# Simulation

- Topics to be covered:
  - Gibbs sampler
  - Metropolis sampler
  - Hastings-Metropolis sampler

# Generating Samples from a Gibbs Distribution

- How do we generate a random variable $X$ with a Gibbs distribution?

$$p(x) = \frac{1}{Z} \exp\{-U(x)\}$$

- Generally, this problem is difficult.
- Markov Chains can be generated sequentially
- Non-causal structure of MRF's makes simulation difficult.

# Gibbs Sampler[4]

- Replace each point with a sample from its conditional distribution

$$p(x_s|x_i^k\ i \neq s) = p(x_s|x_{\partial s})$$

- Scan through all the points in the image.
- Advantage
  - Eliminates need for rejections $\Rightarrow$ faster convergence
- Disadvantage
  - Generating samples from $p(x_s|x_{\partial s})$ can be difficult.

# Gibbs Sampler Algorithm

**Gibbs Sampler Algorithm:**

1. Set $N = \#$ of pixels
2. Order the $N$ pixels as $N = s(0), \cdots, s(N-1)$
3. Repeat for $k = 0$ to $\infty$
   (a) Form $X^{(k+1)}$ from $X^{(k)}$ via

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

where $W \sim p\left(x_{s(k)} \middle| X_{\partial s(k)}^{(k)}\right)$

# The Metropolis Sampler[9, 8]

- How do we generate a sample from a Gibbs distribution?

$$p(x) = \frac{1}{Z} \exp\{-U(x)\}$$

- Start with the sample $x^k$, and generate a new sample $W$ with probability $q(w|x^k)$.

  **Note:** $q(w|x^k)$ must be symmetric.

$$q(w|x^k) = q(x^k|w)$$

- Compute $\Delta E(W) = U(W) - U(x^k)$, then do the following:

  If $\Delta E(W) < 0$

  – Accept: $X^{k+1} = W$

  If $\Delta E(W) \geq 0$

  – Accept: $X^{k+1} = W$ with probability $\exp\{-\Delta E(W)\}$
  – Reject: $X^{k+1} = x^k$ with probability $1 - \exp\{-\Delta E(W)\}$

# Ergodic Behavior of Metropolis Sampler

- The sequence of random fields, $X^k$, form a Markov chain.
- Let $p(x^{k+1}|x^k)$ be the transition probabilities of the Markov chain.
- Then $X^k$ is reversible

$$p(x^{k+1}|x^k)\exp\{-U(x^k)\} = \exp\{-U(x^{k+1})\}p(x^k|x^{k+1})$$

- Therefore, if the Markov chain is irreducible, then

$$\lim_{k\to\infty} P\{X^k = x\} = \frac{1}{Z}\exp\{-U(x)\}$$

- If every state can be reached, then as $k \to \infty$, $X^k$ will be a sample from the Gibbs distribution.

# Example Metropolis Sampler for Ising Model

| | | |
|---|---|---|
| | 0 | |
| 1 | $x_s$ | 0 |
| | 0 | |

- Assume $x_s^k = 0$.
- Generate a binary R.V., $W$, such that $P\{W = 0\} = 0.5$.

$$\begin{aligned}\Delta E(W) &= U(W) - U(x_s^k) \\ &= \begin{cases} 0 & \text{if } W = 0 \\ 2\beta & \text{if } W = 1 \end{cases}\end{aligned}$$

  If $\Delta E(W) < 0$

  – Accept $X_s^{k+1} = W$

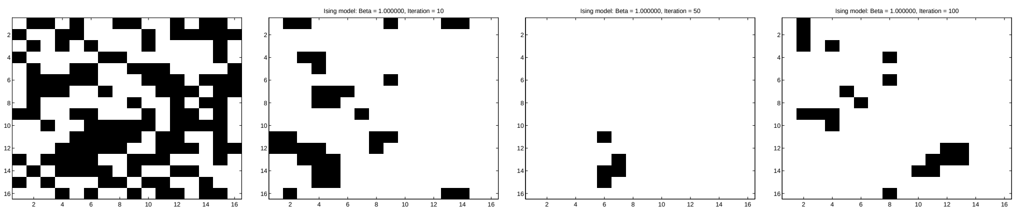
  If $\Delta E(W) \geq 0$

  – Accept: $X_s^{k+1} = W$ with probability $\exp\{-\Delta E(W)\}$
  – Reject: $X_s^{k+1} = x_s^k$ with probability $1 - \exp\{-\Delta E(W)\}$

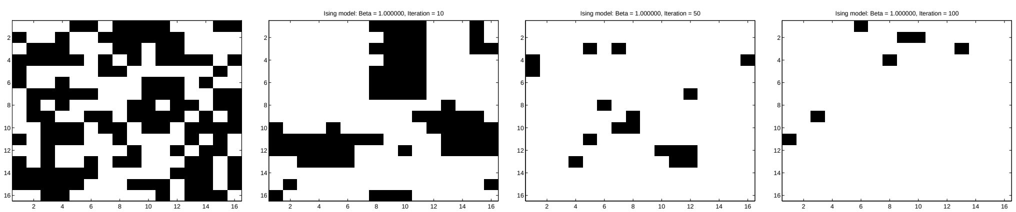
- Repeat this procedure for each pixel.
- **Warning:** for $\beta > \beta_c$ convergence can be extremely slow!

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

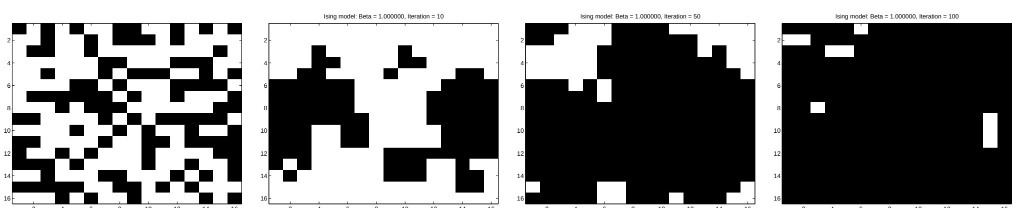
- Test 1



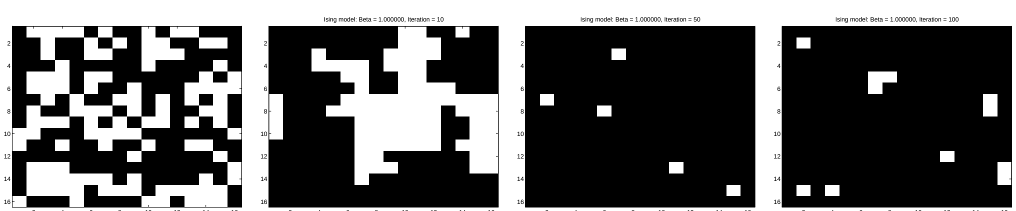
- Test 2



- Test 3



- Test 4



Uniform Random 10 Iterations 50 Iterations 100 Iterations

# Advantages and Disadvantages of Metropolis Sampler

- Advantages
  - Can be implemented whenever $\Delta E$ is easy to compute.
  - Has guaranteed geometric convergence.
- Disadvantages
  - Can be slow if there are many rejections.
  - Is constrained to use a symmetric transition function $q(x^{k+1}|x^k)$.

# Hastings-Metropolis Sampler[7, 10]

- Hastings and Peskun generalized the Metropolis sampler for transition functions $q(w|x^k)$ which are not symmetric.
- The acceptance probability is then

$$\alpha(x_s^k, w) = \min\left\{1, \frac{q(x^k|w)}{q(w|x^k)} \exp\{-\Delta E(w)\}\right\}$$

- Special cases

$$q(w|x^k) = q(x^k|z) \Rightarrow \text{conventional Metropolis}$$
$$q(w_s|x^k) = p(x_s^k|x_{\partial s}^k)\Big|_{x_s^k = w_s} \Rightarrow \text{Gibbs sampler}$$

- Advantage
  - Transition function may be chosen to minimize rejections[6]

# Parameter Estimation for Discrete State MRF's

- Topics to be covered:
  - Why is it difficult?
  - Coding/maximum pseudolikehood
  - Least squares

# Why is Parameter Estimation Difficult?

- Consider the ML estimate of $\beta$ for an Ising model.
- Remember that

$$t_1(x) = (\#\ \text{horz. and vert. neighbors of different value.})$$

- Then the ML estimate of $\beta$ is

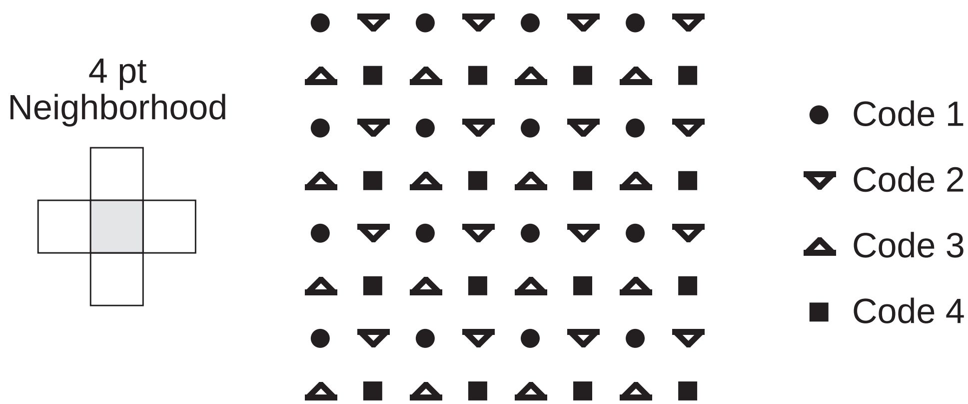
$$\begin{aligned}\hat{\beta} &= \arg\max_{\beta}\left\{\frac{1}{Z(\beta)}\exp\left\{-\beta t_1(x)\right\}\right\} \\ &= \arg\max_{\beta}\left\{-\beta t_1(x) - \log Z(\beta)\right\}\end{aligned}$$

- However, $\log Z(\beta)$ has an intractable form

$$\log Z(\beta) = \log \sum_{x} \exp\left\{-\beta t_1(x)\right\}$$

- Partition function can not be computed.

# Coding Method/Maximum Pseudolikelihood[1, 2]




- Assume a 4 point neighborhood
- Separate points into four groups or codes.
- Group (code) contains points which are conditionally independent given the other groups (codes).

$$\hat{\beta} = \arg\max_{\beta} \prod_{s \in \text{Code}_k} p(x_s | x_{\partial s})$$

- This is tractable (but not necessarily easy) to compute

# Least Squares Parameter Estimation[3]

- It can be shown that for an Ising model

$$\log \frac{P\{X_s = 1|x_{\partial s}\}}{P\{X_s = 0|x_{\partial s}\}} = -\beta \left( V_1(1|x_{\partial s}) - V_1(0|x_{\partial s}) \right)$$

- For each unique set of neighboring pixel values, $x_{\partial s}$, we may compute
  - The observed rate of $\log \frac{P\{X_s=1|x_{\partial s}\}}{P\{X_s=0|x_{\partial s}\}}$
  - The value of $(V_1(1|x_{\partial s}) - V_1(0|x_{\partial s}))$
  - This produces a set of over-determined linear equations which can be solved for $\beta$.
- This least squares method is easily implemented.

# Theoretical Results in Parameter Estimation for MRF's

- Inconsistency of ML estimate for Ising model[11, 12]
  - Caused by critical temperature behavior.
  - Single sample of Ising model cannot distinguish between high $\beta$ with mean 1/2, and low $\beta$ with large mean.
  - Not identifiable
- Consistency of maximum pseudolikelihood estimate[5]
  - Requires an identifiable parameterization.

# References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