{\mathcal{X}}$, we observe that $\nu(n) = \nu(0)P^n$ where P^n is the n-step transition probability matrix.

Definition 2.4. A time homogeneous Markov chain $X : \Omega \to \mathcal{X}^{\mathbb{Z}_+}$ with finite state space $\mathcal{X}$ is called
(a) *irreducible* if for any pair of configurations $x, y \in \mathcal{X}$, there exists a path $(x_0, x_1, \dots, x_n)$ of length n, connecting $x_0 = x$ and $x_n = y$ with non-zero probability, i.e. $(P^n)_{xy} \geqslant \prod_{i=0}^{n-1} p_{x_i, x_{i+1}} > 0$,
(b) *aperiodic* if for any pair of configurations $x, y \in \mathcal{X} \times \mathcal{X}$, there exists a positive integer $n(x,y)$ such that for any $n \geqslant n(x,y)$, there exists a path of length n connecting x and y with non-zero probability,
(c) *positive recurrent* if there exists a distribution $\pi \in \mathcal{M}(\mathcal{X})$ such that $\sum_{x \in \mathcal{Z}^N} \pi_x p_{xy} = \pi_y$ for each $y \in \mathcal{X}$, and
(d) *reversible* if the transition probability satisfy the detailed balance equation $\pi_x p_{xy} = \pi_y p_{yx}$ for each $x, y \in \mathcal{X}$.

Remark 3. We observe the following.
(a) For an irreducible chain, aperiodicity is easily enforced by allowing the configuration to remain unchanged with non-zero probability, i.e. $p_{xx} > 0$ for each configuration $x \in \mathcal{X}$.
(b) For finite state Markov chains irreducibility and aperiodicity implies positive recurrence or stationarity.

2.1 Properties of ergodic Markov chains

Theorem 2.5. *Let $X : \Omega \to \mathcal{X}^{\mathbb{Z}_+}$ be a time homogeneous Markov chain with initial condition $X_0 = x_0$ and transition probability matrix $P \in \mathcal{M}(\mathcal{X})^{\mathcal{X}}$. Let $f : \mathcal{X} \to \mathbb{R}$ be any real valued function. If the Markov chain X satisfies the conditions* (a), (b), (c) *in Definition 2.4, then the following holds true.*
(a) The probability distribution of X_n converges to the stationary distribution, i.e. $\lim_{n\to\infty} P\{X_n = x\} = \pi(x)$ *for each $x \in \mathcal{X}$.*
(b) Time averages converge to averages over the stationary distribution, i.e. $\lim_{t\to\infty} \frac{1}{t} \sum_{s=1}^{t} f(X_s) = \sum_{x \in \mathcal{X}} \pi(x) f(x)$ *almost surely.*

Proposition 2.6. *Let $X : \Omega \to \mathcal{X}^{\mathbb{Z}_+}$ be a time homogeneous Markov chain with symmetric transition probability matrix $P \in \mathcal{M}(\mathcal{X})^{\mathcal{X}}$.*
(a) Uniform distribution is an invariant distribution of P.
(b) X is a reversible Markov chain.

Proof. Since P is symmetric, $P = P^\top$ and it follows that $p_{x,y} = p_{y,x}$ for each $x, y \in \mathcal{X}$.
(a) Since P is symmetric, all one vector is a left eigenvector with eigenvalue unity, and hence the normalized row vector $\frac{1}{|\mathcal{X}|}\mathbf{1}^\top \in \mathcal{M}(\mathcal{Z})$ is an invariant distribution of P.
(b) Further, P satisfies reversibility with respect to uniform distribution on $\mathcal{X}$.

□

2.2 Markov chain as a random walk

Let $X : \Omega \to \mathcal{X}^{\mathbb{Z}_+}$ be a time homogeneous Markov chain with initial condition $X_0 = x_0$ and transition probability matrix $P \in \mathcal{M}(\mathcal{X})^{\mathcal{X}}$. Then we can define a graph $G \triangleq (\mathcal{X}, E, w)$ with set of nodes $\mathcal{X}$, set of edges $E \triangleq \{(x,y) \in \mathcal{X} \times \mathcal{X} : p_{x,y} > 0\}$, and edge weights $w \in [0,1]^E$ defined for each edge $e = (x,y) \in E$ as $w(e) \triangleq p_{x,y}$. It follows that X is a random walk on graph G with initial location $X_0 = x_0$ and transition probability from each state x being the conditional probability distribution $P_x \triangleq \{p_{xy} : y \in \mathcal{X}\}$ which is non zero only over outgoing edges $(x,y) \in E$.

3 Gibbs variational principal

Definition 3.1. Consider a finite state space $\mathcal{X}$ and a discrete random variable $X : \Omega \to \mathcal{X}$ with distribution $P \in \mathcal{M}(\mathcal{X})$. We denote the *entropy* as $H \in \mathbb{R}_+^{\mathcal{M}(\mathcal{X})}$ and define as $H(P) \triangleq \mathbb{E} \ln \frac{1}{P(X)}$ for the distribution $P \in \mathcal{M}(\mathcal{X})$ for random variable X.

Definition 3.2. For a Bernoulli random variable, we can define *binary entropy function* $h : [0,1] \to [0, \ln 2]$ as $h(p) \triangleq H((1-p,p)) = -(1-p)\ln(1-p) - p\ln p$ for each $p \in [0,1]$.

Remark 4. We observe that binary entropy function h is concave with unique maxima of $\ln 2$ achieved at $p = \frac{1}{2}$, and it is increasing for $p \in [0, \frac{1}{2}]$. In general, we observe that entropy is a measure of uncertainty and maximized for a uniform random variable.

Definition 3.3. Consider a state space $\mathcal{X}$ and a random variable $X : \Omega \to \mathcal{X}$. For finite $\mathcal{X}$ and any two distributions $P, Q \in \mathcal{M}(\mathcal{X})$ such that $\mathrm{supp}(Q) \subseteq \mathrm{supp}(P)$, we define *KL divergence* $D : \mathcal{M}(\mathcal{X})^2 \to \mathbb{R}_+$ as

$$D(P \| Q) \triangleq \mathbb{E}_{X \sim P} \ln \frac{P(X)}{Q(X)}.$$

Definition 3.4. For a Bernoulli random variable, we can define *binary relative entropy function* $d : [0,1]^2 \to [0, \ln 2]$ as $d(p\|q) \triangleq D((1-p,p)\|(1-q,q)) = -(1-p)\ln\frac{1-p}{1-q} - p\ln\frac{p}{q}$ for each $p, q \in [0,1]$.

Remark 5. We observe that $d(p\|q) \geqslant 0$ with equality iff $p = q$, and d is convex in both arguments. In general, we observe the following for KL divergence, also referred to as relative entropy.

(a) Relative entropy is a measure of "distance"[1] between two distributions.
(b) Relative entropy is convex in both the arguments, and is always non negative.
(c) Relative entropy is zero when both distributions are identical.

In the following, we consider a system with a discrete configuration space $\mathcal{X}$ and a real-valued energy function $E \in \mathbb{R}^{\mathcal{X}}$ defined on this space.

Definition 3.5 (Boltzmann distribution). Let $\mathcal{X}$ be finite and $E \in \mathbb{R}^{\mathcal{X}}$ be the *energy function*. Then the *partition function* $Z : \mathbb{R}_+ \to \mathbb{R}_+$ is defined for each inverse temperature $\beta \in \mathbb{R}_+$ as $Z(\beta) \triangleq \sum_{x \in \mathcal{X}} e^{-\beta E(x)}$. For each inverse temperature $\beta \in \mathbb{R}_+$, the *Boltzmann distribution* $\mu_\beta \in \mathcal{M}(\mathcal{X})$ is defined for each $x \in \mathcal{X}$ as

$$\mu_\beta(x) \triangleq \frac{1}{Z(\beta)} e^{-\beta E(x)}.$$

We define the *free energy* $F : \mathbb{R}_+ \to \mathbb{R}$ for each inverse temperature $\beta \in \mathbb{R}_+$ as $F(\beta) \triangleq -\frac{1}{\beta}\ln Z(\beta)$, such that

$$\mu_\beta(x) = e^{-\beta(E(x) - F(\beta))}.$$

Definition 3.6 (Gibbs free energy). We define the *Gibbs free energy* $G : \mathcal{M}(\mathcal{X}) \to \mathbb{R}$ as a real-valued functional over the space of probability distributions $\mathcal{M}(\mathcal{X})$ defined over configuration space $\mathcal{X}$, as

$$G(P) \triangleq \mathbb{E}_{X \sim P} E(X) - \frac{1}{\beta} H(P).$$

[1]KL divergence is not a distance strictly speaking since it is not symmetric in P and Q. However, we can define Jensen-Shannon divergence defined as $\mathrm{JS}(P,Q) \triangleq \frac{1}{2} D(P \| \frac{1}{2}(P+Q)) + \frac{1}{2} D(Q \| \frac{1}{2}(P+Q))$, which is a symmetric version of KL divergence.

Proposition 3.7 (Gibbs variational principle). *The Gibbs free energy G is a convex functional of P, and it achieves its unique minimum on the Boltzmann distribution $P = \mu_\beta$. Moreover, $G(\mu_\beta) = F(\beta)$, where F is the free energy.*

Proof. From the definition of relative entropy, entropy, and Boltzmann distribution, we observe that

$$\frac{1}{\beta}D(P\|\mu_\beta) = \frac{1}{\beta}\mathbb{E}_{X\sim P}\ln\frac{P(X)}{\mu_\beta(X)} = -\frac{1}{\beta}H(P) + \mathbb{E}_{X\sim P}(E(X) - F(\beta)) = G(P) - F(\beta).$$

From the convexity of relative entropy, it follows that $G(P)$ is convex in P, and hence has a unique minimum. From non negativity of relative entropy, it follows that $G(P) \geqslant F(\beta)$ with equality at $P = \mu_\beta$. □

Remark 6. We observe the following

(a) Minimizing Gibbs energy is finding the most random distribution P under which mean energy of the system is minimized.
(b) There is a large mass on low energy configuration in Boltzmann distribution.
(c) As the system cools, i.e. inverse temperature grows arbitrary large, energy minimizing configurations $\mathcal{X}_0 \triangleq \{x \in \mathcal{X} : E(x) = \min_{y\in\mathcal{X}} E(y)\}$ are equally likely.
(d) Finding $\min_{x\in\mathcal{X}} E(x)$ is the same as finding the support of Boltzmann distribution at low temperatures.
(e) One approach is to find μ_β at certain inverse temperature β and then increase β. This is called *simulated annealing*.

4 Metropolis Chains

Given state space $\mathcal{X} \triangleq \mathcal{Z}^N$ and stationary distribution $\pi \in \mathcal{M}(\mathcal{Z}^N)$, our goal is to find a Markov chain $X : \Omega \to \mathcal{X}^{\mathbb{Z}_+}$ with transition probability matrix $P \in \mathcal{M}(\mathcal{X})^{\mathcal{X}}$ such that $\pi P = \pi$. The approach of Metropolis chains is to first consider an initial base Markov chain $Y : \Omega \to \mathcal{X}^{\mathbb{Z}_+}$ with certain transition probability matrix $\Psi \in \mathcal{M}(\mathcal{X})^{\mathcal{X}}$ and modify the transition probabilities appropriately so that the new chain X has the desired stationary distribution π.

4.1 Symmetric base chain

Definition 4.1 (Symmetric base chain). Let $Y : \Omega \to \mathcal{X}^{\mathbb{Z}_+}$ be an irreducible time homogeneous Markov chain with state space $\mathcal{X} \triangleq \mathcal{Z}^N$ and symmetric transition probability matrix $\Psi \in \mathcal{M}(\mathcal{X})^{\mathcal{X}}$.

Remark 7. Note that each row $\psi_x \triangleq \{\psi_{xy} : y \in \mathcal{X}\} \in \mathcal{M}(\mathcal{X})$ is the conditional distribution of the next state, starting from state x.

Definition 4.2 (Modification of symmetric base chain). We define $a_{xy} \in [0,1]$ as the *acceptance probability* of transition from state x to state y. We define a new Markov chain $X : \Omega \to \mathcal{X}^{\mathbb{Z}_+}$ with transition probability matrix $P \in \mathcal{M}(\mathcal{X})^{\mathcal{X}}$ that evolves as follows.

(a) When at state x, a candidate move is generated from distribution ψ_x.
(b) If the proposed new state is y, then the move is *accepted* with probability a_{xy} and with remaining probability chain remains at x.

Proposition 4.3. *For a symmetric base chain Y with symmetric transition probability matrix Ψ and acceptance probability matrix $A \in [0,1]^{\mathcal{X}\times\mathcal{X}}$, the resulting Markov chain is reversible if for all $x \neq y$,*

$$\pi(x)a_{xy} = \pi(y)a_{yx}. \tag{1}$$

Proof. The transition probabilities of the new chain X for states $x, y \in \mathcal{X}$, are

$$p_{xy} = \begin{cases} \psi_{xy}a_{xy}, & y \neq x, \\ 1 - \sum_{z\in\mathcal{X}\setminus\{x\}} \psi_{xz}a_{xz}, & y = x. \end{cases}$$

It follows that the transition matrix P is reversible and has invariant distribution π if reversibility condition $\pi(x)\psi_{xy}a_{xy} = \pi(y)\psi_{yx}a_{yx}$ holds for all $x \neq y$. Since Ψ is symmetric, we have $\psi_{xy} = \psi_{yx}$ for each $y \neq x$. □

Corollary 4.4. *The maximum acceptance probability for each state $x, y \in \mathcal{X}$ is bounded above as*

$$a_{xy} \leqslant \min\left\{1, \frac{\pi(y)}{\pi(x)}\right\}.$$

Proof. Defining $b_{xy} \triangleq \pi(x)a_{xy}$ for all $x \neq y$, the condition (1) becomes $b_{xy} = b_{yx}$ for all $x \neq y$. By definition of b, we see that $b_{xy} \leqslant \pi(x)$ and $b_{yx} \leqslant \pi(y)$ for each $x \neq y$, Combining the two conditions, we observe that $b_{xy} = b_{yx} \leqslant \min\{\pi(x), \pi(y)\}$ and the result follows by dividing both sides by $\pi(x)$. □

Remark 8. Recall that the invariant distribution of symmetric base chain is a uniform distribution, and the speed of the mixing for this base chain to a Markov chain with invariant distribution π depends on the acceptance probability. Larger the acceptance probability, the faster is the mixing time.

Definition 4.5 (Metropolis Hastings). Consider a time homogeneous Markov chain Y with symmetric transition probability matrix $\Psi \in \mathcal{M}(\mathcal{X})^{\mathcal{X}}$, and acceptance probability defined for each $x, y \in \mathcal{X}$ as

$$a_{xy} \triangleq 1 \wedge \left(\frac{\pi(y)}{\pi(x)}\right).$$

This choice of acceptance probability is called *Metropolis Hastings*, and the resulting Markov chain is called *Metropolis chain* with invariant distribution $\pi \in \mathcal{M}(\mathcal{X})$ and transition probability matrix $P \in \mathcal{M}(\mathcal{X})$

$$p_{xy} \triangleq \begin{cases} \psi_{xy}\left[1 \wedge \frac{\pi(y)}{\pi(x)}\right], & y \neq x, \\ 1 - \sum_{z \in \mathcal{X}\setminus\{x\}} \psi_{xz}\left[1 \wedge \frac{\pi(z)}{\pi(x)}\right], & y = x. \end{cases}$$

Remark 9. If the desired stationary distribution π is a Boltzmann distribution μ_β, then the Metropolis Hastings acceptance probability is

$$a_{xy} = 1 \wedge e^{-\beta(E(y)-E(x))}.$$

this method has an advantage that we don't need to compute partition function explicitly which is computationally infeasible in many cases.

Example 4.6 (Metropolis algorithm for N-particle system). Consider a system of N Ising spins $\sigma \in \{-1,1\}^N$ with energy function $E(\sigma)$ and inverse temperature β. We call $\sigma^{(i)}$ the configuration which coincides with σ but for the site i, i.e. $\sigma^{(i)} \triangleq \sum_{j \in [N]\setminus\{i\}} \sigma_j e_j - \sigma_i e_i$ where $e_j \in \{0,1\}^N$ is a unit vector in the jth direction. We define the difference in energy for this perturbed configuration as $\Delta E_i(\sigma) \triangleq E(\sigma^{(i)}) - E(\sigma)$.

We are interested in sampling from the Boltzmann distribution $\mu_\beta = \frac{1}{Z(N,\beta)} e^{-\beta E(\sigma)}$. The *Metropolis algorithm* with random updating is defined as follows. At each step $n \in \mathbb{Z}_+$, an *i.i.d.* random integer $I_n : \Omega \to [N]$ is chosen uniformly at random and if $I_n = i$ then the spin σ_i is flipped with probability

$$w_i(\sigma) \triangleq 1 \wedge \frac{\mu_\beta(\sigma^{(i)})}{\mu_\beta(\sigma)} = e^0 \wedge e^{-\beta \Delta E_i(\sigma)} = e^{-\beta(\Delta E_i(\sigma) \vee 0)}.$$

We observe that this corresponds to a symmetric base chain with transition probability $\psi_{\sigma,\tau} = \sum_{i=1}^N \frac{1}{N} \mathbb{1}_{\{\tau = \sigma^{(i)}\}}$ and acceptance probability $a_{\sigma,\tau} = \sum_{i=1}^N w_i(\sigma) \mathbb{1}_{\{\tau=\sigma^{(i)}\}}$. Therefore, we can write the transition probability matrix $P \in \mathcal{M}(\mathcal{X})^{\mathcal{X}}$ associated with the resulting MCMC for each $\sigma, \tau \in \mathcal{X}$, as

$$p_{\sigma,\tau} = \begin{cases} \frac{1}{N} w_i(\sigma), & \tau = \sigma^{(i)}, i \in [N], \\ 1 - \frac{1}{N}\sum_{i=1}^N w_i(\sigma), & \tau = \sigma, \\ 0, & \text{else.} \end{cases}$$

Consider the detailed balance equation with respect to Boltzmann distribution μ_β and for states σ and $\sigma^{(i)}$, as

$$\mu_\beta(\sigma) w_i(\sigma) = \mu_\beta(\sigma) \wedge \mu_\beta(\sigma^{(i)}) = \mu_\beta(\sigma^{(i)}) w_i(\sigma^{(i)}).$$

Thus the chain is irreducible and reversible.

4.2 General base chain

The Metropolis chain can also be defined when the initial transition matrix is not symmetric. For a general irreducible transition matrix $\Psi \in \mathcal{M}(\mathcal{X})^{\mathcal{X}}$ and an arbitrary probability distribution $\pi \in \mathcal{M}(\mathcal{X})$ for $\mathcal{X} \triangleq \mathcal{Z}^N$, the Metropolized chain is executed as follows when at any state $x \in \mathcal{X}$. We first sample the next state y from ψ_x. Chain can move to y with acceptance probability

$$a_{xy} \triangleq \frac{\pi(y)\psi_{yx}}{\pi(x)\psi_{xy}} \wedge 1, \tag{2}$$

or remain at x with the complementary probability. The transition matrix $P \in \mathcal{M}(\mathcal{X})^{\mathcal{X}}$ for this resulting chain is defined for each state $x, y \in \mathcal{X}$ as

$$p_{xy} \triangleq \begin{cases} \psi_{xy}\left[1 \wedge \frac{\pi(y)\psi_{yx}}{\pi(x)\psi_{xy}}\right], & y \neq x, \\ 1 - \sum_{z \in \mathcal{X}\setminus\{x\}} \psi_{xz}\left[1 \wedge \frac{\pi(z)\psi_{zx}}{\pi(x)\psi_{xz}}\right], & y = x. \end{cases}$$

Proposition 4.7. *For an irreducible base chain $Y : \Omega \to \mathcal{X}^{\mathbb{Z}_+}$ with transition probability matrix $\Psi \in \mathcal{M}(\mathcal{X})^{\mathcal{X}}$ and acceptance probability matrix $A \in [0,1]^{\mathcal{X}\times\mathcal{X}}$ defined in* (2)*, the resulting Markov chain $X : \Omega \to \mathcal{X}^{\mathbb{Z}_+}$ is irreducible, reversible, positive recurrent, and has invariant distribution π.*

Proof. The transition probabilities of the new chain X for states $x, y \in \mathcal{X}$, are

$$p_{xy} = \begin{cases} \psi_{xy} a_{xy}, & y \neq x, \\ 1 - \sum_{z \in \mathcal{X}\setminus\{x\}} \psi_{x,z} a_{x,z}, & y = x. \end{cases}$$

We observe that the reversibility condition $\pi(x)p_{xy} = \pi(y)p_{yx}$ holds for all $x \neq y$, and hence it follows that the transition matrix P is irreducible and has invariant distribution π. □

5 Glauber dynamics

Definition 5.1 (Glauber dynamics). Consider and interacting particle system $\mathcal{X} \triangleq \mathcal{Z}^N$, and for each $i \in [N]$ and state $x \in \mathcal{X}$ we define the set of states differing with x only in the state of ith particle as

$$\Omega(x, i) \triangleq \left\{ y \in \mathcal{X} : x_j = y_j, j \neq i \right\}.$$

Define an *i.i.d.* uniform random sequence $I : \Omega \to [N]^{\mathbb{Z}_+}$, and a Markov chain $X : \Omega \to \mathcal{X}^{\mathbb{Z}_+}$ that evolves as follows. At each time $n \in \mathbb{Z}_+$, let $X_n = x$ and $I_n = i$, then move from the current state x to the new state y according to $\pi^{x,i}(y)$ defined as

$$\pi^{x,i}(y) \triangleq \begin{cases} \frac{\pi(y)}{\pi(\Omega(x,i))}, & y \in \Omega(x,i), \\ 0, & y \notin \Omega(x,i). \end{cases}$$

Proposition 5.2. *The Markov chain $X : \Omega \to \mathcal{X}^{\mathbb{Z}_+}$ under Glauber dynamics of Definition 5.1 is irreducible, reversible, and positive recurrent with the invariant distribution $\pi \in \mathcal{M}(\mathcal{X})$.*

Proof. Consider a symmetric base chain $Y : \Omega \to \mathcal{X}^{\mathcal{Z}_+}$ with associated symmetric transition probability matrix $\Psi \in \mathcal{M}(\mathcal{X})^{\mathcal{X}}$ defined as $\psi_{xy} \triangleq \sum_{i=1}^N \sum_{z\in\mathcal{Z}} \frac{1}{N} \mathbb{1}_{\{y \in \Omega(x,i)\}}$. Consider a Metropolis Hastings algorithm with the acceptance probability

$$a_{xy} \triangleq \pi^{x,i}(y).$$

We next observe that for any $y \in \Omega(x,i)$, we have $x \in \Omega(y,i)$. Thus, we have $\Omega(x,i) = \Omega(y,i)$ for all $y \in \Omega(x,i)$. It follows that $\psi_{yx} = \sum_{i=1}^N \frac{1}{N} \mathbb{1}_{\{x \in \Omega(y,i)\}} = \sum_{i=1}^N \frac{1}{N} \mathbb{1}_{\{y \in \Omega(x,i)\}} = \psi_{yx}$ for all x, y, and hence Ψ is a symmetric transition matrix. Further, we have for each $y \neq x$

$$\pi(x)a_{xy} = \pi(y)a_{yx} = \frac{\pi(x)\pi(y)}{\pi(\Omega(x,i))} \mathbb{1}_{\{y \in \Omega(x,i)\}}.$$

That is, this choice of acceptance probability satisfies the condition (1) and hence the resulting Markov chain X is reversible with invariant distribution π from Proposition 4.3. □

Example 5.3 (Glauber dynamics for N-particle system). Consider a system of N Ising spins $\sigma \in \mathcal{X} \triangleq \{-1,1\}^N$ with energy function $E(\sigma)$ and inverse temperature β. Let $\sigma^{(i)}$ the configuration which coincides with σ but for the site i, and the difference in energy for this perturbed configuration be $\Delta E_i(\sigma) \triangleq E(\sigma^{(i)}) - E(\sigma)$. For this system $\Omega(\sigma,i) = \left\{\sigma,\sigma^{(i)}\right\}$. For the desired invariant distribution being Boltzmann distribution μ_β at inverse temperature β, we have

$$w_i(\sigma) \triangleq \pi^{\sigma,i}(\sigma^{(i)}) = \frac{\mu_\beta(\sigma^{(i)})}{\mu_\beta(\sigma^{(i)}) + \mu_\beta(\sigma)} = \frac{e^{-\beta E(\sigma^{(i)})}}{e^{-\beta E(\sigma^{(i)})} + e^{-\beta E(\sigma)}} = \frac{1}{1+e^{\beta \Delta E_i(\sigma)}} = \frac{1}{2}\left[1 - \frac{e^{\beta\Delta E_i(\sigma)} - 1}{e^{\beta\Delta E_i(\sigma)} + 1}\right]$$
$$= \frac{1}{2}\left[1 - \tanh\left(\frac{\beta \Delta E_i(\sigma)}{2}\right)\right].$$

For the resulting Markov chain X, we can write transition probability matrix $P \in \mathcal{M}(\mathcal{X})^{\mathcal{X}}$ for each $\sigma,\tau \in \mathcal{X}$ as

$$p_{\sigma,\tau} \triangleq \sum_{i=1}^N \frac{1}{N} w_i(\sigma) \mathbb{1}_{\left\{\tau = \sigma^{(i)}\right\}} + \Big(1 - \frac{1}{N}\sum_{i=1}^N w_i(\sigma)\Big)\mathbb{1}_{\{\tau=\sigma\}}.$$

Consider the detailed balance equation with respect to invariant Boltzmann distribution μ_β as

$$\mu_\beta(\sigma) w_i(\sigma) = \frac{\mu_\beta(\sigma)\mu_\beta(\sigma^{(i)})}{\mu_\beta(\sigma^{(i)}) + \mu_\beta(\sigma)} = \mu_\beta(\sigma^{(i)}) w_i(\sigma^{(i)})$$

Thus the chain is irreducible and reversible.

5.1 Graph coloring

Definition 5.4. Given a finite set $\mathcal{X} \triangleq \mathcal{Z}^V$ where V is the vertex set of a graph $G = (V,E)$ and $\mathcal{Z}$ is a finite set, we would like to find a transition probability matrix $P \in \mathcal{M}(\mathcal{X})^{\mathcal{X}}$ for which π is an invariant distribution on $\mathcal{M}(\mathcal{X})$. The elements of $\mathcal{X}$ called *configurations* are mappings from V to $\mathcal{Z}$ which can be visualized as labeling of vertices using elements of $\mathcal{X}$.

Remark 10. Given a configuration space $\mathcal{X} \triangleq \mathcal{Z}^V$ for a graph $G = (V,E)$, recall that we can define *Glauber dynamics* or *Gibbs sampler* to be a reversible Markov chain with invariant distribution $\pi \in \mathcal{M}(\mathcal{X})$ if we can define the set of possible transitions $\Omega(x,v)$ appropriately for each configuration x and vertex v. For the graph problems, we define $\Omega(x,v) \triangleq \{y \in \mathcal{X} : y_w = x_w, w \neq v\}$.

Example 5.5 (Graph coloring). Given an undirected graph $G = (V,E)$ and a set of colors $[q] \triangleq \{1,2,\dots,q\}$, a proper q-coloring of G is an assignment of colors to the vertices V such that neighboring vertices do not receive the same color. That is, we define the set of colorings $\mathcal{X} \triangleq [q]^V$, and the set of proper q-colorings as

$$\mathcal{A} \triangleq \{x \in \mathcal{X} : x_v \neq x_w, \{v,w\} \in E\}.$$

Given a proper q-coloring $x \in \mathcal{A}$ the set of *allowable* colors at a vertex $v \in V$ is denoted by $\mathcal{Z}(x,v)$, where a color $j \in [q]$ is *allowable* at vertex v if $j \notin \{x_w : \{v,w\} \in E\}$. That is,

$$\mathcal{Z}(x,v) \triangleq [q] \setminus \cup_{w:\{v,w\}\in E} \{x_w\}.$$

We would like to construct a Markov chain on the set of proper q-coloring of G. Given a proper q-coloring x, a new coloring can be generated by
(a) selecting a vertex $v \in V$ randomly,

(b) selecting an allowable color $j \in \mathcal{Z}(x,v)$ uniformly at random, and
(c) applying the chosen color on v.

Lemma 5.6. *The resulting chain has uniform stationary distribution over all proper q-coloring.*

Proof. The transition probability matrix $P \in \mathcal{M}(\mathcal{A})^{\mathcal{A}}$ of moving from one configuration $x \in \mathcal{A}$ to another configuration $y \in \Omega(x,v)$ differing over the color of a single vertex v, as

$$p_{xy} = \frac{1}{|V|}\frac{1}{|\mathcal{Z}(x,v)|}\mathbb{1}_{\{y \in \Omega(x,v) \cap \mathcal{A}\}}.$$

Let $y \in \Omega(x,v) \cap \mathcal{A}$, then we notice that $x \in \Omega(y,v) \cap \mathcal{A}$ and $\mathcal{Z}(x,v) = \mathcal{Z}(y,v)$ since x and y differ only by the color on vertex v. Therefore, $p_{xy} = p_{yx}$. Substituting this in detailed balance equation, we get $\pi(x) = \pi(y)$, implying that the invariant distribution ofor this chain is uniform. $\square$

Example 5.7 (Hardcore configuration). A hardcore configuration is a placement of particles over a graph $G \triangleq (V,E)$ such that each vertex $v \in V$ is occupied by at most one particle and no two particles are stored on adjacent vertices. Let $\mathcal{Z} \triangleq \{0,1\}$ and $\mathcal{X} \triangleq \mathcal{Z}^V$, then the set of hardcore configurations are

$$\mathcal{A} \triangleq \{b \in \mathcal{X} : b(v)b(w) = 0, \{v,w\} \in E\}.$$

The set of *occupied* vertices are $V_1 \triangleq \{v \in V : b(v) = 1\}$ and set of *vacant* vertices are $V_0 \triangleq \{v \in V : b(v) = 0\}$. To construct a Markov chain $X : \Omega \to \mathcal{A}^{\mathbb{Z}_+}$ on hardcore configurations, we consider the following evolution. Let $X_0 = 0 \in \mathcal{A}$.
(a) A vertex v is chosen independently and uniformly at random.
(b) If any neighboring vertex is occupied, v is left vacant.
(c) Else, a particle is placed on v with probability $\frac{1}{2}$.
We observe that $\Omega(x,v) = \{y \in \mathcal{X} : y_w = x_w, w \neq v\}$ and for any $x \in \mathcal{A}$, the set of allowable transitions at vertex v are

$$\Omega(x,v) \cap \mathcal{A} = \{y \in \mathcal{A} : y_w = x_w, w \neq v\}.$$

By definition, we have $y \in \Omega(x,v) \cap \mathcal{A}$ if and only if $x \in \Omega(y,v) \cap \mathcal{A}$. This implies that $\Omega(x,v) \cap \mathcal{A} = \Omega(y,v) \cap \mathcal{A}$ for all $y \in \Omega(x,v) \cap \mathcal{A}$. It follows that the resulting Markov chain X is reversible and has a uniform distribution on hardcore configurations $\mathcal{A}$.

5.2 Knapsack problem

Definition 5.8 (Kanpsack problem). The $0-1$ knapsack problem is defined as follows. Consider N items with weights $w \in \mathbb{R}_+^N$ and values $v \in \mathbb{R}_+^N$ and a knapsack with weight limit W. The set of feasible assignments to the knapsack is $\mathcal{S} \triangleq \{S \subseteq [N] : \sum_{i \in S} w_i \leqslant W\}$. The goal is to find the most valuable subset of items which satisfy the weight constraint of the knapsack, i.e. find $S^* \triangleq \arg\max\{\sum_{i \in S} v_i : S \in \mathcal{S}\}$. Consider state space $\mathcal{Z} \triangleq \{0,1\}$ for each item to be assigned or not to the knapsack. Then for N items the aggregate state space is $\mathcal{X} \triangleq \mathcal{Z}^N$. We let $x \in \mathcal{X}$ be the indicator vector to each item being assigned to knapsack. The feasible set of vectors that satisfy the weight constraint, and the optimization problem are

$$\mathcal{A} \triangleq \left\{x \in \mathcal{X} : \sum_{i=1}^N w_i x_i \leqslant W\right\}, \qquad x^* \triangleq \arg\max\left\{\sum_{i=1}^N v_i x_i : x \in \mathcal{A}\right\}.$$

Remark 11. This problem has 2^N possible solutions for x, and so is combinatorially hard (exponentially many solutions).

Definition 5.9 (Glauber dynamics for knapsack problem). We define the set of possible next state to transition from a state $x \in \mathcal{X}$, as $\Omega(x,i) \triangleq \{y \in \mathcal{A} : y_j = x_j, j \neq i\}$. We observe that $\Omega(x,i) = \left\{x, x^{(i)}\right\}$ where $x_i^{(i)} = 1 - x_i$. Consider a Markov chain $X : \Omega \to \mathcal{X}^{\mathbb{Z}_+}$ with $X_0 = 0 \in \mathcal{X}$ that evolves as follows.

(a) At each time $n \in \mathbb{Z}_+$, choose an $I_n : \Omega \to [N]$ *i.i.d.* uniform.

(b) Let $X_n = x$ and $I_n = i$, then move from the current state x to the new state y according to probability $\pi^{x,i}(y)$ defined as
$$\pi^{x,i}(y) \triangleq \frac{\pi(y)}{\pi(\Omega(x,i))} \mathbb{1}_{\{y \in \Omega(x,i)\}}.$$

Lemma 5.10. *The Markov chain $X : \Omega \to \mathcal{A}^{\mathbb{Z}_+}$ has an invariant uniform distribution $\pi \in \mathcal{M}(\mathcal{A})$.*

Proof. The transition probability of moving from one configuration $x \in \mathcal{A}$ to another configuration $y \in \mathcal{A}$ differing over assignment of a single item i can be written as $p_{xy} \triangleq \frac{1}{N}\pi^{x,i}(y) = \frac{1}{N}\frac{1}{|A_i(x)|}$ where

$$A_i(x) \triangleq \left\{a \in \{0,1\} : \sum_{j \neq i} w_j x_j + w_i a \leqslant W\right\} = \{a \in \{0,1\} : x + (a - x_i)e_i \in \mathcal{A}\}.$$

is the set of allowable values of x_i given configuration x. Notice that $A_i(x)$ and $A_i(y)$ are the same as x and y differ only by the indicator for assignment of item i. Therefore, $p_{xy} = p_{yx}$ for all $x, y \in \mathcal{A}$. Substituting in detailed balance equation, we obtain $\pi(x) = \pi(y)$ for all $x, y \in \mathcal{A}$, implying that the stationary distribution over this chain is uniform. □

Definition 5.11 (Problem reformulation). For each state $x \in \mathcal{A}$, we define energy of this state as $E(x) \triangleq \sum_{i=1}^N v_i x_i$. An alternative goal could be to sample from a Markov chain $X : \Omega \to \mathcal{A}^{\mathbb{Z}_+}$ such that its invariant distribution is Boltzmann distribution $\mu_\beta \in \mathcal{M}(\mathcal{A})$ defined as $\mu_\beta(x) \triangleq \frac{1}{Z(\beta)}e^{-\beta E(x)}$ for each $x \in \mathcal{A}$, the partition function $Z(\beta) \triangleq \sum_{x \in \mathcal{A}} e^{-\beta E(x)}$, and β is the inverse temperature.

Definition 5.12 (Glauber dynamics). We define the set of possible next state to transition from a state $x \in \mathcal{A}$, as $\Omega(x,i) \triangleq \{y \in \mathcal{X} : y_j = x_j, j \neq i\}$. Defining $x^{(i)} \in \mathcal{X}$ such that $x_j^{(i)} = x_j$ for $j \neq i$ and $x_i^{(i)} = 1 - x_i$, we observe that
$$\Omega(x,i) \triangleq \left\{x, x^{(i)}\right\} \mathbb{1}_{\mathcal{A}}(x^{(i)}) + \{x\} \mathbb{1}_{\mathcal{A}}(x^{(i)}).$$
Consider a Markov chain $X : \Omega \to \mathcal{A}^{\mathbb{Z}_+}$ with $X_0 = 0 \in \mathcal{A}$ that evolves as follows.

(a) At each time $n \in \mathbb{Z}_+$, choose an $I_n : \Omega \to [N]$ *i.i.d.* uniform.

(b) Let $X_n = x$ and $I_n = i$, then move from the current state x to the new state y according to probability $\pi^{x,i}(y)$ defined as
$$\pi^{x,i}(y) \triangleq \frac{\pi(y)}{\pi(\Omega(x,i))} \mathbb{1}_{\{y \in \Omega(x,i)\}}.$$

Remark 12. We can define the energy difference

$$\Delta_i E(x) \triangleq E(x^{(i)}) - E(x) = v_i(1 - 2x_i).$$

For the desired invariant Boltzmann distribution $\pi = \mu_\beta \in \mathcal{M}(\mathcal{A})$, the transition probabilities are

$$\pi^{x,i}(y) = \frac{\mu_\beta(y)}{\mu_\beta(\Omega(x,i))} \mathbb{1}_{\{y \in \Omega(x,i)\}} = \frac{e^{-\beta \sum_{i=1}^N v_i y_i}}{\sum_{z \in \Omega(x,i)} e^{-\beta \sum_{i=1}^N v_i z_i}} \mathbb{1}_{\{\sigma \in \Omega(\rho,i)\}} = \begin{cases} \frac{1}{1+e^{\beta \Delta_i E(x)}}, & y = x^{(i)} \in \mathcal{A}, \\ \frac{1}{1+e^{-\beta \Delta_i E(x)}}, & y = x, x^{(i)} \in \mathcal{A}, \\ 1, & y = x, x^{(i)} \notin \mathcal{A}. \end{cases}$$

From Proposition 5.2, it follows that $X : \Omega \to \mathcal{X}^{\mathbb{Z}_+}$ is a time homogeneous irreducible, aperiodic, and positive recurrent Markov chain which is reversible at stationarity with invariant Boltzmann distribution $\mu_\beta \in \mathcal{M}(\mathcal{X})$.

5.3 Travelling Salesman Problem (TSP)

Definition 5.13 (Travelling Salesman Problem). Consider a totally connected graph $G = ([N], E, d)$ with N number of nodes, and set of edges $E = [N] \times [N]$ and distance function $d : E \to \mathbb{R}_+$ defined for each pair $(v, w) \in E$. We define the set of permutations $\mathcal{X} \triangleq \left\{\rho \in [N]^{[N]} : \rho \text{ is a bijection}\right\}$ such that $((\rho_1, \rho_2), \dots, (\rho_N, \rho_1))$ is a cycle and $E(\rho) \triangleq \sum_{i=1}^{N} d(\rho_i, \rho_{i+1}) + d(\rho_N, \rho_1)$ is the minimum among all permutations.

Definition 5.14 (Problem reformulation). We observe that the state space of all permutations is denoted by $\mathcal{X} \triangleq \left\{\rho \in [N]^{[N]} : \rho \text{ bijection } \right\}$. For each state $\rho \in \mathcal{X}$, we define energy of this state as

$$E(\rho) \triangleq \sum_{i=1}^{N-1} d(\rho_i, \rho_{i+1}) + d(\rho_N, \rho_1).$$

An alternative goal could be to sample from a Markov chain $X : \Omega \to \mathcal{X}^{\mathbb{Z}_+}$ such that its invariant distribution is Boltzmann distribution $\mu_\beta \in \mathcal{M}(\mathcal{X})$ defined as $\mu_\beta(\rho) \triangleq \frac{1}{Z(\beta)} e^{-\beta E(\rho)}$ where partition function $Z(\beta) \triangleq \sum_{\rho \in \mathcal{X}} e^{-\beta E(\rho)}$ and β is the inverse temperature.

Definition 5.15. We can define Glauber dynamics for this system as follows. We define $N + 1 = 1$ and for each $i \in [N]$ and state $\rho \in \mathcal{X}$ we define the set of permutations differing with ρ only at locations in $\{i, i+1\}$ as

$$\Omega(\rho, i) \triangleq \left\{\sigma \in \mathcal{X} : \sigma_j = \rho_j, j \notin \{i, i+1\}\right\}.$$

Define an *i.i.d.* uniform random sequence $I : \Omega \to [N]^{\mathbb{Z}_+}$, and a Markov chain $X : \Omega \to \mathcal{X}^{\mathbb{Z}_+}$ that evolves as follows. At each time $n \in \mathbb{Z}_+$, let $X_n = \rho$ and $I_n = i$, then move from the current permutation ρ to the new permutation σ according to $\pi^{\rho,i}(\sigma)$ defined as

$$\pi^{\rho,i}(\sigma) \triangleq \frac{\pi(\sigma)}{\pi(\Omega(\rho, i))} \mathbb{1}_{\{\sigma \in \Omega(\rho, i)\}}.$$

Remark 13. We observe that $\Omega(\rho, i) = \{\rho, (\rho_1, \dots, \rho_{i+1}, \rho_i, \dots, \rho_N)\}$. We define the energy difference

$$\Delta_i E(\rho) \triangleq d(\rho_{i-1}, \rho_{i+1}) - d(\rho_{i-1}, \rho_i) + d(\rho_{i+1}, \rho_i) - d(\rho_i, \rho_{i+1}) + d(\rho_i, \rho_{i+2}) - d(\rho_{i+1}, \rho_{i+2}).$$

For the desired invariant Boltzmann distribution $\pi = \mu_\beta \in \mathcal{M}(\mathcal{A})$, the transition probabilities are

$$\pi^{\rho,i}(\sigma) = \frac{\mu_\beta(\sigma)}{\mu_\beta(\Omega(\rho, i))} \mathbb{1}_{\{\sigma \in \Omega(\rho, i)\}} = \frac{e^{-\beta \sum_{i=1}^{N} d(\sigma_i, \sigma_{i+1})}}{\sum_{\sigma \in \Omega(\rho, i)} e^{-\beta \sum_{i=1}^{N} d(\sigma_i, \sigma_{i+1})}} \mathbb{1}_{\{\sigma \in \Omega(\rho, i)\}} = \begin{cases} \frac{1}{1 + e^{-\beta \Delta_i E(\rho)}}, & \sigma = \rho, \\ \frac{1}{1 + e^{\beta \Delta_i E(\rho)}}, & \sigma \in \Omega(\rho, i) \setminus \{\rho\}. \end{cases}$$

From Proposition 5.2, it follows that $X : \Omega \to \mathcal{X}^{\mathbb{Z}_+}$ is a time homogeneous irreducible, aperiodic, and positive recurrent Markov chain which is reversible at stationarity with invariant Boltzmann distribution $\mu_\beta \in \mathcal{M}(\mathcal{X})$.