Lecture 9: Markov Chain Monte Carlo

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Last Time

- Rejection sampling
- Markov chain review

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This time: Markov chain Monte Carlo

- Gibbs sampling
- Metropolis-Hastings

Gibbs Sampling: Motivation

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  - Proposal distribution $q(x_1, \ldots, x_n)$ for all x_i at once
  - Issue: too slow (typically exponentially small acceptance rate in n)
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- Idea behind Gibbs sampling: change one variable at a time (Markov chain)

Gibbs Sampling: Algorithm

Algorithm:

- Initialize $(x_1, \dots, x_n)$ arbitrarily
- Repeat:
  - Pick i (randomly or sequentially)
  - Re-sample x_i from $p(x_i \mid x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_n)$ (often denote $p(x_i \mid x_{-i})$)

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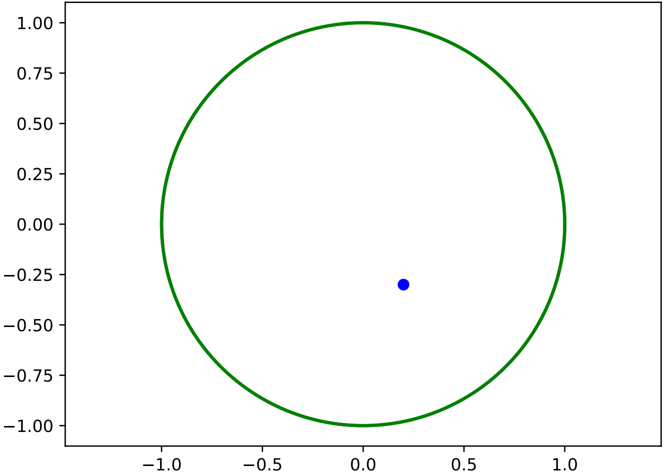
Defines a Markov chain, and can prove that the stationary distribution is $p(x_1, \ldots, x_n)$ (!!).

Gibbs Sampling: Unit Circle Example



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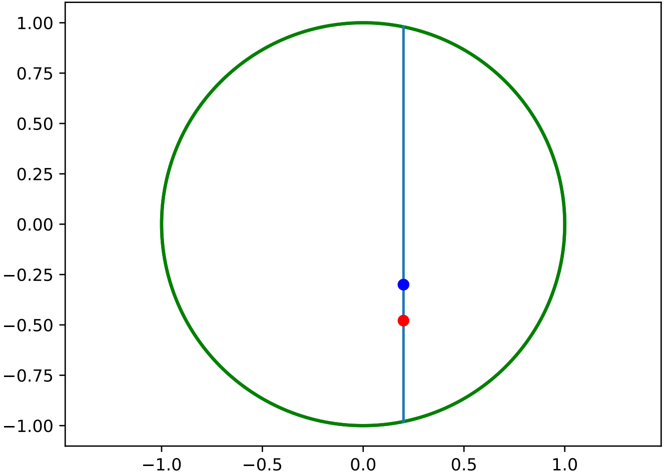

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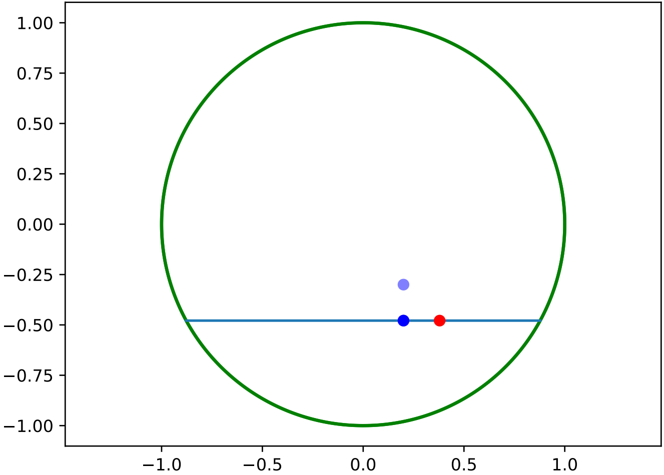

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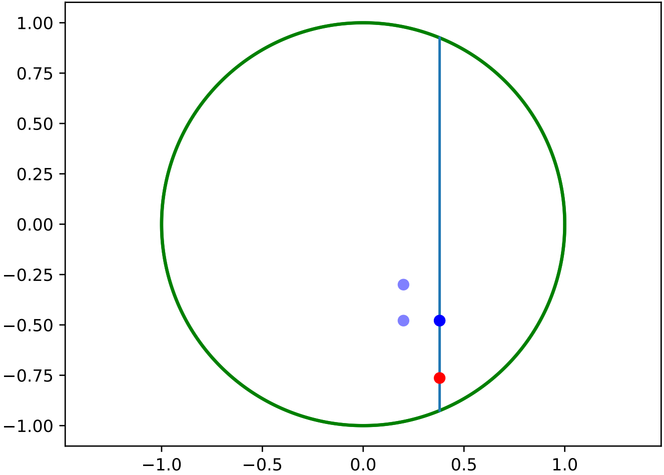

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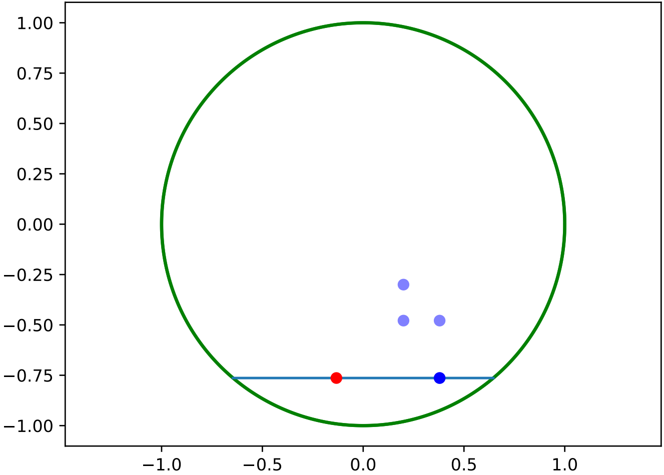

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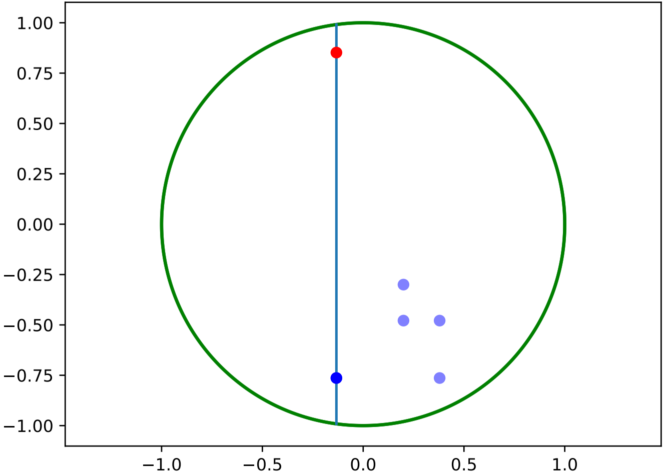

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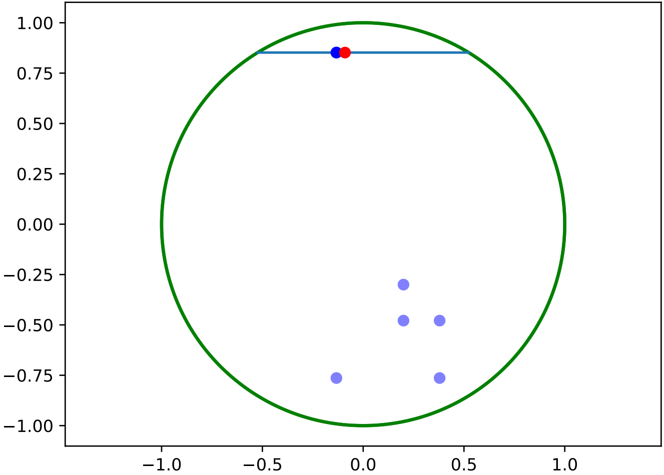

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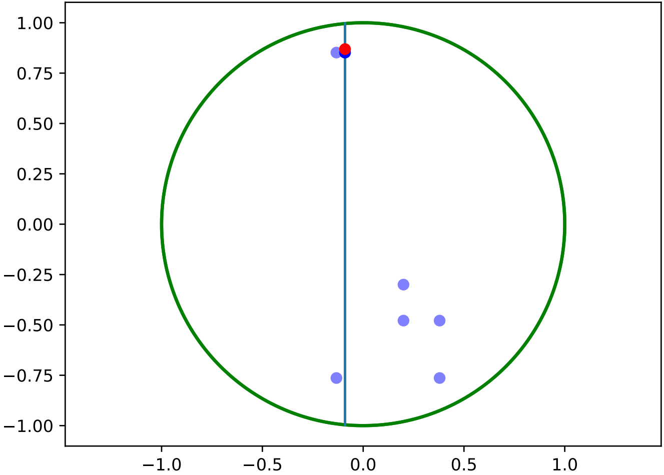

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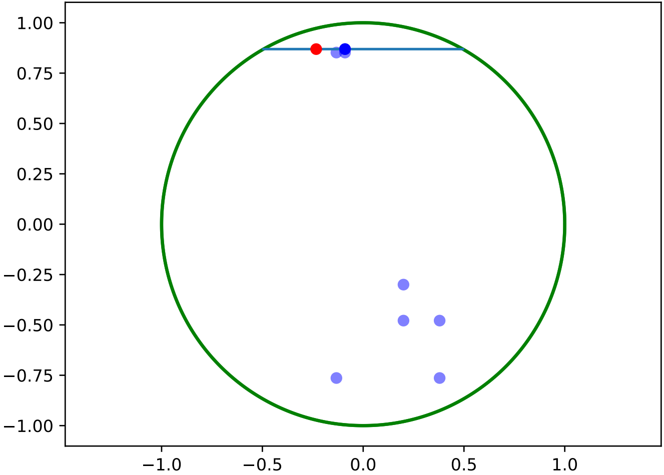

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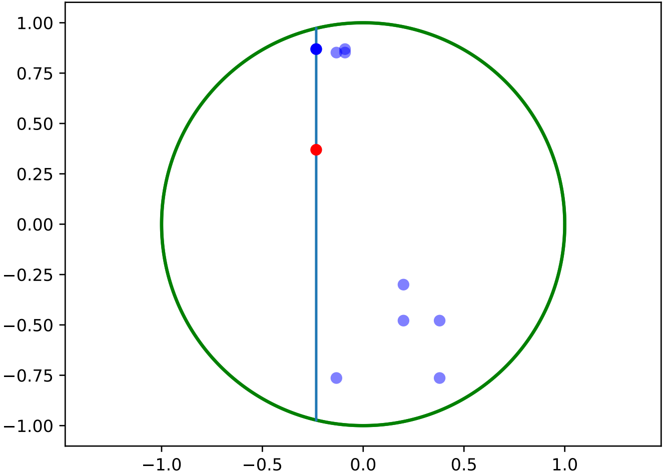

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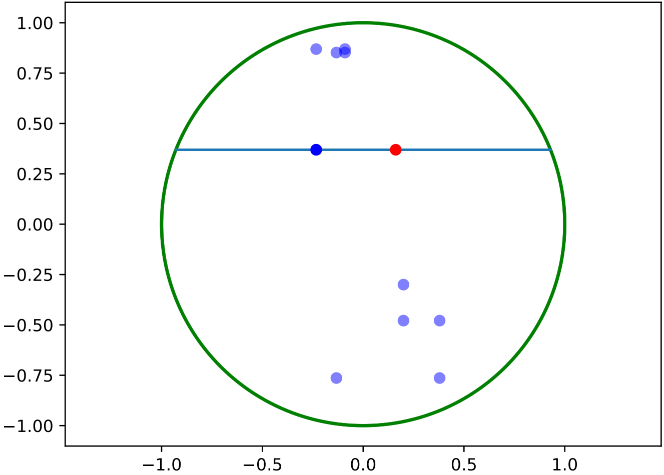

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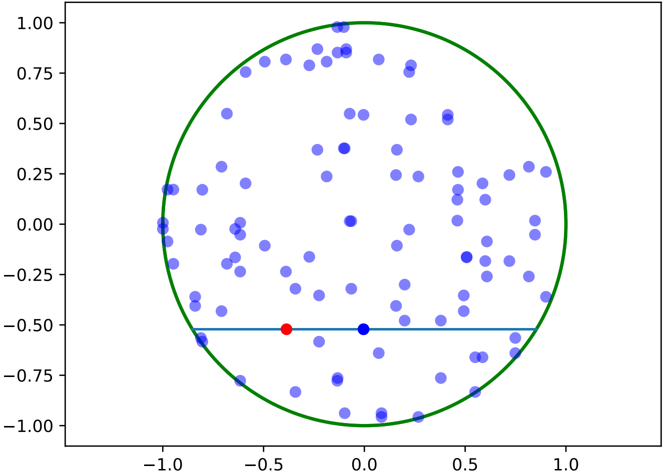

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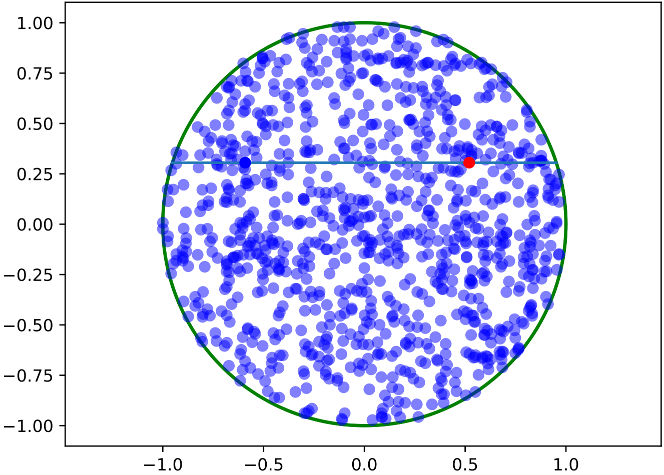
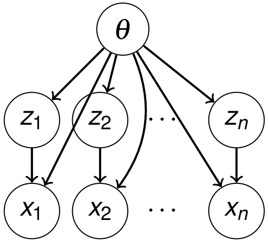


Gibbs Sampling for Hierarchical Models

Recall hierarchical models (e.g. height and gender example)



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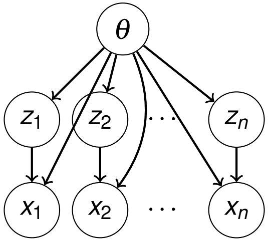

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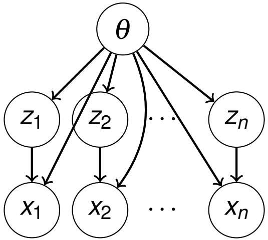

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- Sample z_i: $p(z_i \mid x_i, \theta) \propto \underbrace{p(z_i \mid \theta)}_{\text{prior}} \underbrace{p(x_i \mid z_i)}_{\text{likelihood}}$

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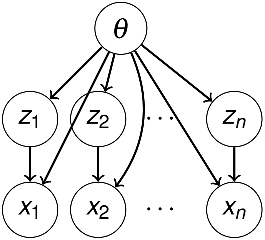

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- Sample z_i: $p(z_i \mid x_i, \theta) \propto \underbrace{p(z_i \mid \theta)}_{\text{prior}} \underbrace{p(x_i \mid z_i)}_{\text{likelihood}}$
- Sample θ (e.g. μ_0 for height/gender model):

$$p(\mu_0 \mid z_{1:n}, x_{1:n}) \propto \underbrace{p(\mu_0)}_{\text{prior}} \cdot \underbrace{\prod_{i:z_i=0} \exp(-(x_i - \mu_0)^2/2\sigma^2)}_{\text{likelihood}}$$

Proof of stationary distribution

Assuming chain is ergodic, just need to show stationary distribution is preserved.

Suppose $x \sim p$ and x' is obtained from x by Gibbs sampling update. Want to show that x' is also distributed according to p.

If index i is updated, then $x' = (x_1, \ldots, x_{i-1}, x'_i, x_{i+1}, \ldots)$, where $x'_i \sim p(x_i \mid x_1, \ldots, x_{i-1}, x_{i+1}, \ldots)$.

Indices $\neq i$ distributed according to p, and $x'_i \mid x'_{\neq i}$ is as well, so x' follows p.

Ergodicity: counterexample

Suppose that $x_1, x_2 \in \{0, 1\}$ with following probability table:

	0	1
0	0.5	0.0
1	0.0	0.5

What will Gibbs sampling do?

Gibbs Sampling: Summary

- Repeatedly sample from $p(x_i \mid x_{-i})$
- Creates Markov chain whose stationary distribution is $p(x_1, \dots, x_n)$
- Flexible: conditional $p(x_i \mid x_{-i})$ one-dimensional, easy to sample from
- Don't need to "get lucky" with graphical model structure
- Extensions, e.g. block Gibbs sampling

Metropolis-Hastings: Idea

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- Is there a more general strategy?
- Yes! Combine with idea of rejection sampling
- Given any “proposed Markov chain” $q(x^{\text{new}} \mid x^{\text{old}})$, will combine with an accept/reject step to create new Markov chain with the correct stationary distribution

Metropolis-Hastings: Algorithm

Proposal distribution: $q(x^{\text{new}} \mid x^{\text{old}})$

Given x^{old}:

- Sample x^{new} from q
- With probability [ ], accept (replace x^{old} with x^{new})
- Otherwise, reject (keep x^{old})

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Gibbs sampling: special choice of q where we always accept!

Proof sketch: Detailed balance

Can show that if an ergodic Markov chain satisfies
$\bar{p}(x)A(x' \mid x) = \bar{p}(x')A(x \mid x')$ for all x, x', then it has stationary distribution $\bar{p}$.

This condition is called **detailed balance**.

Metropolis-Hastings sets probabilities so that detailed balance holds.

Mixing time

Performance of MCMC algorithms governed by **mixing time**: how long it takes to get close to stationary distribution.

Mixing time can vary dramatically, from nearly linear to exponential in number of variables.

[mixing time examples: on board]