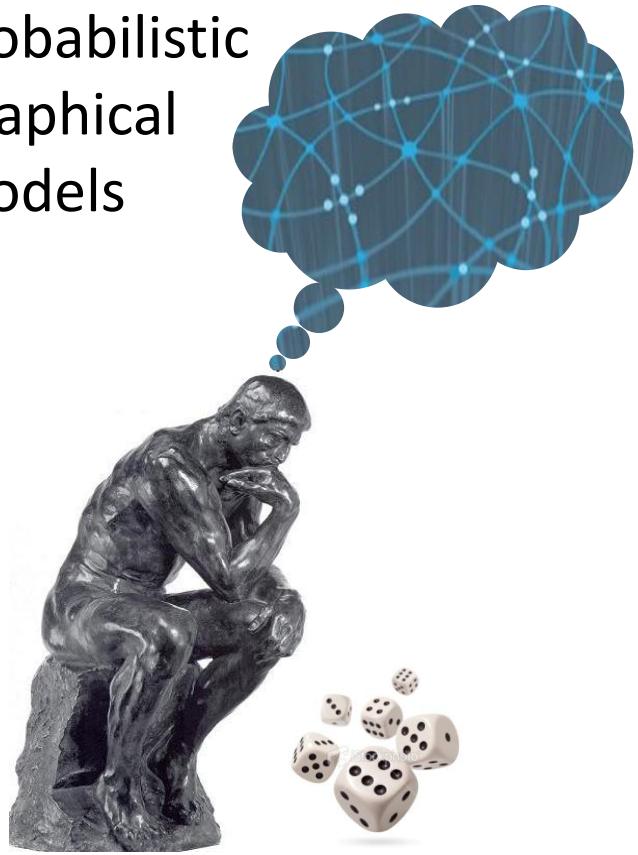
Probabilistic Graphical Models



Inference

Sampling Methods

Simple Sampling

Sampling-Based Estimation

$\mathcal{D} = \{x[1], \ldots, x[M]\}$ sampled IID from P

independent, identically distributed

If P(X=1) = p

$= E_P[\mathbb{1}_{X=1}]$

fraction of 1's

Estimator for p: $T_{\mathcal{D}} = \frac{1}{M} \sum_{m=1}^{M} x[m]$

More generally, for any distribution P, function f:

indicator function

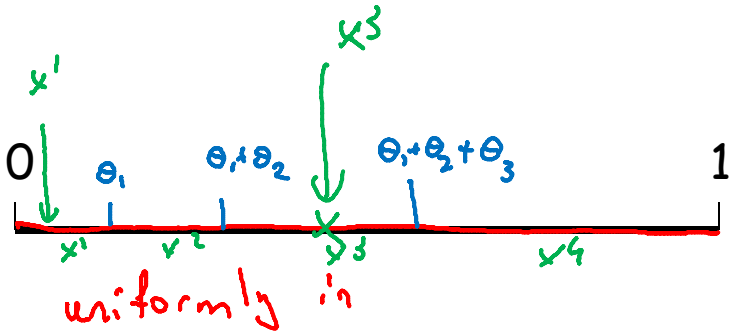
$$\boldsymbol{E}_P[f] \approx \frac{1}{M} \sum_{m=1}^{M} f(x[m])$$

f on samples

empirical expectation

Sampling from Discrete Distribution

$Val(X) = \{x^1, \ldots, x^k\}$ $\quad\quad$ $P(x^i) = \theta^i$



Sampling-Based Estimation

$$T_{\mathcal{D}} = \frac{1}{M}\sum_{m=1}^{M} X[m]$$

Hoeffding Bound:

$$P_{\mathcal{D}}(T_{\mathcal{D}} \notin [p-\epsilon, p+\epsilon]) \leq 2e^{-2M\epsilon^2}$$

additive · # samples · estimate · prob. of sample a bad set · is ε-away from p

Chernoff Bound:

$$P_{\mathcal{D}}(T_{\mathcal{D}} \notin [p(1-\epsilon), p(1+\epsilon)]) \leq 2e^{-Mp\epsilon^2/3}$$

multiplicative

Sampling-Based Estimation

Hoeffding Bound:

$$T_{\mathcal{D}} = \frac{1}{M}\sum_{m=1}^{M} X[m]$$

$$P_{\mathcal{D}}(T_{\mathcal{D}} \notin [p-\epsilon, p+\epsilon]) \leq 2e^{-2M\epsilon^2} < \delta$$

For additive bound ε on error with probability > 1-δ:

$$M \geq \frac{\ln(2/\delta)}{2\epsilon^2}$$

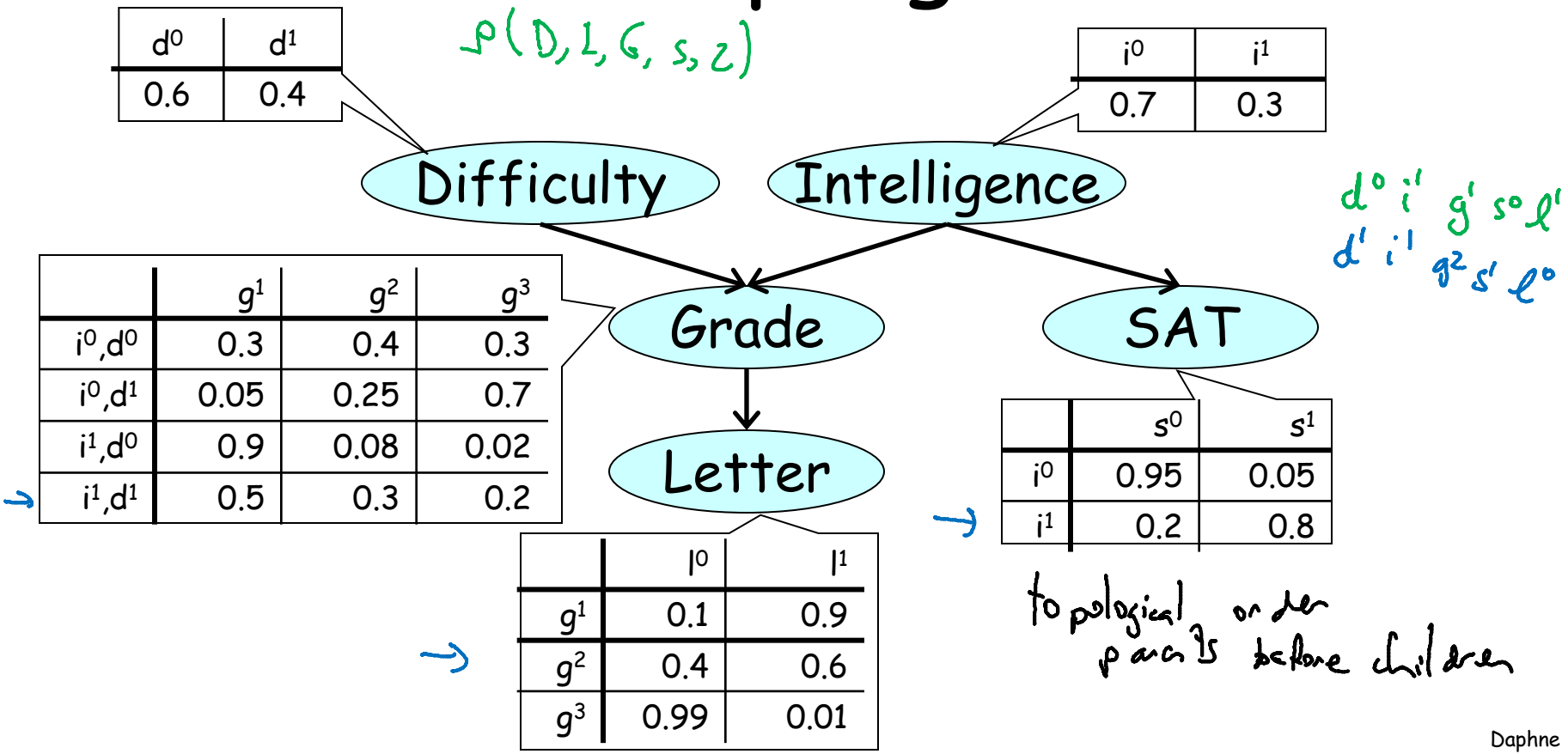
Chernoff Bound:

$$P_{\mathcal{D}}(T_{\mathcal{D}} \notin [p(1-\epsilon), p(1+\epsilon)]) \leq 2e^{-Mp\epsilon^2/3}$$

For multiplicative bound ε on error with probability > 1-δ:

$$M \geq 3\frac{\ln(2/\delta)}{p\epsilon^2}$$

Forward sampling from a BN



$p(D, I, G, S, L)$

$d^0\ i^1\ g^1\ s^0\ l^1$
$d^1\ i^1\ g^2\ s^1\ l^0$

topological order
parents before children

Forward Sampling for Querying

- Goal: Estimate P(Y=y)
  - Generate samples from BN
  - Compute fraction where Y=y

# of samples

For additive bound ε on error with probability > 1-δ: $M \geq \frac{\ln(2/\delta)}{2\epsilon^2}$

For multiplicative bound ε on error with probability > 1-δ: $M \geq 3\frac{\ln(2/\delta)}{P(y)\epsilon^2}$

Queries with Evidence

- Goal: Estimate $P(Y=y \mid \mathbf{E}=\mathbf{e})$
- Rejection sampling algorithm
  - Generate samples from BN
  - Throw away all those where $\mathbf{E} \neq \mathbf{e}$
  - Compute fraction where $Y=y$

remaining samples are sampled from $P(\cdot \mid E=e)$

Expected fraction of samples kept ~ $P(\mathbf{e})$

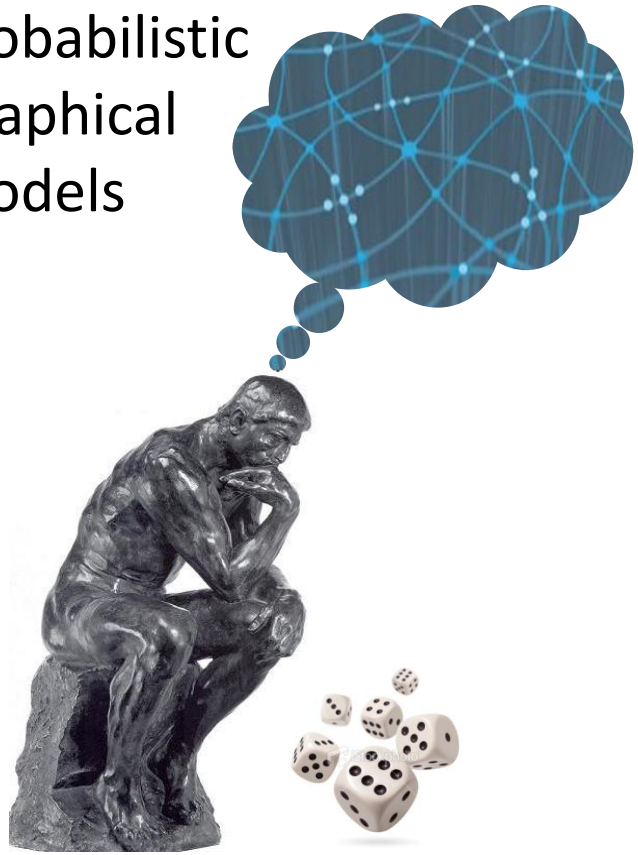
samples needed grows exponentially with # of observed variables

Summary

- Generating samples from a BN is easy
- (ε,δ)-bounds exist, but usefulness is limited:
  - Additive bounds: useless for low probability events
  - Multiplicative bounds: # samples grows as 1/P(y)
- With evidence, # of required samples grows exponentially with # of observed variables

- Forward sampling generally infeasible for MNs

Probabilistic Graphical Models



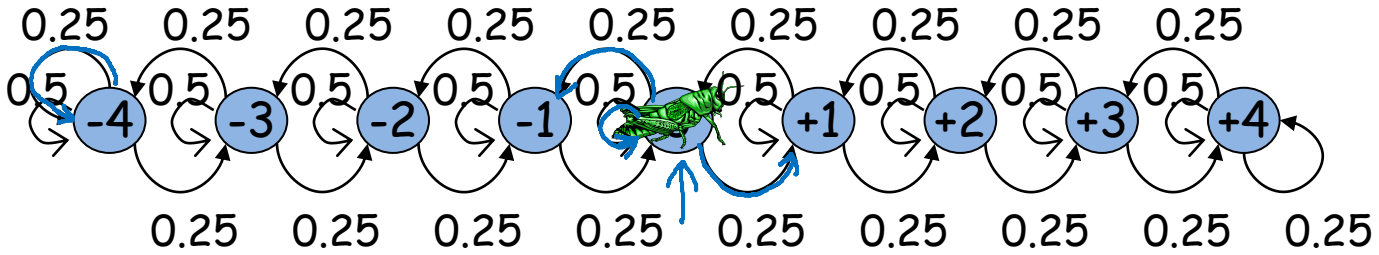
Inference

Sampling Methods

Markov Chain

Monte Carlo

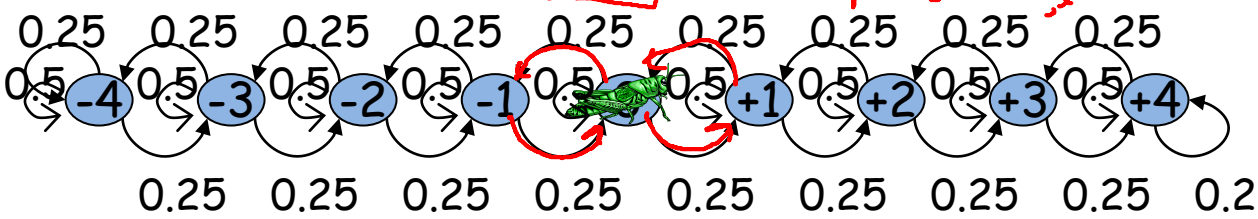
Markov Chain



- A Markov chain defines a probabilistic transition model $T(x \rightarrow x')$ over states x:
  - for all x: $\sum_{x'} T(x \rightarrow x') = 1$

Temporal Dynamics

$$P^{(t+1)}(X^{(t+1)} = x') = \sum_{x} P^{(t)}(X^{(t)} = x) T(x \to x')$$



	-2	-1	0	+1	+2
$P^{(0)}$	0	0	1	0	0
$P^{(1)}$	0	.25	.5	.25	0
$P^{(2)}$	$.25^2$= .0625	2×(.5×.25) = .25	$.5^2+2\times.25^2$ = .375	2×(.5×.25) = .25	$.25^2$= .0625

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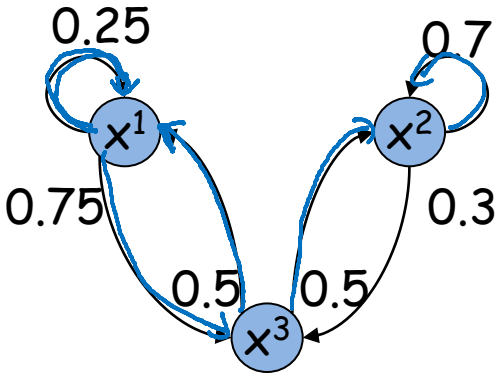
Stationary Distribution

$$P^{(t)}(x') \approx P^{(t+1)}(x') = \sum_x P^{(t)}(x) T(x \to x')$$

$$\pi(x') = \sum_x \pi(x) T(x \to x')$$



$$\begin{aligned}
\pi(x^1) &= 0.25\pi(x^1) + 0.5\pi(x^3) \\
\pi(x^2) &= 0.7\pi(x^2) + 0.5\pi(x^3) \\
\pi(x^3) &= 0.75\pi(x^1) + 0.3\pi(x^2)
\end{aligned}$$

$$\pi(x^1) + \pi(x^2) + \pi(x^3) = 1$$

$$\begin{aligned}
\pi(x^1) &= 0.2 \\
\pi(x^2) &= 0.5 \\
\pi(x^3) &= 0.3
\end{aligned}$$

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Regular Markov Chains

- A Markov chain is regular if there exists k such that, for every x, x', the probability of getting from x to x' in exactly k steps is > 0

- Theorem: A regular Markov chain converges to a unique stationary distribution regardless of start state

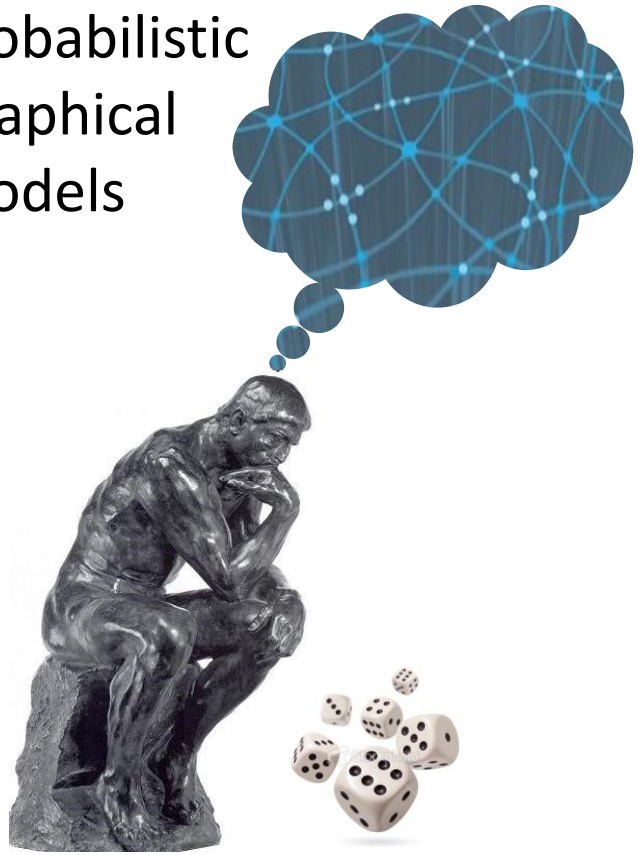
Regular Markov Chains

- A Markov chain is regular if there exists k such that, for every x, x', the probability of getting from x to x' in exactly k steps is > 0

  k = distance between furthest x, x'

- Sufficient conditions for regularity:
  - Every two states x, x' are connected with path of prob > 0
  - For every state, there is a self-transition

Probabilistic Graphical Models



Inference

Sampling Methods

Using a Markov Chain

Using a Markov Chain

- Goal: compute $P(x \in S)$
  - but P is too hard to sample from directly
- Construct a Markov chain T whose unique stationary distribution is P
- Sample $x^{(0)}$ from some $P^{(0)}$
- For t = 0, 1, 2, …
  - Generate $x^{(t+1)}$ from $T(x^{(t)} \rightarrow x')$

Using a Markov Chain

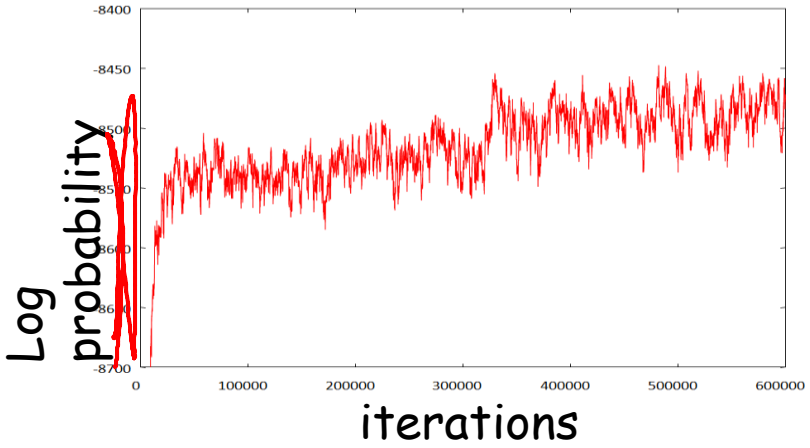
- We only want to use samples that are sampled from a distribution close to P
- At early iterations, $P^{(t)}$ is usually far from P
- Start collecting samples only after the chain has run long enough to "mix" $p^{(t)}$ close enough to π

Mixing

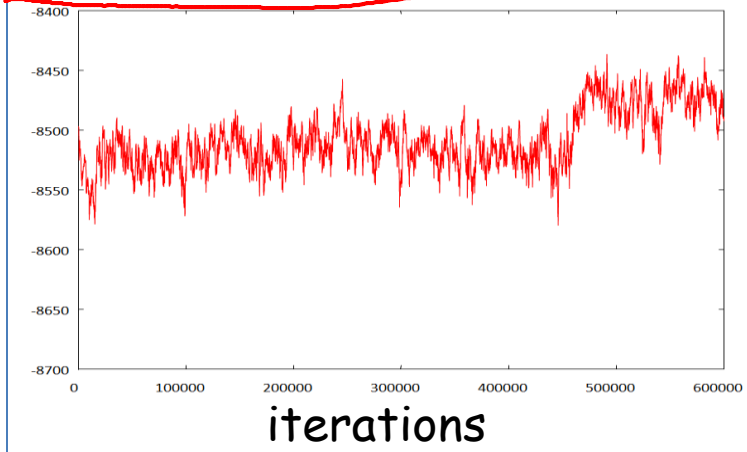
- How do you know if a chain has mixed or not?
  - In general, you can never "prove" a chain has mixed
  - But in many cases you can show that it has NOT

- How do you know a chain has not mixed?
  - Compare chain statistics in different windows within a single run of the chain
  - and across different runs initialized differently

Initialized from an arbitrary state

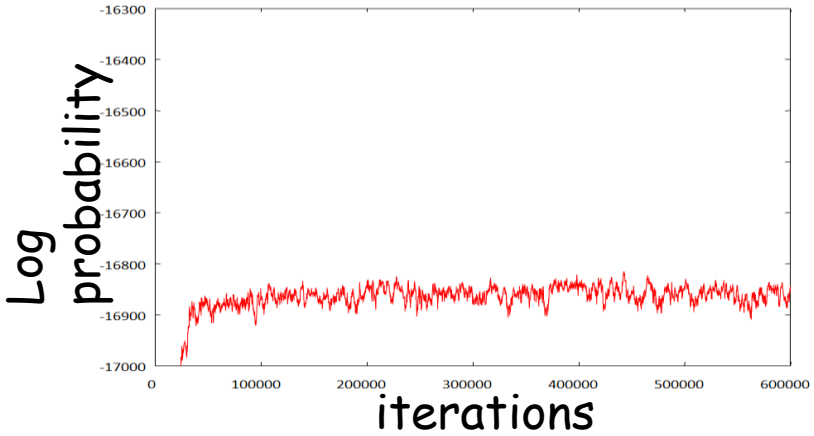


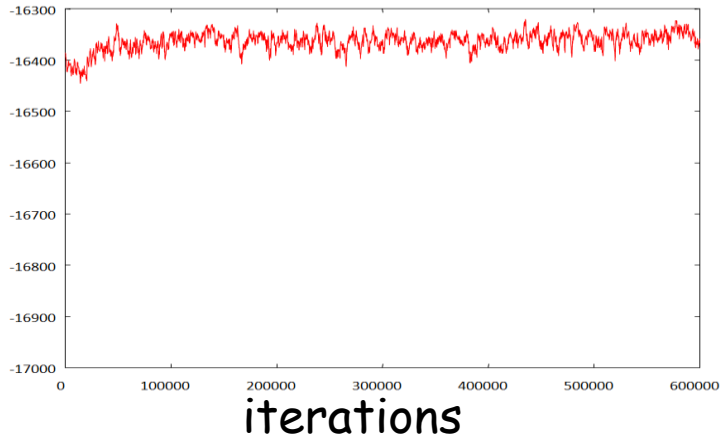
Initialized from a high-probability state



Mixing?

Maybe





NO

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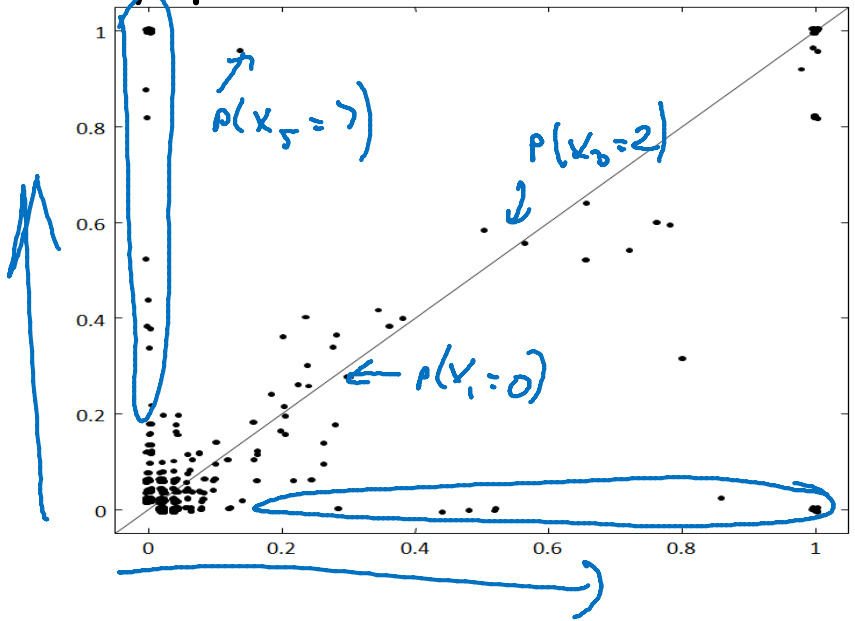
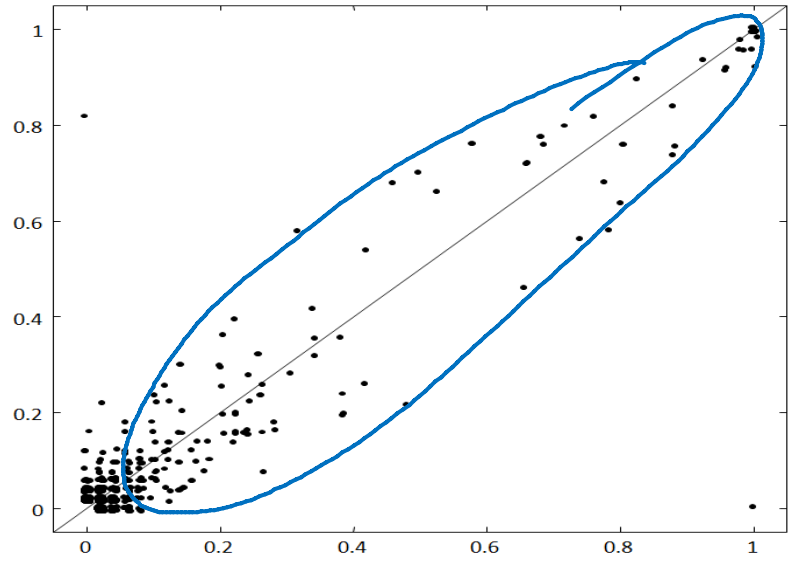
- Each dot is a statistic (e.g., $P(x \in S)$)
- x-position is its estimated value from chain 1
- y-position is its estimated value from chain 2





Mixing? **NO** **Maybe**

Using the Samples

- Once the chain mixes, all samples $x^{(t)}$ are from the stationary distribution π
  - So we can (and should) use all $x^{(t)}$ for $t > T_{mix}$
- However, nearby samples are correlated!
  - So we shouldn't overestimate the quality of our estimate by simply counting samples
- The faster a chain mixes, the less correlated (more useful) the samples

not IID

MCMC Algorithm Summary I

- For c=1,…,C
  - Sample $x^{(c,0)}$ from $P^{(0)}$
- Repeat until mixing
  - For c=1,…,C
    - Generate $x^{(c,\,t+1)}$ from $T(x^{(c,t)} \rightarrow x')$
  - Compare window statistics in different chains to determine mixing
  - t := t+1

MCMC Algorithm Summary II

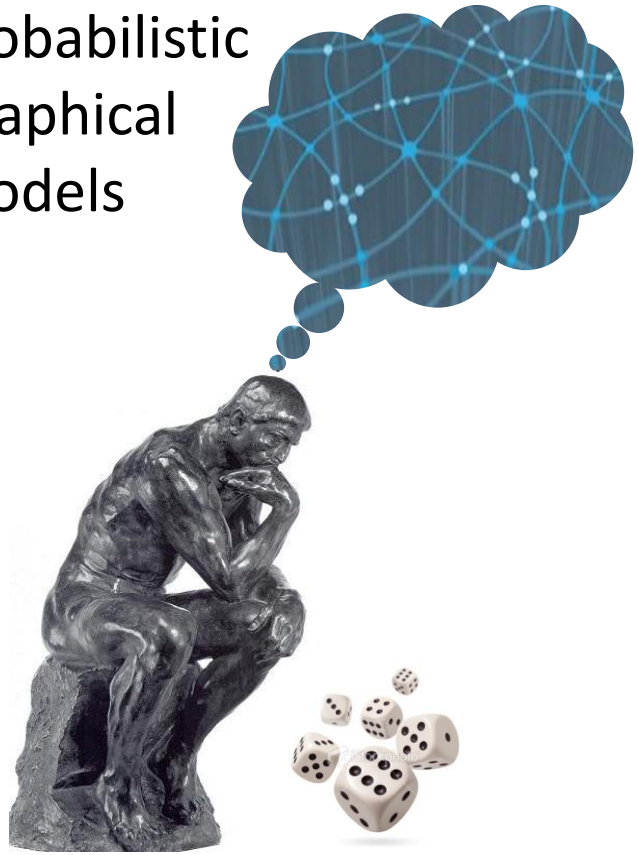
- Repeat until sufficient samples
  - D := $\emptyset$
  - For c=1,…,C
    - Generate $x^{(c,t+1)}$ from $T(x^{(c,t)} \rightarrow x')$
    - D := D $\cup$ $\{x^{(c,t+1)}\}$
  - t := t+1
- Let D = {x[1],…,x[M]}
- Estimate

$$\boldsymbol{E}_P[f] \approx \frac{1}{M} \sum_{m=1}^{M} f(x[m])$$

Summary

- Pros:
  - Very general purpose
  - Often easy to implement
  - Good theoretical guarantees as $t \to \infty$
- Cons:
  - Lots of tunable parameters / design choices
  - Can be quite slow to converge
  - Difficult to tell whether it's working

Probabilistic Graphical Models



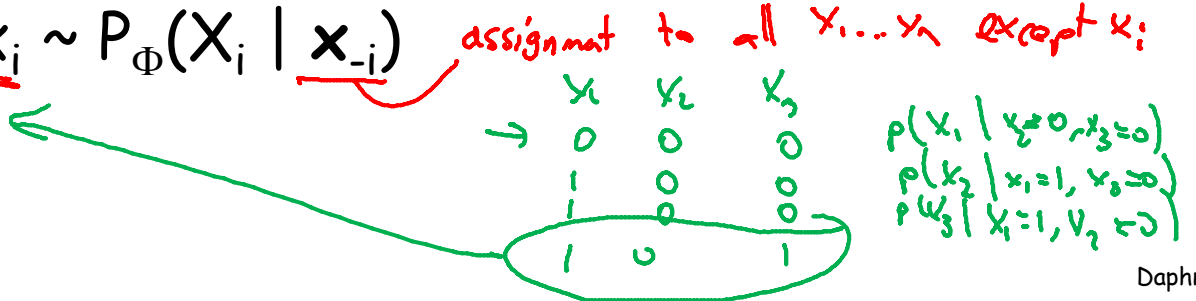
Inference

Sampling Methods

MCMC for PGMs: The Gibbs Chain

Gibbs Chain

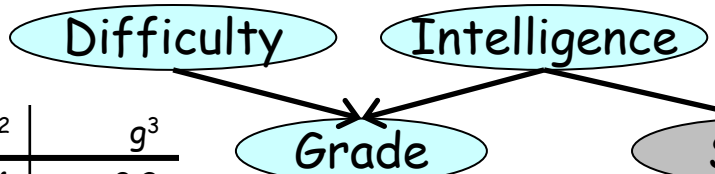
- Target distribution $P_\Phi(X_1,\ldots,X_n)$
- Markov chain state space: complete assignments $\mathbf{x}$ to $\mathbf{X} = \{X_1,\ldots,X_n\}$
- Transition model given starting state $\mathbf{x}$:
  - For i=1,…,n
    - Sample $x_i \sim P_\Phi(X_i \mid \mathbf{x}_{-i})$
  - Set $\mathbf{x}' = \mathbf{x}$



Example

d^0	d^1
0.6	0.4

i^0	i^1
0.7	0.3



	g^1	g^2	g^3
i^0,d^0	0.3	0.4	0.3
i^0,d^1	0.05	0.25	0.7
i^1,d^0	0.9	0.08	0.02
i^1,d^1	0.5	0.3	0.2

	s^0	s^1
i^0	0.95	0.05
i^1	0.2	0.8

	l^0	l^1
g^1	0.1	0.9
g^2	0.4	0.6
g^3	0.99	0.01

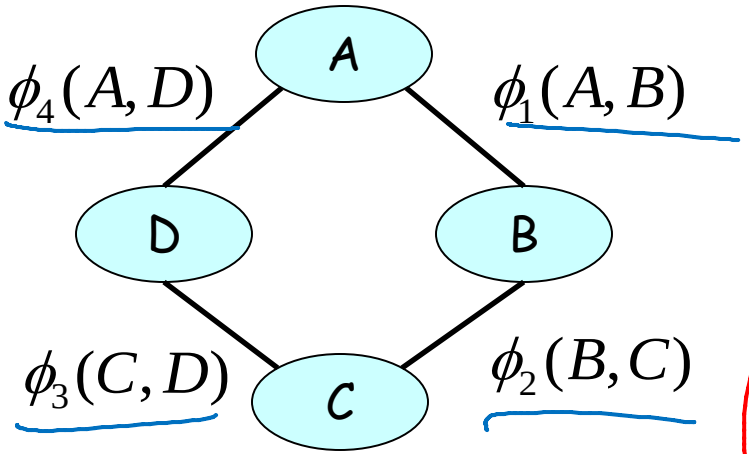
Computational Cost

- For i=1,…,n
  - Sample $x_i \sim P_\Phi(X_i \mid \mathbf{x}_{-i})$

$$P_\Phi(X_i \mid \boldsymbol{x}_{-i}) = \frac{P_\Phi(X_i, \boldsymbol{x}_{-i})}{P_\Phi(\boldsymbol{x}_{-i})} = \frac{\frac{1}{Z}\tilde{P}_\Phi(X_i, \boldsymbol{x}_{-i})}{\frac{1}{Z}\tilde{P}_\Phi(\boldsymbol{x}_{-i})}$$

complete assignment product of factors

Another Example



$$P_\Phi(A \mid b,c,d) = \frac{\tilde{P}_\Phi(a,b,c,d)}{\sum_{A'} \tilde{P}_\Phi(A',b,c,d)}$$

$$\frac{\phi_1(A,b)\phi_2(b,c)\phi_3(c,d)\phi_4(A,d)}{\sum_{A'} \phi_1(A',b)\phi_2(b,c)\phi_3(c,d)\phi_4(A',d)}$$

normalizing constant

$\propto \phi_1(A,b)\,\phi_4(A,d)$

factors that involve A

Computational Cost Revisited

- For i=1,…,n
  - Sample $x_i \sim P_\Phi(X_i \mid \mathbf{x}_{-i})$

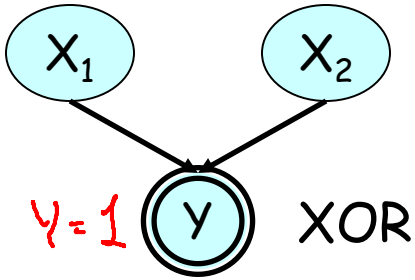
$$P_\Phi(X_i \mid \boldsymbol{x}_{-i}) = \frac{P_\Phi(X_i, \boldsymbol{x}_{-i})}{P_\Phi(\boldsymbol{x}_{-i})} = \frac{\tilde{P}_\Phi(X_i, \boldsymbol{x}_{-i})}{\tilde{P}_\Phi(\boldsymbol{x}_{-i})}$$

only X_i and its neighbors

$$\propto \prod_{j: X_i \in Scope[C_j]} \phi_j(X_i, \boldsymbol{x}_{j,-i})$$

factors that involve x_i

Gibbs Chain and Regularity



X_1	X_2	Y	Prob
~~0~~	~~0~~	~~0~~	~~0.25~~
0	1	1	0.25
1	0	1	0.25
~~1~~	~~1~~	~~0~~	~~0.25~~

- If all factors are positive, Gibbs chain is regular
- However, mixing can still be very slow

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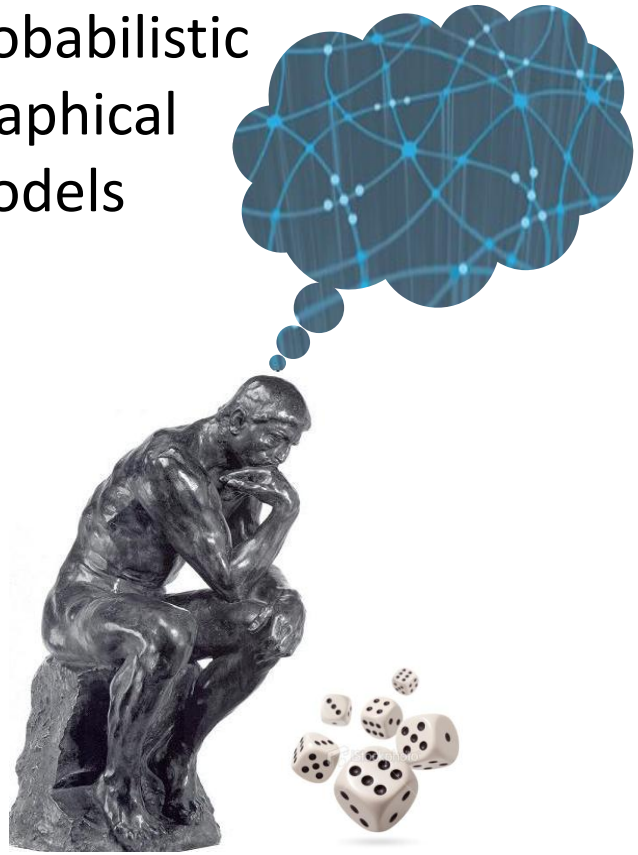
Summary

- Converts the hard problem of inference to a sequence of "easy" sampling steps
- Pros:
  - Probably the simplest Markov chain for PGMs
  - Computationally efficient to sample
- Cons:
  - Often slow to mix, esp. when probabilities are peaked
  - Only applies if we can sample from product of factors

Probabilistic Graphical Models

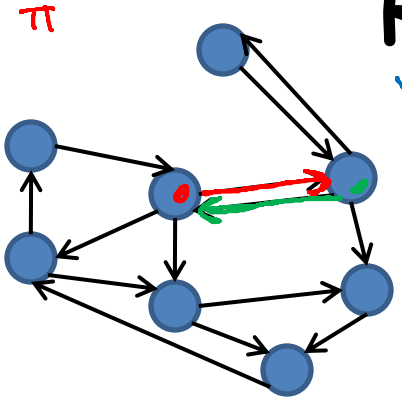


Inference

Sampling Methods

Metropolis-Hastings Algorithm

Reversible Chains



$$\pi(x)T(x \to x') = \pi(x')T(x' \to x)$$

detailed balance

Theorem: If detailed balance holds, and T is regular, then T has a unique stationary distribution π

Proof:

$$\sum_x \pi(x)T(x \to x') = \sum_x \pi(x')T(x' \to x) = \pi(x') \cdot \underbrace{\sum_x T(x' \to x)}_{1}$$

$$\to \sum_x \pi(x)T(x \to x') = \pi(x')$$ definition of π

Metropolis Hastings Chain

Proposal distribution $Q(x \to x')$

Acceptance probability: $A(x \to x')$

- At each state x, sample x' from $Q(x \to x')$
- Accept proposal with probability $A(x \to x')$
  - If proposal accepted, move to x'
  - Otherwise stay at x

$$T(x \to x') = Q(x \to x')\, A(x \to x') \quad \text{if } x' \neq x$$

$$T(x \to x) = Q(x \to x) + \Sigma_{x' \neq x}\, Q(x \to x')\,(1 - A(x \to x'))$$

Acceptance Probability

$$\pi(\boldsymbol{x})T(\boldsymbol{x} \to \boldsymbol{x}') = \pi(\boldsymbol{x}')T(\boldsymbol{x}' \to \boldsymbol{x})$$

construct A s.t. holds for Q, π

$x \neq x'$ $\quad \pi(\boldsymbol{x})Q(\boldsymbol{x} \to \boldsymbol{x}')A(\boldsymbol{x} \to \boldsymbol{x}') = \pi(\boldsymbol{x}')Q(\boldsymbol{x}' \to \boldsymbol{x})A(\boldsymbol{x}' \to \boldsymbol{x})$

$A(x \to x') = p$
$A(x' \to x) = 1$

$$\frac{A(\boldsymbol{x} \to \boldsymbol{x}')}{A(\boldsymbol{x}' \to \boldsymbol{x})} = \frac{\pi(\boldsymbol{x}')Q(\boldsymbol{x}' \to \boldsymbol{x})}{\pi(\boldsymbol{x})Q(\boldsymbol{x} \to \boldsymbol{x}')} = p < 1$$

$$\mathcal{A}(\boldsymbol{x} \to \boldsymbol{x}') = \min\left[1, \frac{\pi(\boldsymbol{x}')Q(\boldsymbol{x}' \to \boldsymbol{x})}{\pi(\boldsymbol{x})Q(\boldsymbol{x} \to \boldsymbol{x}')}\right]$$

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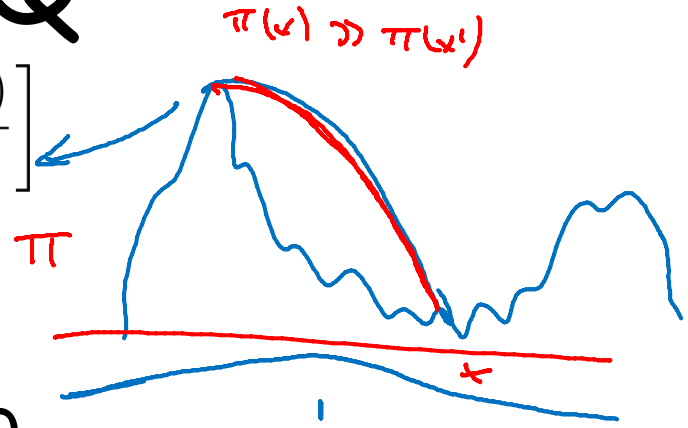
Choice of Q

$$\mathcal{A}(\boldsymbol{x} \to \boldsymbol{x}') = \min\left[1, \frac{\pi(\boldsymbol{x}')Q(\boldsymbol{x}' \to \boldsymbol{x})}{\pi(\boldsymbol{x})Q(\boldsymbol{x} \to \boldsymbol{x}')}\right]$$

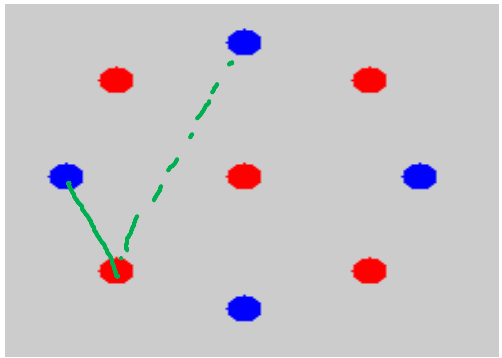


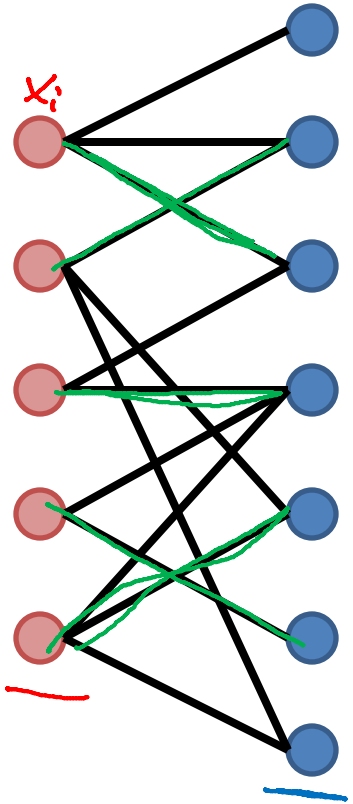
- Q must be reversible:
  - $Q(\boldsymbol{x} \to \boldsymbol{x}') > 0 \Rightarrow Q(\boldsymbol{x}' \to \boldsymbol{x}) > 0$
- Opposing forces
  - Q should try to spread out, to improve mixing
  - But then acceptance probability often low

MCMC for Matching

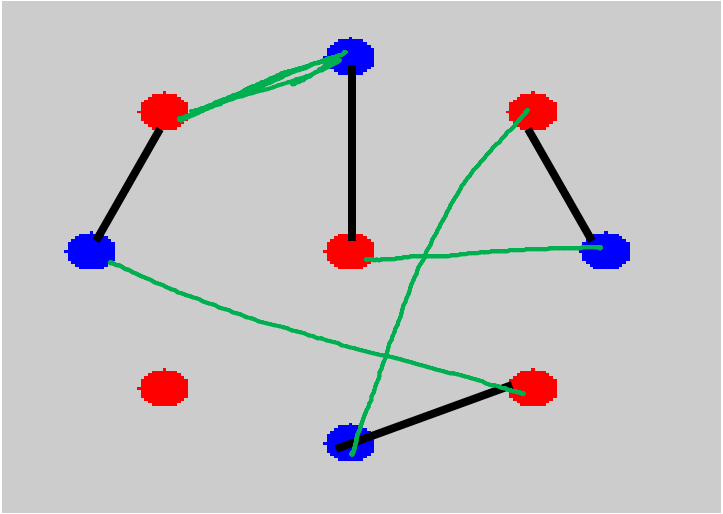
$X_i = j$ if i matched to j

$$P(X_1 = v_1, \ldots, X_4 = v_4) \propto \begin{cases} \exp(-\sum_i \text{dist}(i, v_i)) & \text{if every } X_i \text{ has different value} \\ 0 & \text{otherwise} \end{cases}$$





MH for Matching: Augmenting Path

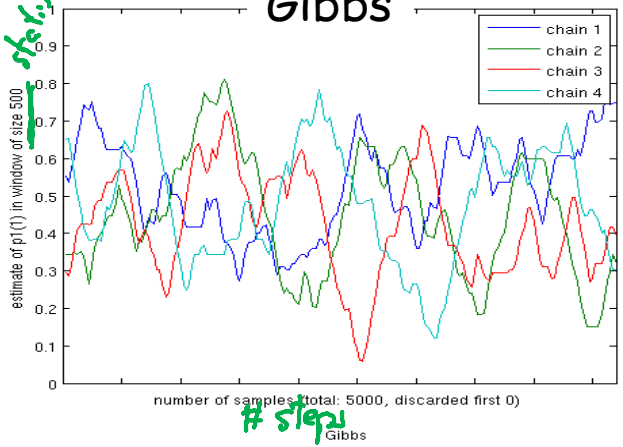


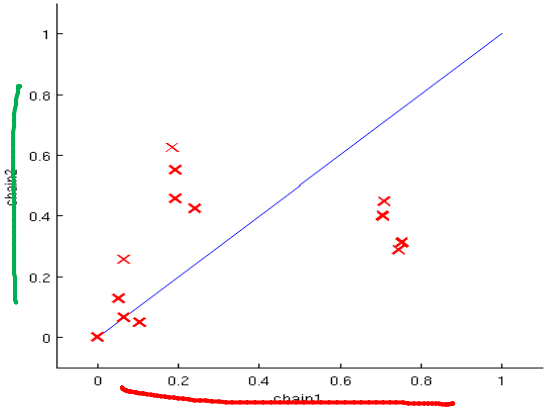
1) randomly pick one variable X_i
2) sample X_i, pretending that all values are available
3) pick the variable whose assignment was taken (conflict), and return to step 2

- When step 2 creates no conflict, modify assignment to flip augmenting path

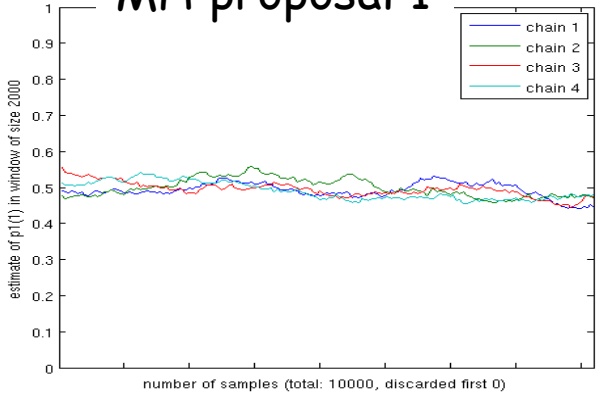
Example Results

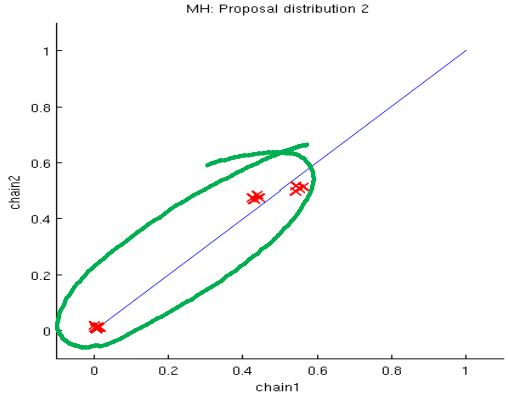
Gibbs



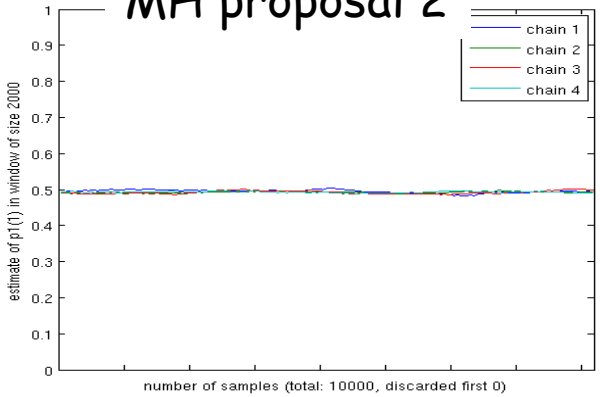


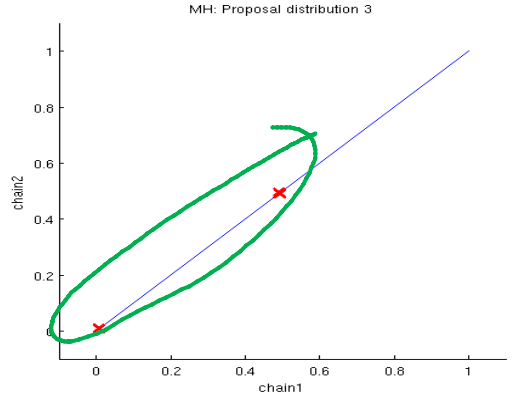
MH proposal 1





MH proposal 2





Summary

- MH is a general framework for building Markov chains with a particular stationary distribution
  - Requires a proposal distribution
  - Acceptance computed via detailed balance
- Tremendous flexibility in designing proposal distributions that explore the space quickly
  - But proposal distribution makes a big difference
  - and finding a good one is not always easy