Stochastic Modeling 14, 20.10.09

Note Title 20.10.2009

Burn-in period for MCMC methods

$$\frac{1}{n}\sum_{j=\cancel{1}\ 1000}^{n+1000} F(f_j) \xrightarrow[n\to\infty]{} \mathbb{E}_S F$$

a.s.

in practice

Theorem Let $(f_i)_{i=0}^{\infty}$ be a homogeneous Markov chain with $X = \{0,..,K\}$ and $T = (p_{k\ell})_{k,\ell=0}^{K}$ and assume

$$\varepsilon = \min_{k,\ell} p_{k\ell} > 0.$$

If $(s_0, \dots, s_K)$ is the unique stationary distribution, $T^n = (p_{ke}^{(n)})$, then

$$|p_{ke}^{(n+1)} - s_e| \le (1-\varepsilon)^n \sup_{k,e} p_{ke}.$$

Proof

$$M_e^{(n+1)} - m_e^{(n+1)} \le (1-\varepsilon)^n (M_e^{(1)} - m_e^{(1)})$$

max $= M_e^{(n)}$

$T^n = \Big(\quad e \quad \Big)$

min $= m_e^{(n)}$

$$m_e^{(n)} \le s_e \le M_e^{(n)} \quad \forall n$$

$$m_e^{(n+1)} \le p_{ke}^{(n+1)} \le M_e^{(n+1)}$$

$$\Rightarrow \quad |p_{ke}^{(n+1)} - s_e| \le M_e^{(n+1)} - m_e^{(n+1)}$$

$$\le (1-\varepsilon)^n (M_e^{(1)} - m_e^{(1)})$$

$$\le (1-\varepsilon)^n M_e^{(1)}$$

$$\leq (1-\varepsilon)^n \max_{k,\ell} p_{k\ell} .$$

$\square$

The hard-core model

$X = \{$ feasible configuration $\}$

10×10 Lattice $\Rightarrow \# X \geq 2^{50} \approx 1{,}1 \times 10^{15}$

Assume $\underset{= X_0}{f_0} \in X$ = we start with

one feasible configuration

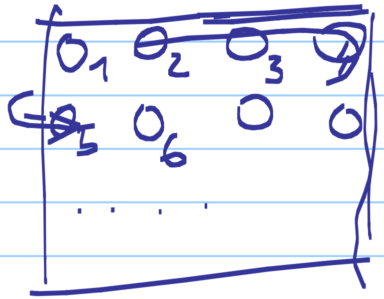
algorithm:

1. pick a vertex at random

2. toss a fair coin

3. $$X_{n+1}(v) = \begin{cases} \text{'black'} & \text{if coin = "heads" and all direct neighbors of } v \text{ are white} \\ \text{'white'} & \text{otherwise} \end{cases}$$

4. $$X_{n+1}(w) = X_n(w) \quad \forall w \neq v$$



Metropolis algorithm

1953 Metropolis et al.

$X = \{0, \dots, K\}$

$s = (s_0, \dots, s_K)$ a distribution on X

with $s_\ell > 0$

How to construct an ergodic Markov chain with state space X and stationary distribution s?

We choose an auxiliary matrix

$$\tilde{T} = (q_{k,\ell})_{k,\ell=0}^{K}$$

a transition matrix, symmetric:

$$q_{k\ell} = q_{\ell k} \quad \forall \ell, k$$

and $\quad q_{k,\ell} > 0 \quad \forall k, \ell$

$\boxed{\text{Step } n \to \text{Step } n+1}$

$f_n(\omega) = \xi_n \in X$

generate η according to the distribution

$$(q_{\xi_n,\ell})_{\ell=0}^{K}$$

i.e. $\mathbb{P}(\eta = \ell) = q_{\xi_n, \ell} \qquad \ell = 0, \dots, K$

$$r = \frac{s_\eta}{s_{\xi_n}}$$

$$\xi_{n+1} = \begin{cases} \eta & \text{if } r \geq 1 \\ \eta & \text{with probability } r, \text{ if } r \in (0,1) \\ \xi_n & \text{with} \text{ ---''} \ 1-r, \text{ if } r \in (0,1) \end{cases}$$

$$f_n(\omega) = \xi_n$$

Theorem

$(f_i)_{i=0}^{\infty}$ is an ergodic Markov chain with stationary distribution $s = (s_0, \dots, s_K)$.

Proof Assume that
$0 < s_0 \leq s_1 \leq \dots \leq s_K$.

and $\xi_n = e$ and $T = (p_{ek})$

$$p_{ek} = \begin{cases} q_{ek} & \text{if } s_k \geq s_e \Leftarrow \text{if } k > e \\ \frac{s_k}{s_e} q_{ek} & \text{if } s_k < s_e \Leftrightarrow \text{if } k < e \end{cases}$$

$$p_{ee} = q_{ee} + \left(1 - \frac{s_0}{s_e}\right) q_{e0} + \dots + \left(1 - \frac{s_{e-1}}{s_e}\right) q_{e,e-1}$$

T has only positive entries $\Rightarrow$

Markov chain is ergodic.

We have to check that

$$s \circ T = s$$

LHS =

$s_0 q_{0e} + \dots s_{e-1} q_{e-1,e} + s_e p_{ee}$

$$+ s_{\cancel{\ell}+1} \frac{s_\ell}{s_{\cancel{\ell}+1}} q_{\ell+1,\ell} + \cdots + \cancel{s_k} \frac{s_\ell}{s_{\cancel{k}}} q_{k,\ell} \overset{?}{=} s_\ell$$

$$\underbrace{\qquad\qquad\qquad\qquad}_{\text{symmetric } \tilde{T}}$$

$$= s_\ell \left[q_{\ell,\ell+1} + \cdots + q_{\ell,k} \right]$$

$$s_\ell p_{\ell\ell} = s_\ell \left[q_{\ell 0} + \cdots + q_{\ell\ell} \right] - \left[s_0 q_{\ell 0} + s_1 q_{\ell 1} + \cdots + s_{\ell-1} q_{\ell,\ell-1} \right]$$

$$\Rightarrow \text{LHS} = s_\ell \left[q_{\ell 0} + \cdots + q_{\ell\ell} \right] + s_\ell \left[q_{\ell,\ell+1} + \cdots + q_{\ell,k} \right]$$

$= s_\ell$ since $\tilde{T}$ is a transition matrix

$\square$

Application of the Metropolis algorithm

Assume we have an irreducible and homogeneous Markov chain $(f_i)_{i=0}^{\infty}$ with

- $X = \{0, \ldots, K\}$
- $s = \left(\frac{1}{K+1}, \ldots, \frac{1}{K+1}\right)$
- K is not known

Problem: estimate K

Define $F : X \to \mathbb{R}$ by

$$F = \mathbb{1}_{\{k_0\}} \qquad \text{where } k_0 \in X$$

Then

$$\frac{1}{n}\sum_{i=1}^{n} \mathbb{1}_{\{k_0\}}(f_i) \xrightarrow[n\to\infty]{} E_S \mathbb{1}_{\{k_0\}} \quad \text{a.s.}$$

$$\| $$

$$\sum_{k=0}^{K} \mathbb{1}_{\{k_0\}}(k)\, s_k$$

$$\| $$

$$s_{k_0} = \frac{1}{K+1}$$