

Markov chain Monte Carlo idea

★ Situation:

- Given a target distribution $f(x)$
- Want to estimate

$$\mu = E_f[g(X)] = \int g(x)f(x)dx$$

- Want to generate samples from $f(x)$

★ Idea:

- construct a Markov chain $\{X_i\}_{i=1}^{\infty}$ so that

$$\lim_{i \rightarrow \infty} P(X_i = x) = f(x)$$

- simulate the Markov chain for many iterations
- for m large enough x_m, x_{m+1}, \dots are (essentially) from $f(x)$
- estimate μ by

$$\tilde{\mu} = \frac{1}{n} \sum_{i=m}^{m+n-1} g(x_i)$$

Markov chain Monte Carlo: questions to answer

- ★ Questions to answer:
 - how to construct such a Markov chain?
 - how to simulate the Markov chain?
 - how to find the value of m ?
 - how to estimate $\text{Var}[\hat{\mu}]$?

Markov chain Monte Carlo: questions to answer

★ Questions to answer:

- how to construct such a Markov chain?
- how to simulate the Markov chain?
- how to find the value of m ?
- how to estimate $\text{Var}[\hat{\mu}]$?

★ How to construct such a Markov chain? ($x \in \Omega$ discrete)

- Markov chain transition probabilities:
 $P(y|x) = P(X_{i+1} = y | X_i = x)$
- Need to have

$$f(y) = \sum_{x \in \Omega} f(x)P(y|x) \quad \text{for all } y \in \Omega$$

- Sufficient condition: Detailed balance condition

$$f(x)P(y|x) = f(y)P(x|y) \quad \text{for all } x, y \in \Omega$$

Metropolis–Hastings

- ★ Detailed balance condition:

$$f(x)P(y|x) = f(y)P(x|y) \quad \text{for all } x, y \in \Omega$$

- ★ Metropolis–Hastings setup for $P(y|x)$:

$$P(y|x) = Q(y|x)\alpha(y|x) \quad \text{when } y \neq x$$

$$P(x|x) = 1 - \sum_{y \neq x} Q(y|x)\alpha(y|x)$$

where

- $Q(y|x)$ is a transition matrix (proposal kernel)
 - $\alpha(y|x) \in [0, 1]$ is an acceptance probability
- ★ Questions:
 - how to simulate the Markov chain with this setup?
 - for given $Q(y|x)$, what can $\alpha(y|x)$ be?

Limiting distribution of a Markov chain

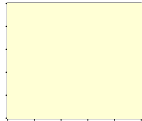
- ▶ Theorem: A Markov chain has a unique limiting distribution $f(x)$ if the chain is **irreducible**, **aperiodic** and **positive recurrent**. If so the limiting distribution $f(x) = \lim_{i \rightarrow \infty} P(X_i = x)$, is given from the equations

$$f(y) = \sum_{x \in \Omega} f(x)P(y|x) \quad \text{for all } y \in \Omega,$$

$$\sum_{x \in \Omega} f(x) = 1.$$

Ising model ($\beta = 0.87, x^0 = 0$)

$0n$ iterations

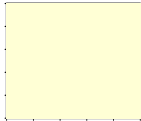


$200n$ iterations

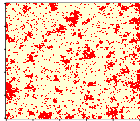
$400n$ iterations

Ising model ($\beta = 0.87, x^0 = 0$)

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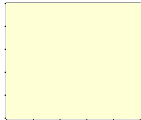
$200n$ iterations



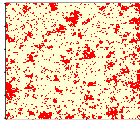
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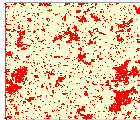
$0n$ iterations



$200n$ iterations

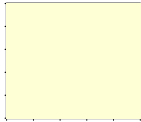


$400n$ iterations

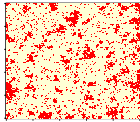


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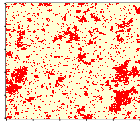
$0n$ iterations



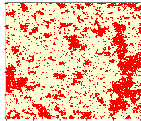
$200n$ iterations



$400n$ iterations



$600n$

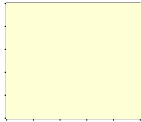


$800n$ iterations

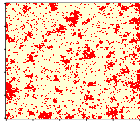
$1000n$ iterations

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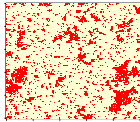
$0n$ iterations



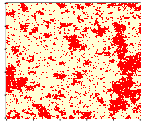
$200n$ iterations



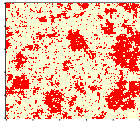
$400n$ iterations



$600n$



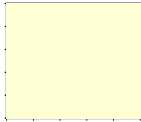
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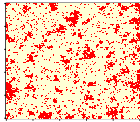
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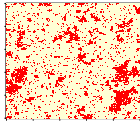
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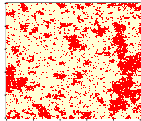
$200n$ iterations



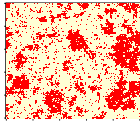
$400n$ iterations



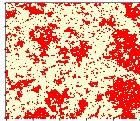
$600n$



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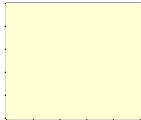


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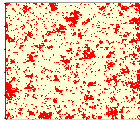


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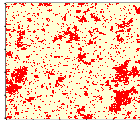
$0n$ iterations



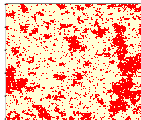
$200n$ iterations



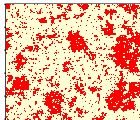
$400n$ iterations



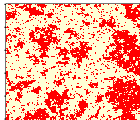
$600n$



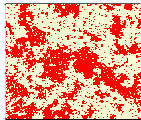
$800n$ iterations



$1000n$ iterations



$5000n$

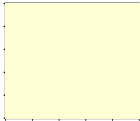


$10000n$ iterations

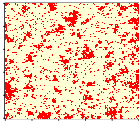
$15000n$ iterations

Ising model ($\beta = 0.87, x^0 = 0$)

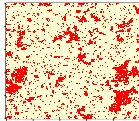
$0n$ iterations



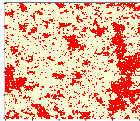
$200n$ iterations



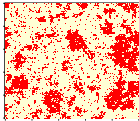
$400n$ iterations



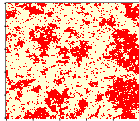
$600n$



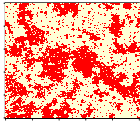
$800n$ iterations



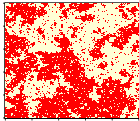
$1000n$ iterations



$5000n$



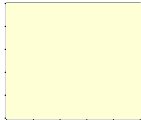
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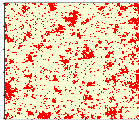
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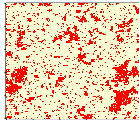
0n iterations



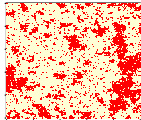
200n iterations



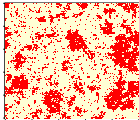
400n iterations



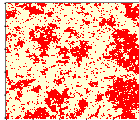
600n



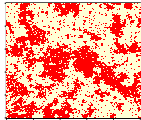
800n iterations



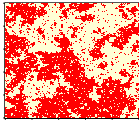
1000n iterations



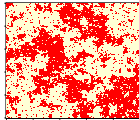
5000n



10000n iterations

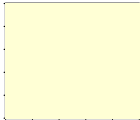


15000n iterations

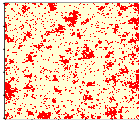


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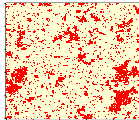
0n iterations



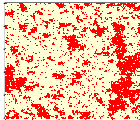
200n iterations



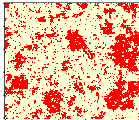
400n iterations



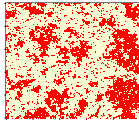
600n



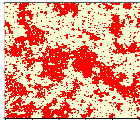
800n iterations



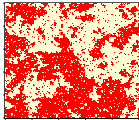
1000n iterations



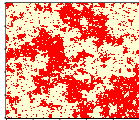
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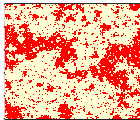
10000n iterations



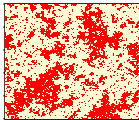
15000n iterations



20000n



25000n iterations



30000n iterations

