Monte Carlo - Recap

- Monte Carlo methods we have discussed so far
  - Inverse CDF works for 1D
  - Analytic transformations for some distributions
  - Grid evaluation and sampling works in low dimensions
  - Rejection sampling
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  - Rejection sampling
  - Importance sampling
- What to do in high dimensions?
  - Markov chain Monte Carlo (Ch 11-12 in BDA 3rd)

Markov Chain

- The probability of each event depends only on the state attained in the previous event
  - Sequence $x_1, x_2, \dots, x_T$ where distribution of x_t depends only on x_{t-1}
- Defined by transition distribution $A(x^{new}|x^{old})$, together with initial state x_1

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- Example of a simple Markov chain on black board
  - Random walk
  - Repeatedly shuffling a deck of cards

Markov Chain

- The Markov property is such that given the present, the future is independent of the past. Let the state space be Ω, a Markov chain on Ω is determined by the transition probability

  $$K(x,y) = P(X_{t+1} = y | X_t = x, X_{t-1}, ..., X_0) = P(X_{t+1} = y | X_t = x).$$

  Let $p^{(t)}(x)$ be the marginal distribution of X_t. Then

  $$\begin{aligned} p^{(t+1)}(y) &= P(X_{t+1} = y) \\ &= \sum_x P(X_{t+1} = y, X_t = x) \\ &= \sum_x P(X_{t+1} = y | X_t = x) P(X_t = x) \\ &= \sum_x p^{(t)}(x) K(x,y). \end{aligned}$$

- Let K be the matrix $(K(x,y))$. Let $p^{(t)}$ be the row vector $(p^{(t)}(x))$. Then $p^{(t+1)} = p^{(t)}K$. By induction, $p^{(t)} = p^{(0)}K^t$.

Markov Chain: Two-step transition

$$
\begin{aligned}
K^{(2)}(x,y) &= P(X_{t+2}=y|X_t=x) \\
&= \sum_z P(X_{t+2}=y, X_{t+1}=z|X_t=x) \\
&= \sum_z P(X_{t+2}=y|X_{t+1}=z, X_t=x)P(X_{t+1}=z|X_t=x) \\
&= \sum_z K(x,z)K(z,y) = K^2(x,y).
\end{aligned}
$$

In general, $K^{(t)} = K^t$.

Markov Chain: Stationary Distribution

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- The distribution $\pi(x)$ is also what we get if we count how many times x_t visits each state, as $T \to \infty$.
- The mixing time is how long it takes for x_T to be close to the stationary distribution (we won't define this formally).
  - Mixing time is how many shuffles we need for deck to be "almost random"

Markov Chain: Reversibility

- A special case is the reversible Markov chain where

$$\pi(x)K(x,y) = \pi(y)K(y,x)$$

It is also called the detailed balance condition.

- If a chain is reversible with respect to π, then π is the stationary distribution, because

$$\sum_x \pi(x)K(x,y) = \sum_x \pi(y)K(y,x) = \pi(y)\sum_x K(y,x) = \pi(y).$$

Markov Chain: Transition Matrix

The transition matrix K contains the transition probabilities. We can interpret it as follows:

(1) Forward meaning as mixing. In $p^{(t+1)} = p^{(t)}K$, K acts on a row vector, and its verb meaning is mixing $p^{(t)}$ into $p^{(t+1)}$.

(2) Backward meaning as smoothing. We can also let K act on a column vector so that $g = Kh$. Both g and h can be considered functions defined on the state space Ω.

$$
\begin{aligned}
g(x) &= \sum_y K(x,y)h(y) \\
&= \sum_y h(X_{t+1}=y)P(X_{t+1}=y|X_t=x) \\
&= \mathrm{E}(h(X_{t+1})|X_t=x),
\end{aligned}
$$

which is local average of h around x. So K is smoothing h into g.

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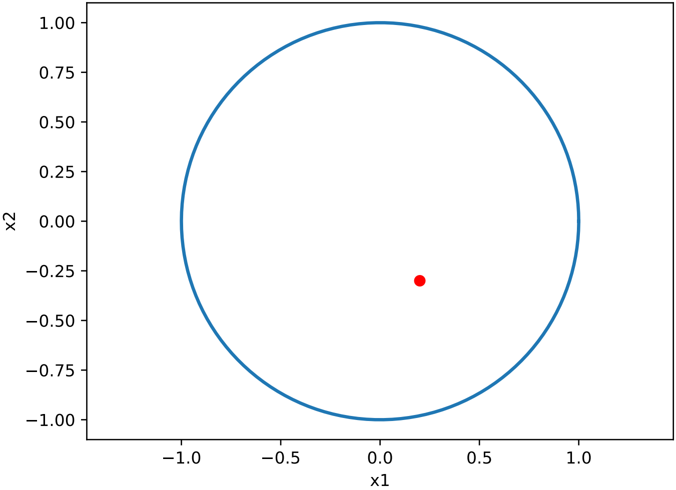
  - Issue: too slow (typically exponentially small acceptance rate in d)
- Idea behind Gibbs sampling: change one variable at a time (Markov chain)
- Algorithm
  - Initialize $(\theta_1, \ldots, \theta_n)$ arbitrarily
  - Repeat:
    Pick j (randomly or sequentially)
    Re-sample θ_j from $p(\theta_j | \theta_1^t, \ldots, \theta_{j-1}^t, \theta_{j+1}^{t-1}, \ldots, \theta_d^{t-1})$ (often denote as $p(\theta_j | \theta_{-j})$)

Gibbs Sampling: Unit Circle Example



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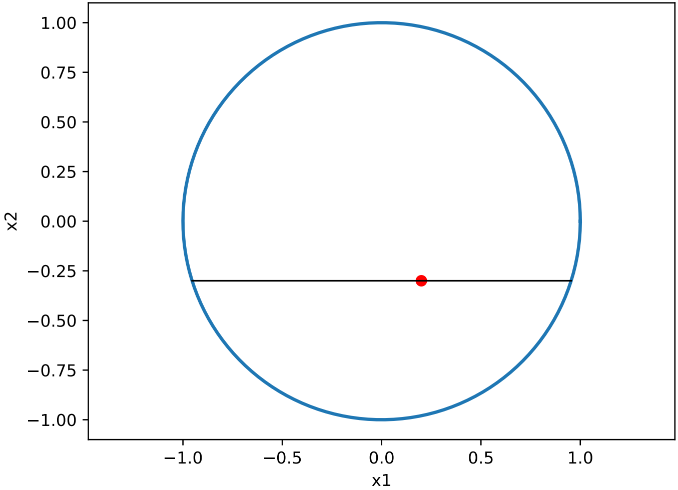

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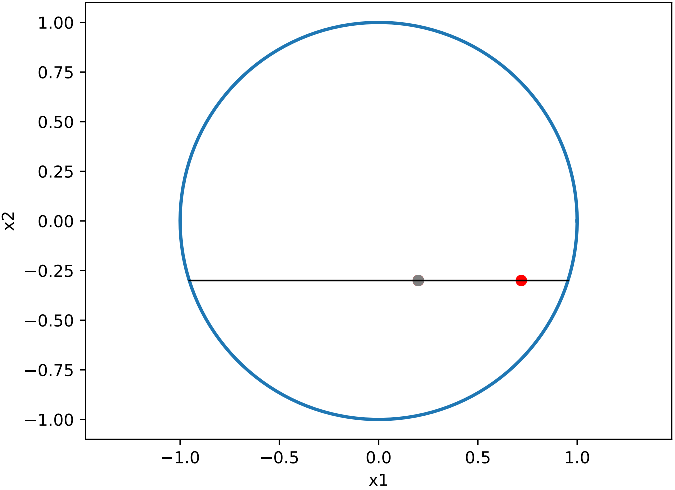

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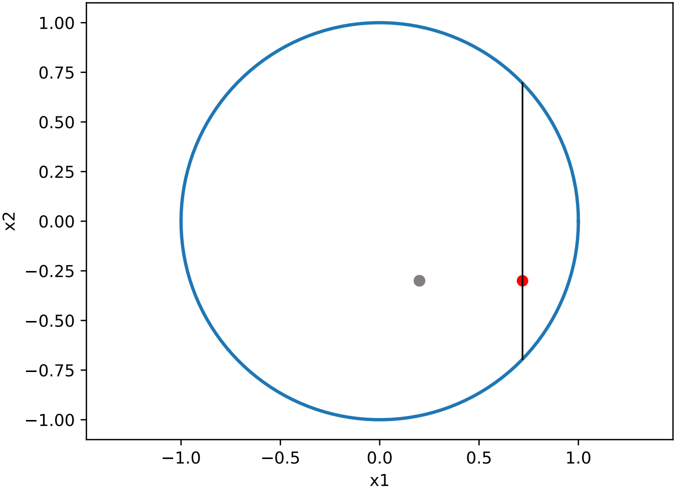

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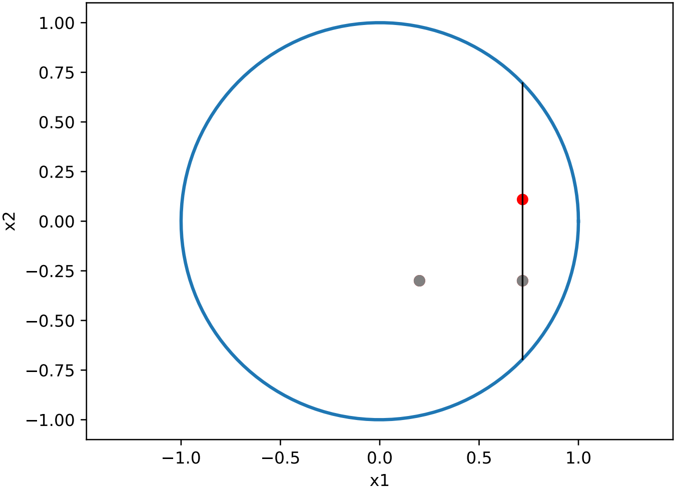

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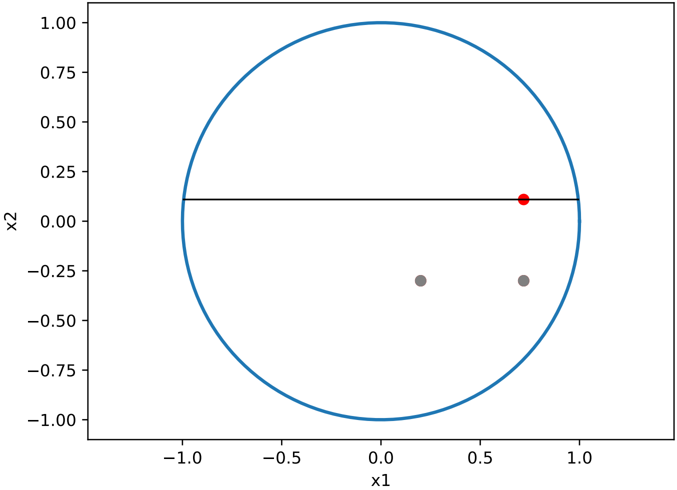

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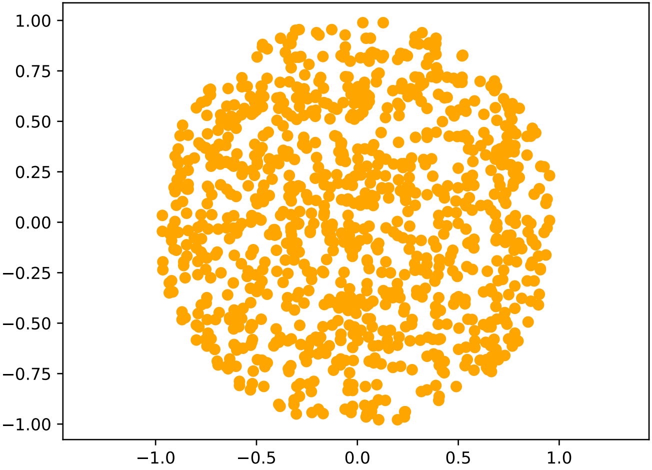

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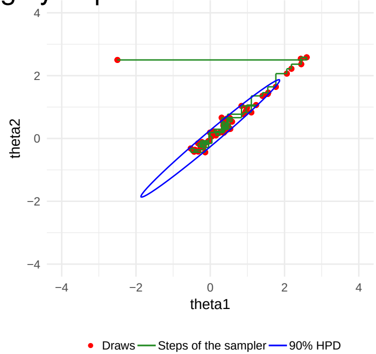
- If conditional distribution is not straight forward, use e.g. inverse-CDF
- Several parameters can be updated in blocks (*blocking*)
- Slow if parameters are highly dependent



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Metropolis algorithm

- Algorithm
  1. starting point θ^0
  2. $t = 1, 2, \ldots$
     (a) pick a proposal θ^* from the proposal distribution $J_t(\theta^*|\theta^{t-1})$.
     Proposal distribution has to be symmetric, i.e.
     $J_t(\theta_a|\theta_b) = J_t(\theta_b|\theta_a)$, for all θ_a, θ_b

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     ie, if $p(\theta^*|y) > p(\theta^{t-1}|y)$, always accept the proposal and otherwise accept the proposal with probability r

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  - step c is executed by generating a random number from U(0, 1)
  - $p(\theta^*|y)$ and $p(\theta^{t-1}|y)$ have the same normalization terms, and thus instead of $p(\cdot|y)$, unnormalized $q(\cdot|y)$ can be used, as the normalization terms cancel out!

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- Theoretically
  1. Prove that simulated series is a Markov chain which has unique stationary distribution
  2. Prove that this stationary distribution is the desired target distribution

Metropolis-Hastings algorithm

- Generalization of Metropolis algorithm for non-symmetric proposal distributions
  - acceptance ratio includes ratio of proposal distributions

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    $\rightarrow$ many steps accepted, but the chain moves slowly due to small steps
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- Generic rule for rejection rate is 60-90% (but depends on dimensionality and a specific algorithm variation)

Gibbs sampling

- Specific case of Metropolis-Hastings algorithm
  - single updated (or blocked)
  - proposal distribution is the conditional distribution
    $\rightarrow$ proposal and target distributions are same
    $\rightarrow$ acceptance probability is 1