ADVANCED STOCHASTIC PROCESSES - 9° LECTURE

Monte Carlo Markov Chains (MCMC)

The construction is basically divided in two steps: proposal (irreducibility) and acceptance (reversibility w.r.t π).

1° STEP: Consider an arbitrary irreducible transition matrix Q, s.t. $q_{x,y} > 0 \iff q_{y,x} > 0$. If $X_n = x$, with probability $q_{x,y}$ we propose the transition to y. PROPOSAL

2° STEP: We accept the transition with prob. $\alpha(x,y) \in (0,1)$, so that

$$P_{x,y} = \mathbb{P}(X_{n+1}=y \mid X_n = x) = \begin{cases} q_{xy} \cdot \alpha(x,y) & \text{if } x \neq y \\ 1 - \sum_{z \neq x} P_{x,z} & \text{if } x = y \end{cases}$$

(ACCEPTANCE)

We only have to find $\alpha(x,y)$ to obtain reversibility w.r.t π, which is the following:

$$\forall x \neq y \text{ s.t. } q_{x,y} \neq 0 : \quad \boxed{\pi(x)\alpha(x,y)q_{x,y} = \pi(y)\alpha(y,x)q_{y,x}}$$

otherwise, trivial identity

$\pi(x) = \not{c} \cdot h(x)$, $\pi(y) = \not{c}\, h(y)$

$$\Longrightarrow \quad \alpha(x,y) = \frac{\pi(y)\, q_{y,x}}{\pi(x)\, q_{x,y}} \cdot \alpha(y,x) = \frac{h(y)\, q_{y,x}}{h(x)\, q_{x,y}}\, \alpha(y,x) \quad (b)$$

Example: The hard-core model

- Consider a finite graph $G = (V,E)$ with $V = \{1,2,\dots,N\}$
- At each vertex $i \in V$ is associated a value $x_i \in \{0,1\}$ that tell us if the vertex is free ($x_i = 0$) or occupied ($x_i = 1$)
- The whole configuration of particles on G is described by $x = (x_i)_{i \in V} \in \{0,1\}^V =: S$

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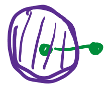
- The allowed (or feasible) configurations are a subset $F \subset S$: $F = \{x \in S : x_i \cdot x_j = 0 \ \forall\, i \sim j\}$
  where $i \sim j$ means that $(i,j) \in E$.
  Equivalently $x \in F$ if particles are not in neighboring vertices (hard constraint : )
- Let $\pi \in \mathcal{P}(S)$ s.t. $\pi(x) = \frac{1}{|F|} \mathbb{1}_F(x)$

Goal: Approximate π by constructing a MC (on F) which is irreducible and reversible w.r.t. π.

Construction:

1. Start with $x \in F$ (for example, the empty configuration)
   ↳ $X_0 \sim \delta_x$ (e.g. $x = \underline{0} = (0, \dots, 0)$)
2. Given $X_n = x \in F$, we construct X_{n+1} in two steps:
   i. Choose a vertex $i \in V$ uniformly at random (with prob. $\frac{1}{N}$) and propose to update $X_n(i)$ (update only at site i).
   ii. * if $x_j = 0 \ \forall\, j \sim i$, then set $X_{n+1}(i) = \begin{cases} 1 - x_i & \text{with prob } \frac{1}{2} \\ x_i & \text{with prob } \frac{1}{2} \end{cases}$
   (and $X_{n+1}(j) = x_j \ \forall\, j \neq i$)
   * if $x_j = 1$ for some $j \sim i$, then set $X_{n+1} = X_n = x$.

In conclusion, $P_{x,y} = \begin{cases} 0 & \text{if } d(x,y) = \#\{i : x_i \neq y_i\} \geq 2 \text{ or if } y \notin F \\ \frac{1}{2N} & \text{if } d(x,y) = 1 \text{ and } y \in F \\ 1 - \sum_{z \neq x} P_{x,z} & \text{if } y = x \end{cases}$

The described MC is irreducible (check!) and reversible w.r.t. π.

Indeed $\pi(x) P \ ? \ \pi(y) P$

The described MC is irreducible (check!) and reversible w.r.t. π.

Indeed: $\pi(x) P_{x,y} \overset{?}{=} \pi(y) P_{y,x}$

if $d(x,y) \geq 2$ $\quad 0 = 0$

if $d(x,y) = 1$ $\quad \frac{1}{|F|} \mathbb{1}_F(x) \cdot \frac{1}{2|V|} \mathbb{1}_F(y) = \frac{1}{F} \mathbb{1}_F(y) \cdot \frac{1}{2|V|} \mathbb{1}_F(x)$ ✓

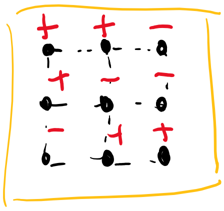
There are many solution to (b). For example:

Hastings - Metropolis algorithm $\longrightarrow \alpha(x,y) = \min\left\{1, \frac{h(y) q_{y,x}}{h(x) q_{x,y}}\right\}$

↓

Example: Ising model on a lattice $\Lambda = \{0, \dots, N-1\}^d$

↳ ferromagnetism in cristals



$\Lambda \subset \mathbb{Z}^2$

$|\Lambda| = N^d$

General assumptions:
- The sites of Λ are where atoms are placed
- each atom has a magnetic spin $x(i) \in \{+1, -1\}$, $\forall i \in \Lambda$
- neighboring atoms in Λ interact

  $i = (i_1, \dots, i_d)$ and $j = (j_1, \dots, j_d)$ are neighbors if $\sum_{\ell=1}^{d} |i_\ell - j_\ell| = 1$. Then write $i \sim j$

Let $S = \{+1, -1\}^{|\Lambda|}$ (so that $|S| = 2^{N^d}$) $\longrightarrow$ compare with voter model

The Ising probability measure on Λ on S is defined by the density

Gibbs probability measure $\rightarrow$ $\pi(x) = \frac{e^{-\beta H(x)}}{Z_\beta}$, where $\beta > 0$ is a fixed parameter (inverse temperature)

$H(x) = -\sum_{i \in \Lambda} \sum_{j \sim j} x(i) x(j)$ (energy of the state x)

and $Z_\beta = \sum_{x \in S} e^{-\beta H(x)}$ (normalization costant, called partition function)

While is difficult to get the precise value of Z_β, following the

While is difficult to get the precise value of τ_p, following the Metropolis procedure it is easy to construct an ergodic MC to sample from π: * Let $q_{xy} = \begin{cases} \frac{1}{|\Lambda|} & \text{if } \sum_{i \in \Lambda} |x(i) - y(i)| = 1 \\ 0 & \text{otherwise} \end{cases}$, $\forall x, y \in S$

Exercise

Determine $\alpha(x,y)$ to get a reversible measure w.r.t. π.