Simmulation

Hindermann + Snell pp 53-61

- How do we generate a MRF X?

For a Markov Chain:

- generate in order using transition probability

- Does not work for MRF

Solution:

- Iteratively generate points and hope for steady state

Outline of approach

- Generate a Markov chain of images
- At each time m

$$p_{m+1}(y^{(m+1)}) = \sum_{y^{(m)}} p(y^{(m+1)} | y^{(m)}) \, p_m(y^{(m)})$$

- Assuming steady state

$$\lim_{m \to \infty} p_m(y) = p(y)$$

- $p(y)$ must be the solution to

$$p(y) = \sum_{y'} p(y | y') \, p(y')$$

Approach in book → Metropolis method
In class → Gibbs sampler (Geman + Geman)

1) Order the pixels from 1 to N
$s(0), \ldots, s(N-1)$

2) $$X_r^{(k+1)} = \begin{cases} X_r^{(k)} & \text{if } r \neq s(k \bmod N) \\ W_r & \text{if } r = s(k \bmod N) \end{cases}$$

Generate W with distribution
$$p(x_s \mid x_i \; i \neq s)$$

For Ising $= \dfrac{1}{1 + \exp\{-2\beta(V(x_s, x_{\partial s}) - 2)\}}$

$X^{(0)} \to X^{(1)} \to X^{(2)} \to \ldots$

Notice:
1) $X^{(k)}$ is a Markov Chain in k
2) $X^{(k)}$ is nonhomogeneous.

Define $Y^{(m)} = X^{(mN)}$ $N = \#$ of pixels

Then

1) $Y^{(m)}$ is a Markov Chain
   - Any subsample MC is a Markov Chain

2) $Y^{(m)}$ is homogeneous
   - Each update replaces all pixels

$$p(y^{(m+1)} | y^{(m)})$$

3) $Y^{(m)}$ is irreducible.

That means that $\forall y^{(m+1)}$ and $y^{(m)}$

$$p(y^{(m+1)} | y^{(m)}) > 0$$

We can get between any two states

$\boxed{\text{Lecture 17}}$

4) Must show that

$$p(y) = \sum_{y'} p(y|y')\, p(y')$$

where

$$p(y) = \frac{1}{Z} \exp\left\{ -\sum_{c \in \mathcal{C}} V_c(y) \right\}$$

$$= g(y)$$

Gibbs distribution

- It is enough to show that

$$g(y) = \sum_{y'} p_s(y|y')\, g(y')$$

where $p_s(y|y')$ is the replacement of a single pixel.

$$p_s(y|y') = g_s(y_s | y'_{\partial s})\, \delta(y_i - y'_i \;\; i \neq s)$$

$$g(y') = g_s(y'_s | y'_{\partial s})\, g(y'_i \;\; i \neq s)$$

$$g(y) = \sum_{y'} p_s(y|y')\, g(y')$$

$$= \sum_{y'_s} \sum_{y'_i\, i\neq s} g_s(y_s|y'_{\partial s})\, \delta(y_i - y'_i\ i\neq s)\, g_s(y'_s|y'_{\partial s}) \cdot g(y'_i\ i\neq s)$$

$$= \sum_{y'_s} g_s(y_s|y_{\partial s})\, g_s(y'_s|y_{\partial s})\, g(y_i\ i\neq s)$$

$$= g_s(y_s|y_{\partial s})\, g(y_i\ i\neq s)$$

$$= g(y)$$

Theorem: 1) + 2) + 3) + 4) ⇒ For any initial $y^{(0)}$

$$\lim_{m\to\infty} P_m(y) = g(y)$$

- From result of 4)

$$\lim_{k\to\infty} p_k(x) = g(x)$$

Metropolis Sampler

It may be difficult to generate a RV with distribution

$$X_s \sim p(x_s | X_{\partial s})$$

In this case, the Gibbs sampler is not practical.

Alternatively, we may use a Metropolis Sampler

Objective: Generate a random (field) X with distribution

$$p(x) = \frac{1}{z} e^{-u(x)}$$

Select a sampling function with two properties

1) $$q(x, x') = q(x', x)$$
which is the probability of selecting x' given an initial state x

so $$\sum_{x'} q(x, x') = 1$$

2) The MC generated by $q(x_n, x_{n+1})$ is irreducible i.e. all states may be reached

Metropolis algorithm

1) Randomly generate a new state x' given the current state x by using the distribution

$$q(x, x')$$

2) If $U(x') \leq U(x)$

set $x \leftarrow x'$

If $U(x') > U(x)$

compute $\alpha = \exp\{-(U(x') - U(x))\}$

set $x \leftarrow x'$ with probability α

set $x \leftarrow x$ with probability $1-\alpha$

3) Repeat process starting at step 1)

Theorem: The metropolis algorithm converges to a ergodic distribution of

$$\lim_{n\to\infty} p_n(x) = \frac{1}{2} e^{-u(x)}$$

proof:

1) MC is irreducible

2) MC is homogeneous

3) need to show that

$$\sum_i \pi_i P_{ij} = \pi_i$$

where

$$\pi_i = \frac{1}{2} e^{-u(x=i)}$$

$$P_{ij} = \underbrace{p(X_{n+1}=j \mid X_n=i)}_{\text{Metropolis algorithm.}}$$

- To do this, we will need the concept of a reversible MC

Definition: A MC is reversible iff

$$\begin{cases} p(X_n=i, X_{n+1}=j) = p(X_n=j, X_{n+1}=i) \\ \text{and it is stationary} \end{cases}$$

$$\Leftrightarrow \quad p(X_n=i)\, p(X_{n+1}=j \mid X_n=i)$$
$$= p(X_n=j)\, p(X_{n+1}=i \mid X_n=j)$$

$$\Leftrightarrow \quad \underbrace{\pi_i P_{ij} = \pi_j P_{ji}}_{\text{known as detailed Balance equations}}$$

$$\text{Reversible} \Leftrightarrow \left\{ \begin{array}{c} \text{stationary} \\ + \\ \pi_i P_{ij} = \pi_j P_{ji} \end{array} \right\}$$

Notice that

$$\pi_i P_{ij} = \pi_j P_{ji}$$

$$\Rightarrow \sum_i \pi_i P_{ij} = \pi_j \sum_i P_{ji} = \pi_j$$

$$\underbrace{\sum_i \pi_i P_{ij} = \pi_j}_{\text{Full balance equations}}$$

Conclusion: If we find a solution to the detailed balance equations, then π_i is an ergodic distribution for the MC.

Consider two states x and x'

Without loss of generallity assume $u(x) \geq u(x')$

Then the detailed balance equations are:

$$\underbrace{\tfrac{1}{Z} e^{-u(x)}}_{\pi_i} \underbrace{q(x,x') \cdot 1}_{P_{ij}} \stackrel{?}{=} \underbrace{\tfrac{1}{Z} e^{-u(x')}}_{\pi_j} \underbrace{q(x',x)\,\alpha}_{P_{ji}}$$

where $\alpha = e^{-(u(x)-u(x'))}$

so

$$e^{-u(x)} \stackrel{?}{=} e^{-u(x')} e^{-(u(x)-u(x'))}$$

$$e^{-u(x)} = e^{-u(x)}$$

yes! QED

Hastings - Metropolis Sampler

Can we use Metropolis algorithm when
$$q(x,x') \neq q(x',x) \; ?$$

Yes, if we choose an a acceptance probability of

$$\alpha(x,x') = \min\left\{1, \frac{\pi(x')\, q(x',x)}{\pi(x)\, q(x,x')}\right\}$$

Notice that $\alpha(x,x')$ compensates for bias in $q(x,x')$

Special Cases:

1) $q(x',x) = q(x,x')$

$$\alpha(x,x') = \min\left\{1, \frac{\pi(x')}{\pi(x)}\right\}$$

$$= \begin{cases} 1 & \text{if } \pi(x') \leq \pi(x) \\ \frac{\pi(x')}{\pi(x)} & \text{if } \pi(x') > \pi(x) \end{cases}$$

for $\pi(x) = \frac{1}{Z} e^{-u(x)}$

$$= \begin{cases} 1 & \text{if } u(x') \leq u(x) \\ e^{-(u(x')-u(x))} & \text{if } u(x') > u(x) \end{cases}$$

$\Rightarrow$ Metropolis sampler

2) $q(x, x') = p(x_s \mid x_{\partial s})\, \delta(x'_r - x_r \text{ for } r \neq s)$

$$\frac{q(x', x)}{q(x, x')} = \frac{p(x_s \mid x_{\partial s})}{p(x'_s \mid x_{\partial s})}$$

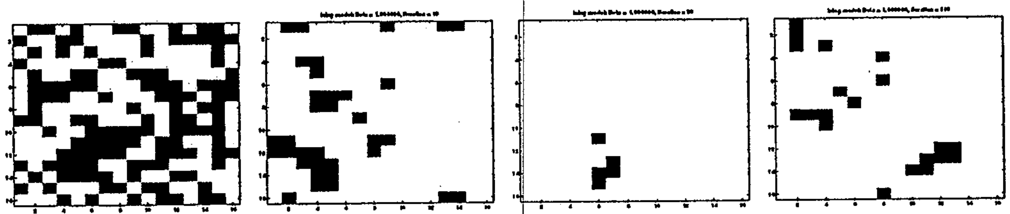
$$\frac{\pi(x')}{\pi(x)} = \frac{p(x'_s \mid x_{\partial s})}{p(x_s \mid x_{\partial s})}$$

$$\frac{\pi(x')\, q(x', x)}{\pi(x)\, q(x, x')} = 1 \Rightarrow \alpha(x, x') = 1$$

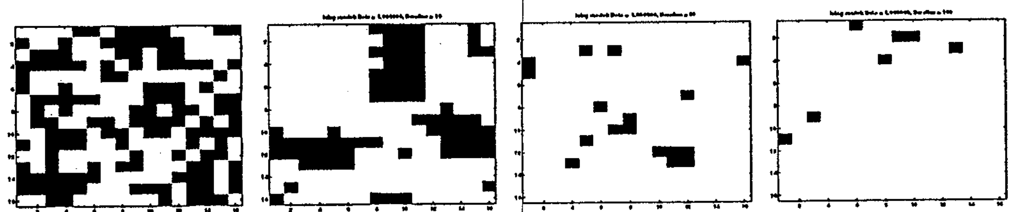
$\Rightarrow$ Gibbs sampler

Example Simulation for Ising Model($\beta = 1.0$)

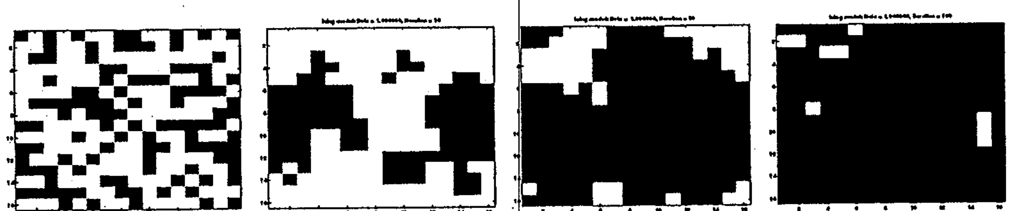
- Test 1



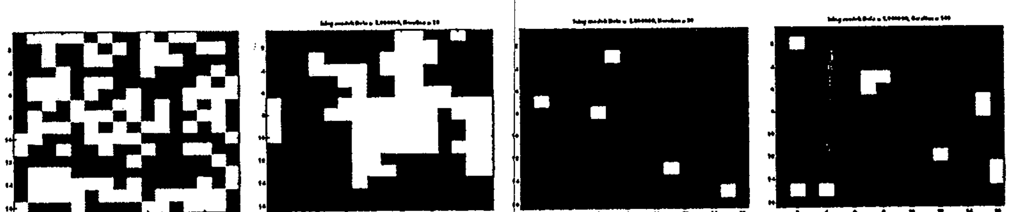
- Test 2



- Test 3



- Test 3



Critical Temperature Behavior

Markov Chains

- Steady State distribution does not depend on initial state

$$\lim_{K\to\infty} p_K(X^{(K)} \mid \underbrace{X^{(0)}}_{\text{initial state}}) = p(X^{(K)})$$

- Not true in 2-D!

Define $\mathcal{B} = \{ s \in S : s \text{ is on boundary} \}$

$$\lim_{\substack{N\to\infty \\ \text{of pixels}}} p(X_{(0,0)} \mid X_{\mathcal{B}}) \leftarrow \text{depends on } X_{\mathcal{B}}$$

Example Ising model

Let $X^{(N)}$ be a Ising MRF with pixels $X_{(s_1, s_2)}$ where $-N \le s_1, s_2 \le N$

$$\mathcal{B} = \{ s = (s_1, s_2) : |s_1| = N \text{ or } |s_2| = N \}$$

What is $p\{ X_{(0,0)} \mid X_{\mathcal{B}} = 1 \}$?

We might expect that

$$\lim_{N \to \infty} p\{ X_{(0,0)} = 1 \mid X_{\mathcal{B}} = 1 \} = \frac{1}{2}$$

ONLY true when $\beta < \beta_c$ = critical temperature $\cong .88$

For $\beta > \beta_c$

$$\lim_{N \to \infty} p\{ X_{(0,0)} = 1 \mid X_{\mathcal{B}} = 1 \} > 1/2$$

Intuition:

- Above the critical temperature the Ising model is

1) - Mostly 1 with spots of -1

2) Mostly -1 with spots of 1

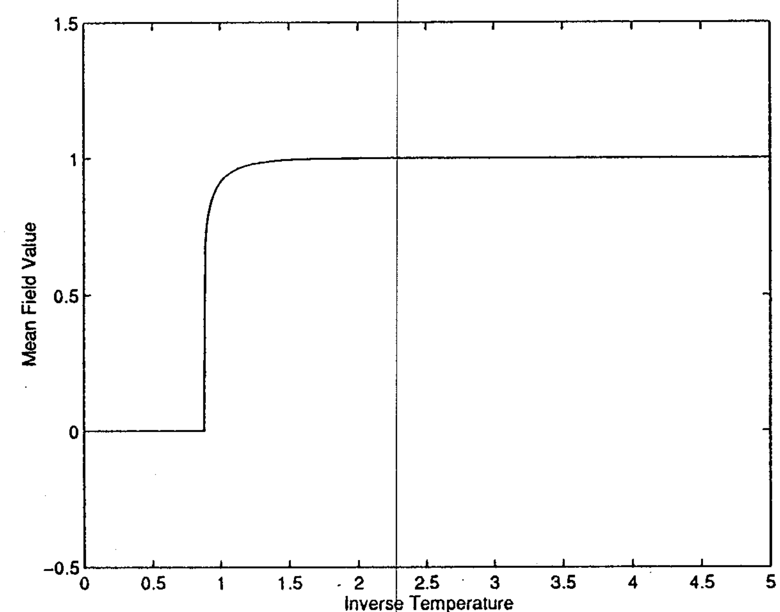
If $X_{\mathcal{B}} = 1 \Rightarrow 1) \Rightarrow P(X_{(0,0)} = 1) > \frac{1}{2}$

If $X_{\mathcal{B}} = -1 \Rightarrow 2) \Rightarrow P(X_{(0,0)} = 1) < \frac{1}{2}$

Critical Temperature Analysis[122]

- Amazingly, Onsager was able to compute

$$E[X_0|B=1] = \begin{cases} \left(1 - \frac{1}{(\sinh(\beta))^4}\right)^{1/8} & \text{if } \beta > \beta_c \\ 0 & \text{if } \beta < \beta_c \end{cases}$$



- Onsager also computed an analytic expression for $Z(T)$!