Sampling Methods

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with slides by Prof.Dr. Cristobal Curio, FH Reutlingen

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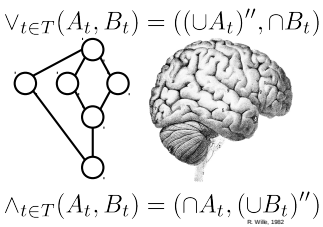

Outline

1. Why sampling?
2. Basic Sampling Algorithms
   - Rejection sampling
   - Importance sampling
3. Markov Chain Monte Carlo (MCMC)
   - Markov Chain methods
   - Gibbs Sampling

Sampling Methods Motivation

Why:

- Useful when deterministic approximations don't work (or we're too lazy)
- Stochastic approximations (Sampling methods)

Pro:

- Given infinite computational resources, they can generate exact results.
- Approximation arises from the use of a finite amount of processor time.
- Enable the use of Bayesian techniques across many domains.

Con: computationally demanding, often limited to small-scale problems.

Why sampling?
The summation/ integration problem

Almost everything we have learned about summation is valid for integration.

Normalization (Θ: e.g. parameters of a model, $\mathbf{x}$: evidence/data)
To obtain the posterior $p(\Theta|\mathbf{x})$ given the prior $p(\Theta)$ and the likelihood $p(\mathbf{x}|\Theta)$, the normalizing factor in Bayes theorem needs to be computed.

$$p(\Theta|\mathbf{x}) = \frac{p(\mathbf{x}|\Theta)\, p(\Theta)}{\int_{states} p(\mathbf{x}|\Theta)\, p(\Theta)\, d\Theta}$$

Example: making a prediction (Θ: est. model parameters, x: state, $\mathcal{D}$: evidence)

$$p(x|\mathcal{D}) = \int P(x|\Theta, \mathcal{D})\, P(\Theta|\mathcal{D})\, d\Theta$$

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Monte Carlo principle

Simple Monte Carlo

Idea: Sample from $p(x)$, average values of $f(x)$:

$$\textit{Estimator}: \int f(x)\, p(x)\, dx \approx \hat{f} \equiv \frac{1}{S} \sum_{s=1}^{S} f\left(x^{(s)}\right),\ x^{(s)} \sim p(x)$$

where $x^{(s)}$ are (independent) samples drawn from $p(x)$.

Attractions:

Estimator is unbiased:

$$\mathbb{E}_{P(\{x^{(s)}\})}\left[\hat{f}\right] = \frac{1}{S} \sum_{s=1}^{S} \mathbb{E}_{P(x^{(s)})}\left[f(x^{(s)})\right] = \mathbb{E}_{P(x)}\left[f(x)\right]$$

Variance shrinks $\propto 1/S$ independent of dimension!:

$$var_{P(\{x^{(s)}\})}\left[\hat{f}\right] = \frac{1}{S^2} \sum_{s=1}^{S} var_{P(x^{(s)})}\left[f(x^{(s)})\right] = var_{P(x)}\left[f(x)\right]/S$$

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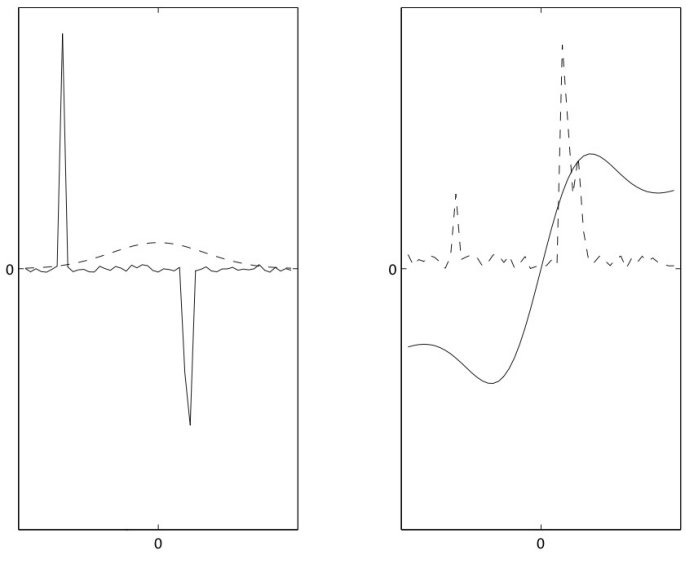
Why sampling?
The integration problem.



Z. Ghahramani

We often need to compute integrals of the form

$$\int f(x)\, p(x)\, dx$$

where $f(x)$ is some function of a random variable X which has probability density $p(x)$.

Three typical difficulties can arise:

left panel:

full line is some complicated function, dashed is density;

right panel:

full line is some function and dashed is complicated density;

not shown: integral (or sum) very high dimensions.

Monte Carlo sampling
Difficulties

Monte Carlo Estimator:

$$\int f(x) P(x) dx \approx \hat{f} \equiv \frac{1}{S} \sum_{s=1}^{S} f\left(x^{(s)}\right), x^{(s)} \sim P(x)$$

Problems with Monte Carlo sampling:

- it may be difficult (impossible) to obtain the samples directly from $P(x)$
- regions of high density $P(x)$ may not correspond to regions where $f(x)$ varies a lot

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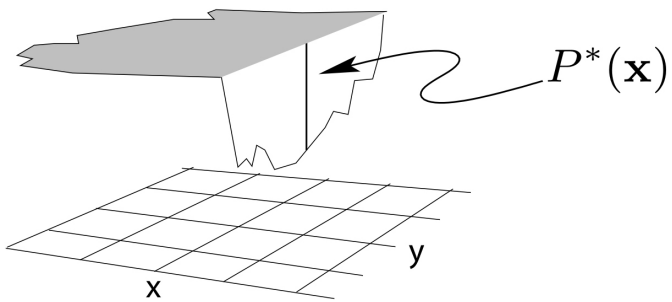
A real-world problem

Task: draw random water samples from a lake and find the average plankton concentration.



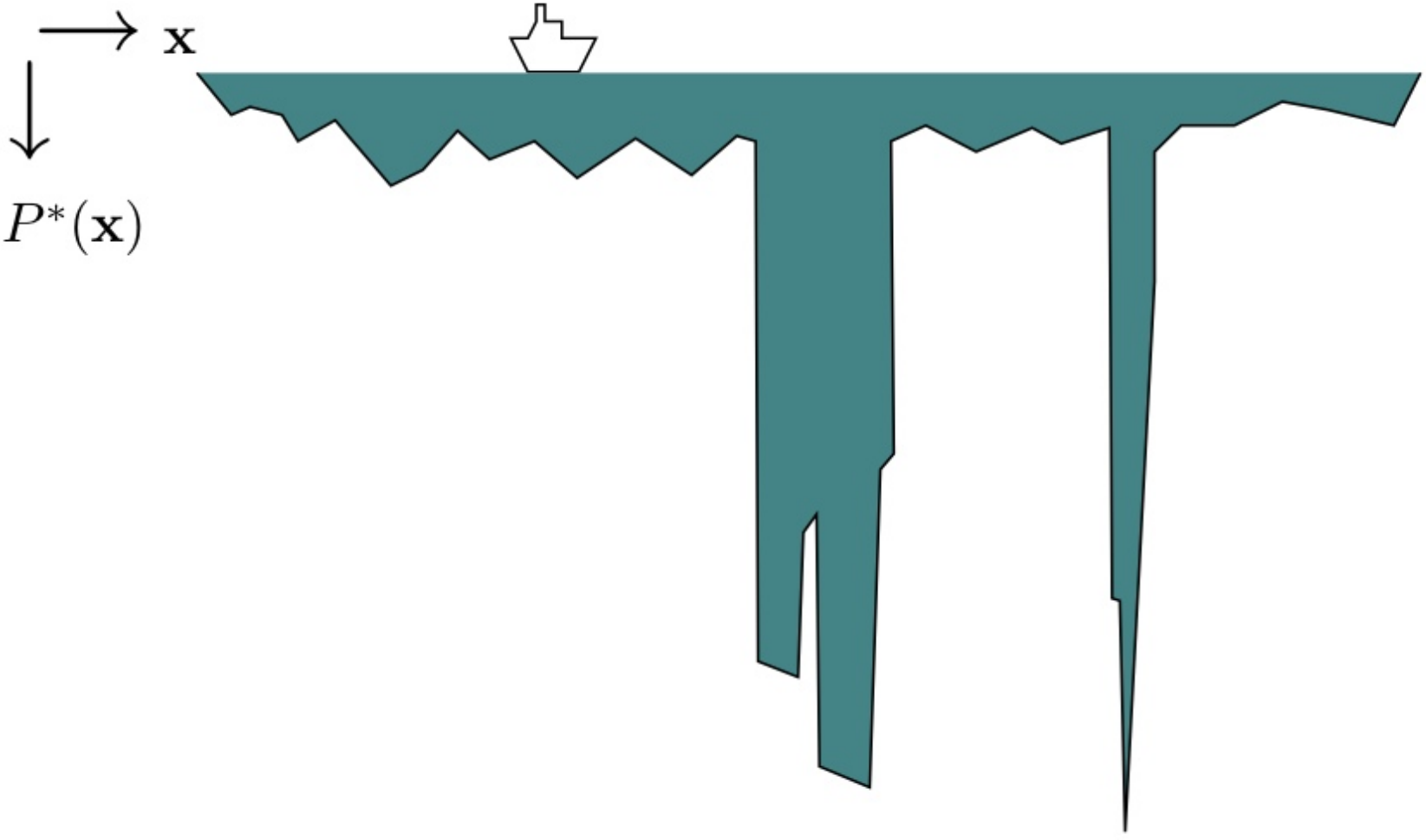
Assume we can measure

- The depth of the lake: $P^{\star}(\mathbf{x}), \mathbf{x} = (x, y)$
- Plankton concentration: $f(\mathbf{x})$

The required average concentration is an integral of the above form, namely

$$< f(\mathbf{x}) > \quad = \quad \frac{1}{Z} \int f(\mathbf{x}) P^{\star}(\mathbf{x}) \, d\mathbf{x} \quad Z = \int P^{\star}(\mathbf{x}) \, dxdy$$

Difficult samples



Sampling discrete distributions

Sampling from a univariate discrete distribution p with K states

Fundamental to understand how to sample probability distributions:
How can we "sample from a distribution"?
Assume for now:
univariate discrete (not conditional) distribution p, with K states, e.g.

$$p(x) = \begin{cases} 0.6 & x = 1 \\ 0.1 & x = 2 \\ 0.3 & x = 3 \end{cases}$$

Throw uniformly a dart to this partition of distribution and determine the corresponding $k \in 1, 2, 3$ as state of the sample

1	×	2	3

Sampling discrete distributions

Sampling from a univariate discrete distribution p with K states

Implementation

1: Label the K states as $i = 1, \ldots, K$, with associated probabilities p_i.
2: Calculate the *cumulant*

$$c_i = \sum_{j \leq i} p_j$$

and set $c_0 = 0$.
3: Draw a value u uniformly at random from the unit interval $[0, 1]$.
4: Find that i for which $c_{i-1} \leq u \leq c_i$.
5: Return state i as a sample from p.

First, compute the discrete cumulative histogram and then draw a uniform random variable $u \sim U[0, 1]$, and select a discrete **state** i, c.f. denoting *the sample*.

Sampling discrete distributions

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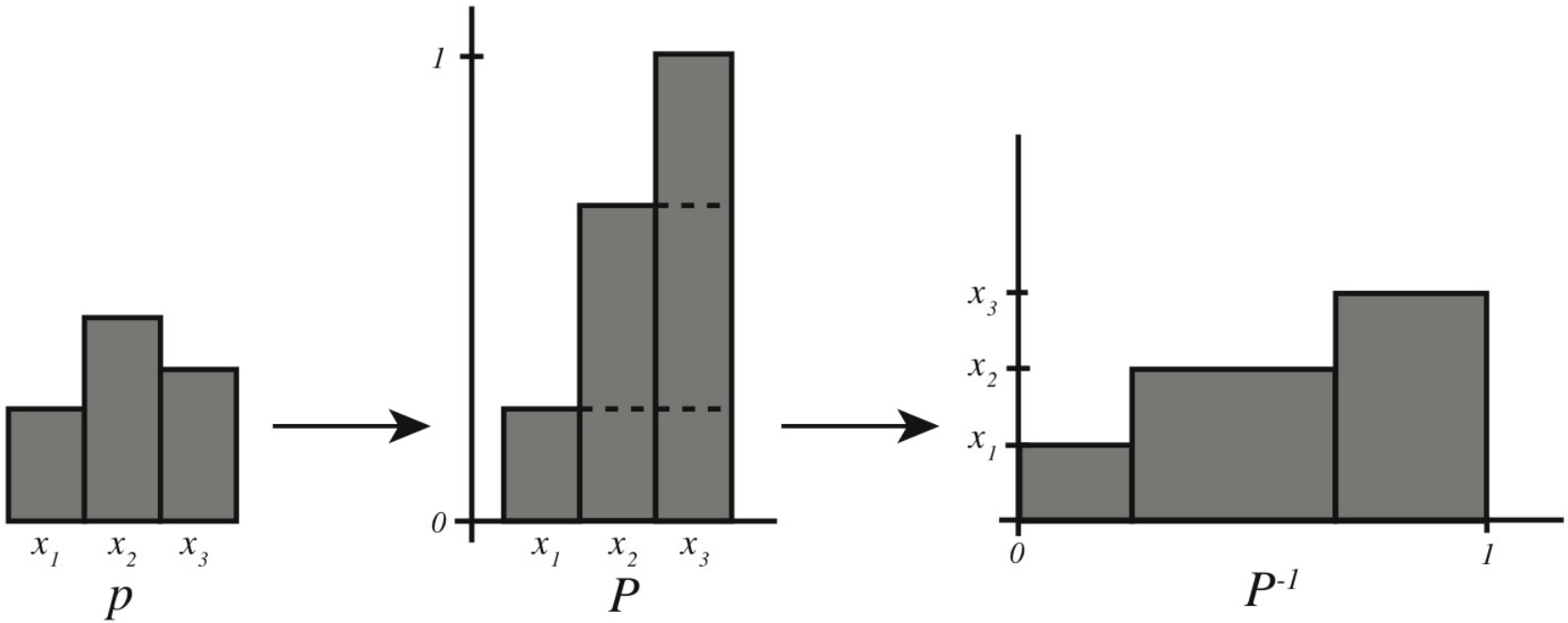
Another illustration of sampling from discrete distribution:



1. Distribution is given by p with discrete states $x = 1, 2, 3$ or $x_1, x_2,$ and x_3
2. $\rightarrow$ derive the cumulative distribution P
3. $\rightarrow$ Map uniform sample $U[0, 1]$ via inverse cumulative function P^{-1} to state 1, 2 or 3

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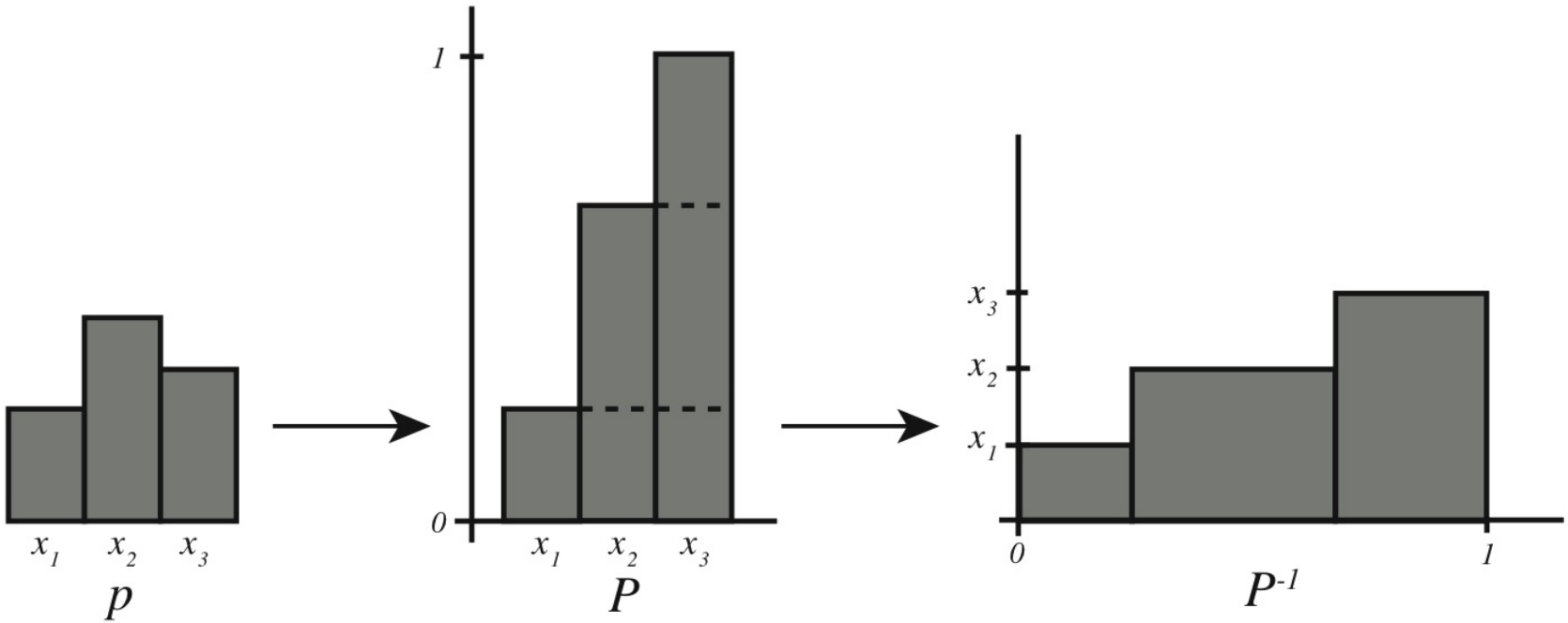

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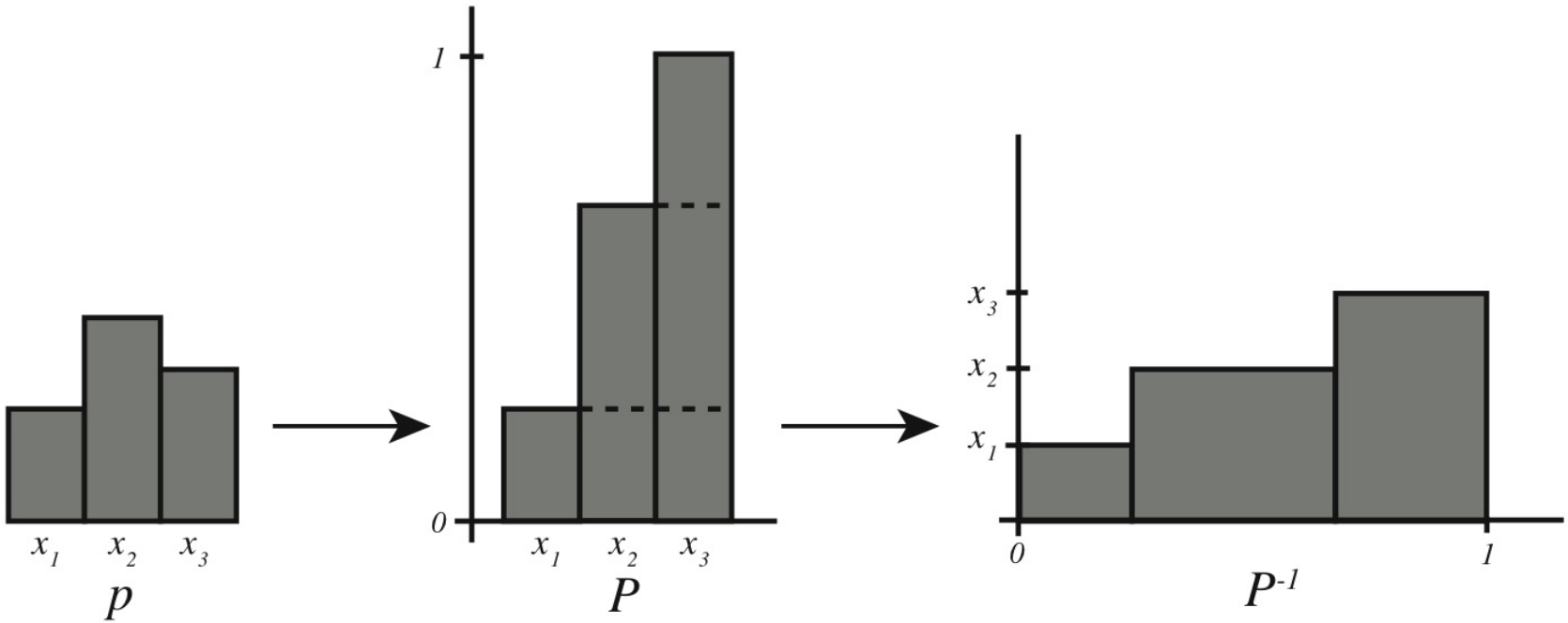

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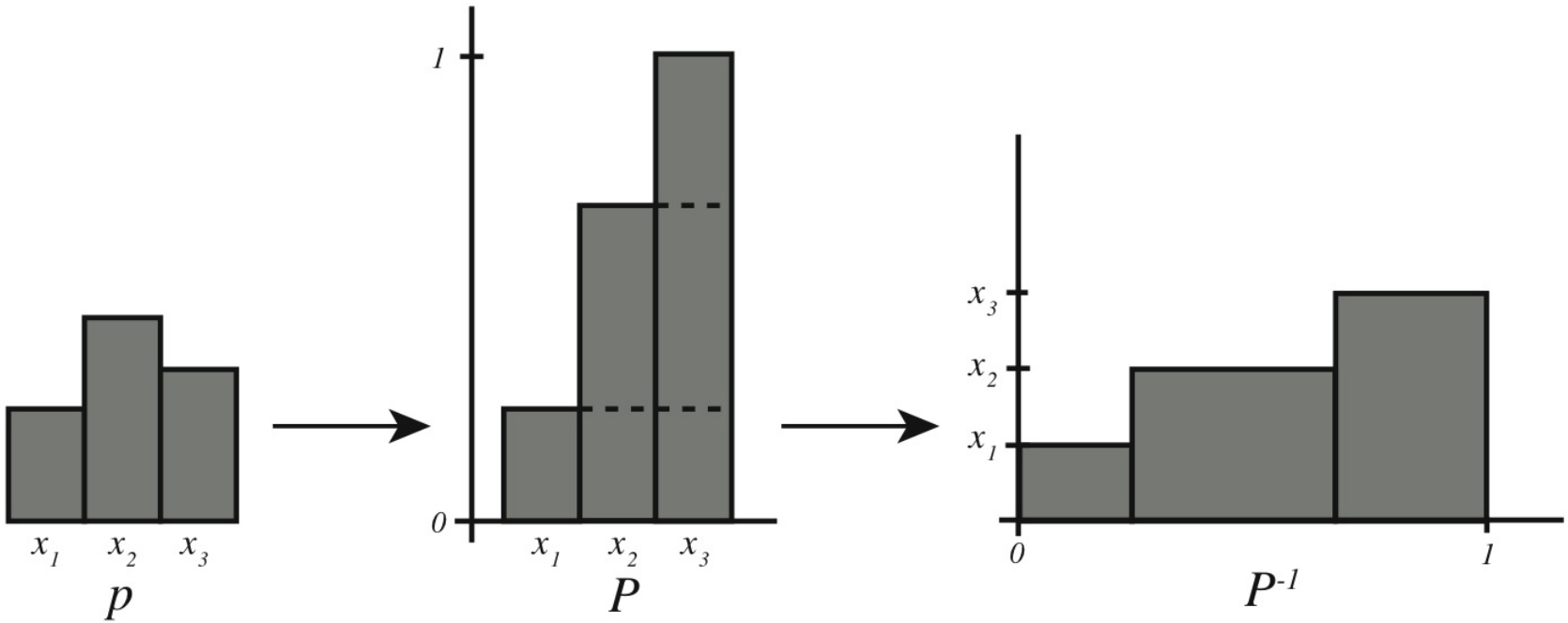

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Sampling discrete distributions

Multidimensional distributions

Problem: Sample from $p(x_1, \ldots, x_n)$ We can sample from the joint distribution $p(x_1, \ldots, x_n)$ by

1. sampling a state for x_1 from the one-dimensional $p(x_1)$
2. with x_1 clamped/ fixed to this state, sampling from the one-dimensional $p(x_2|x_1)$ a state for x_2

We can generalize this scheme by cascading this approach by decomposition into conditional probability distributions

$$p(x_1, \ldots, x_n) = p(x_n|x_{n-1}, \ldots, x_n)\, p(x_{n-1}|x_{n-2}, \ldots, x_1) \ldots p(x_2|x_1)\, p(x_1)$$

In **Belief Networks**, however, these conditionals are computationally tractable and specified which leads to ancestral sampling

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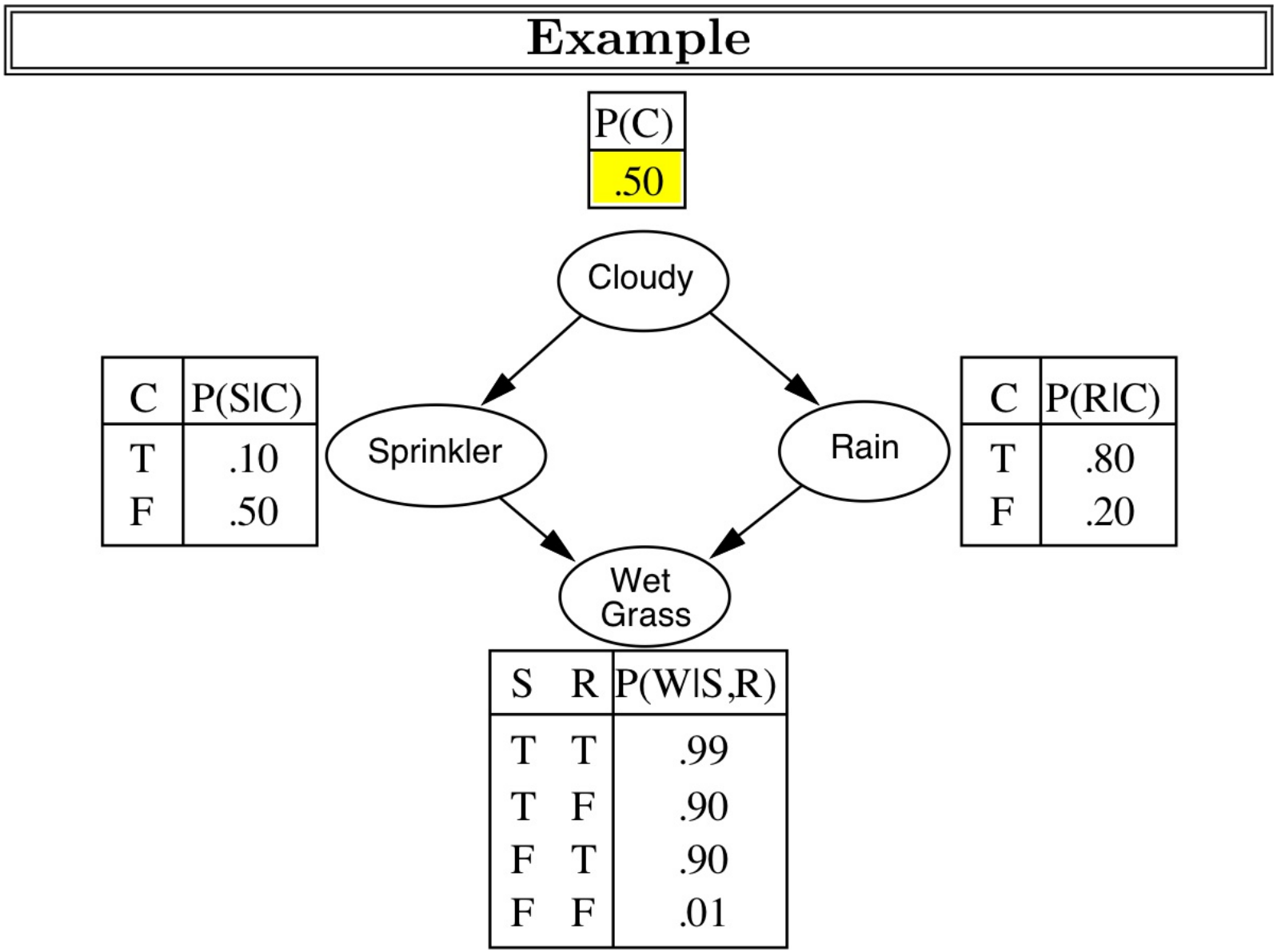
Sampling from an empty Network



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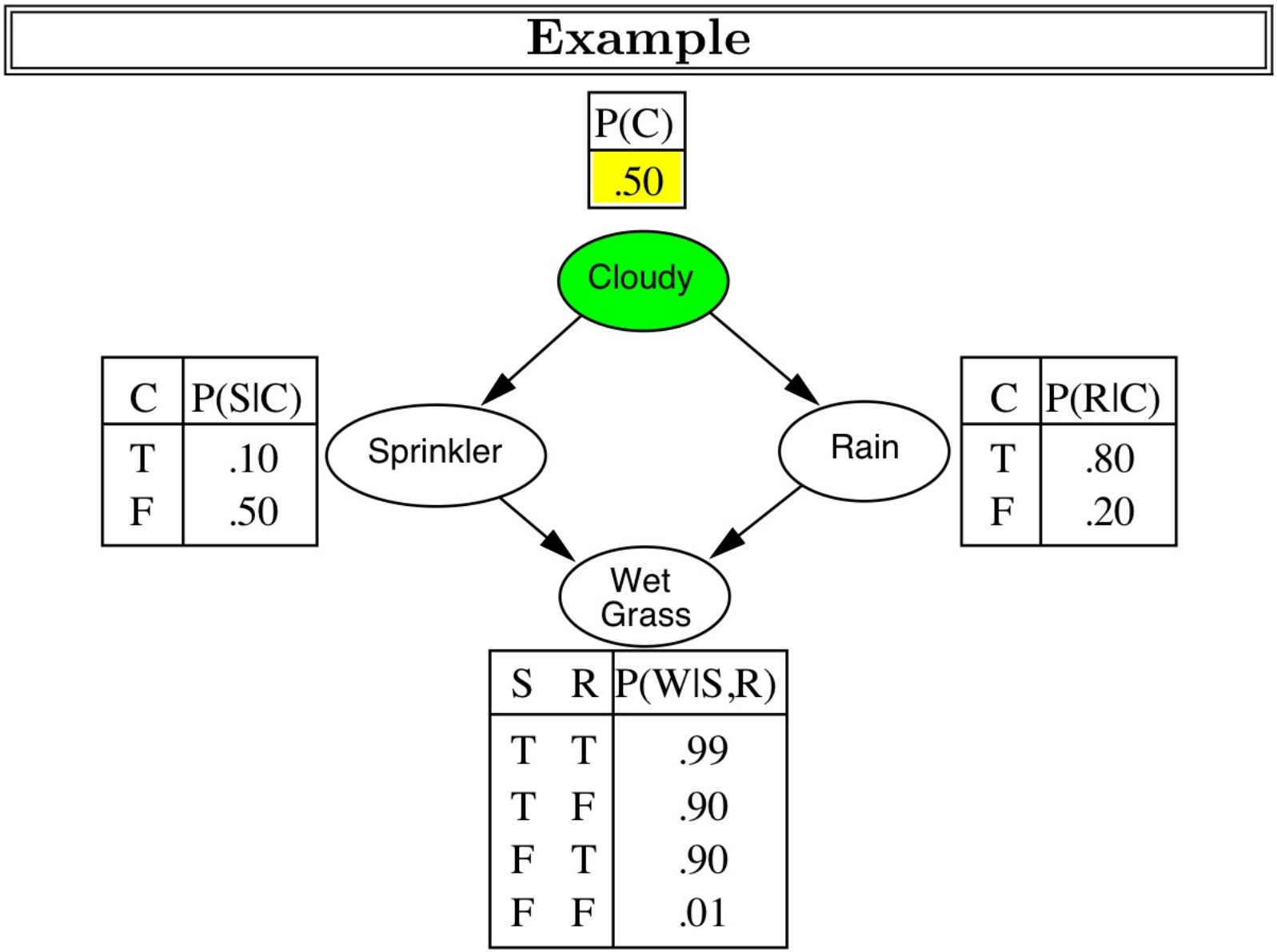

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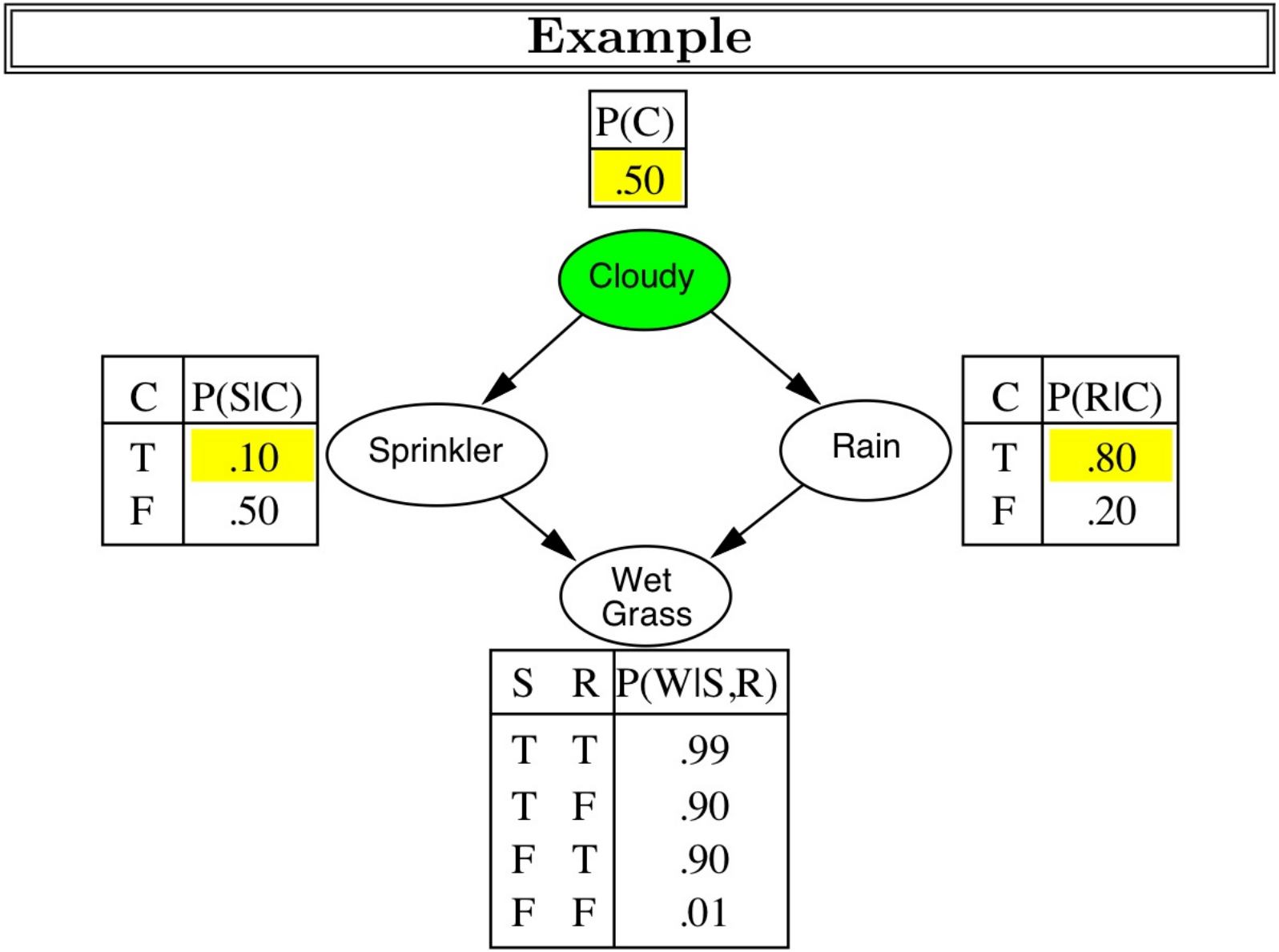

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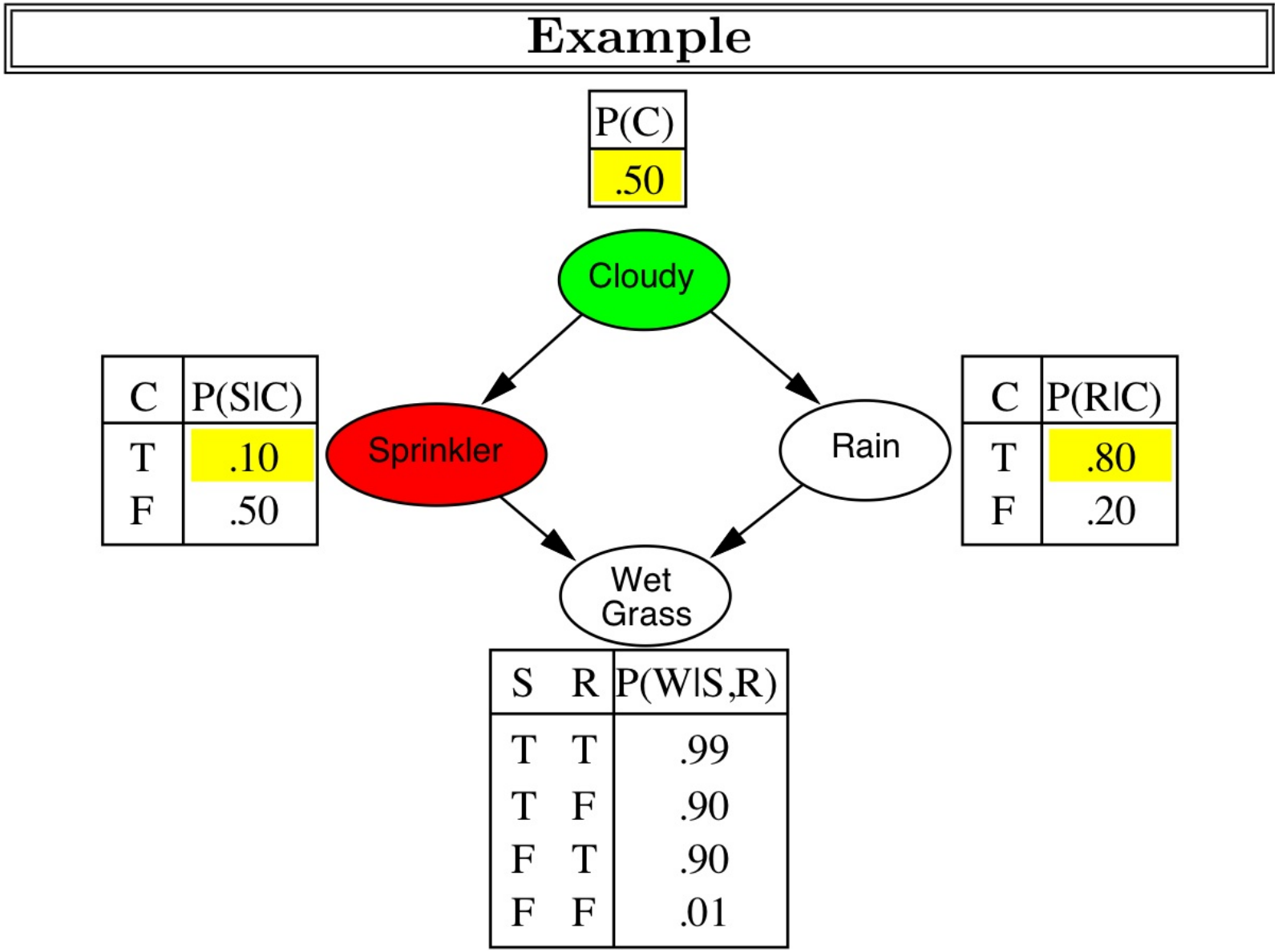

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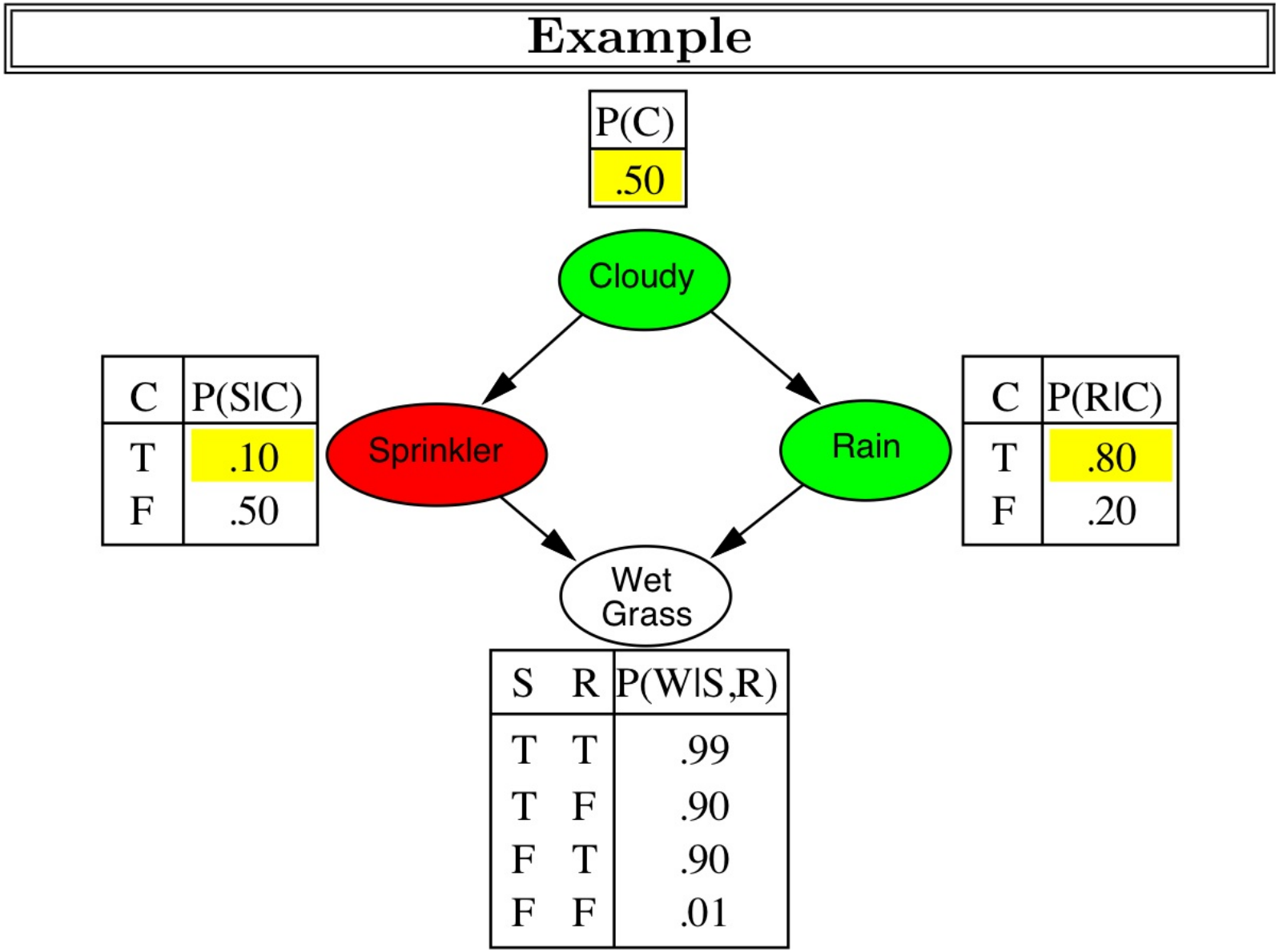

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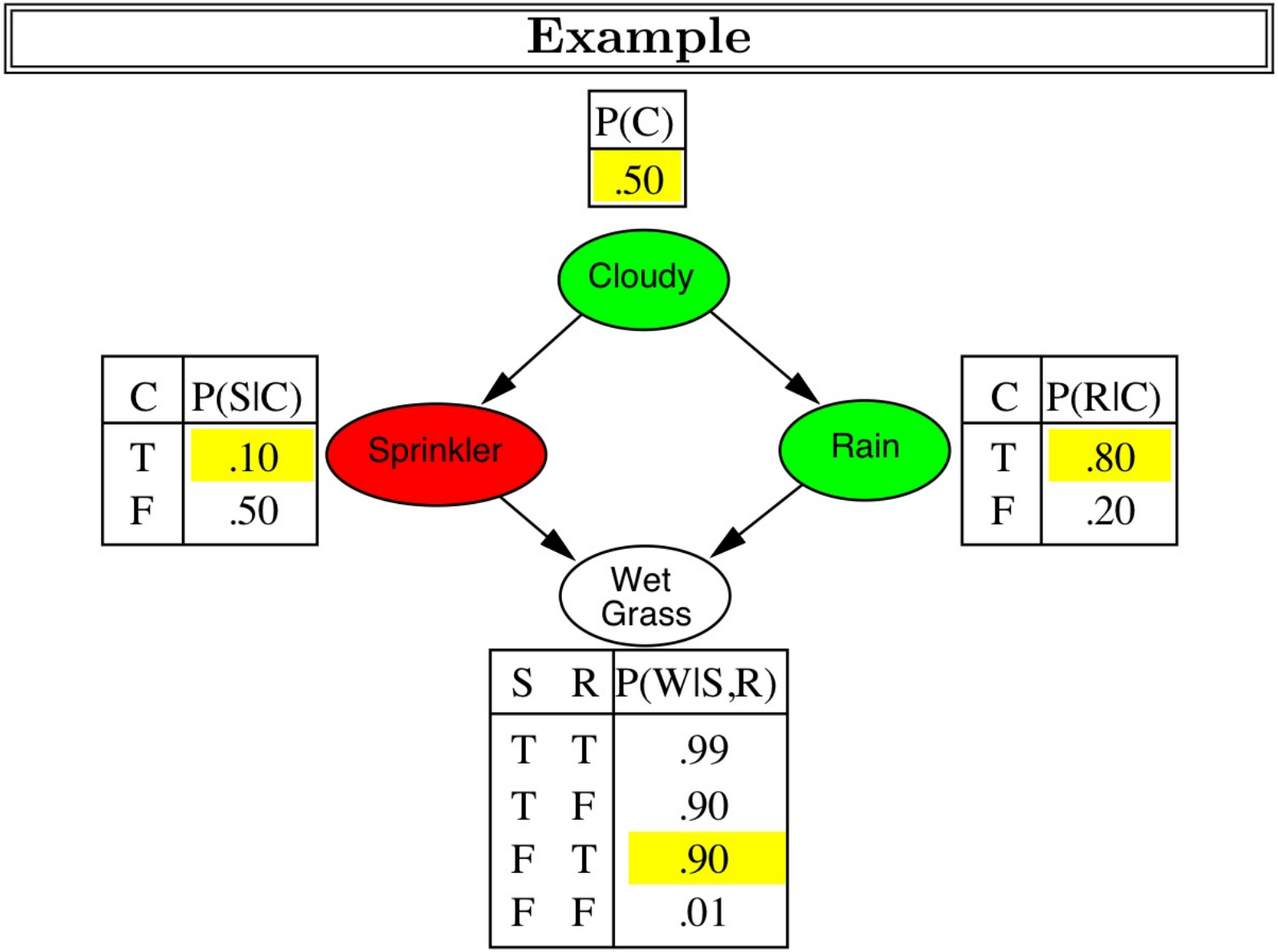

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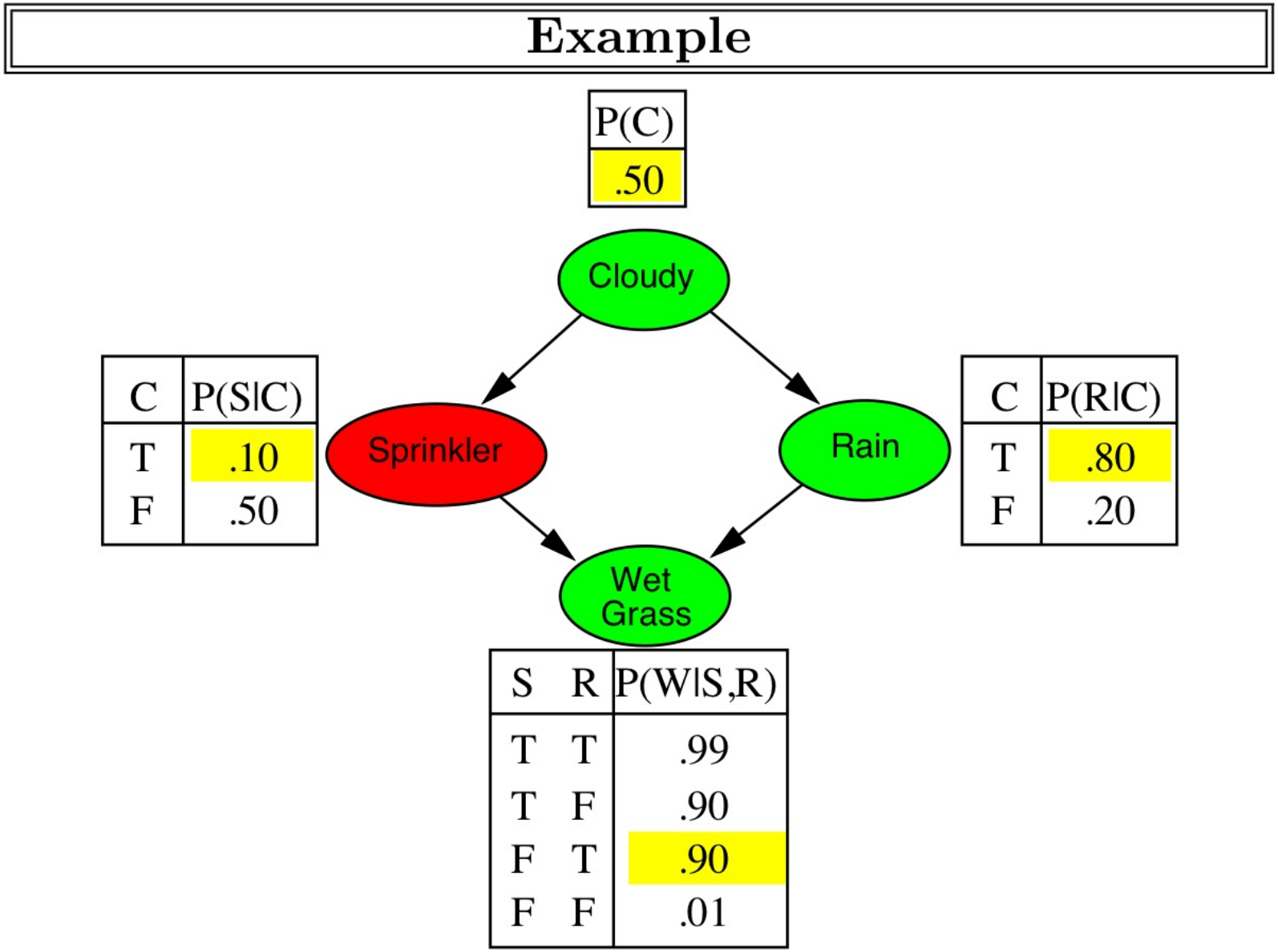

Ancestral sampling (Prior Sampling) from empty network

Probability that this prior sampling (PS) scheme generates a particular event

$$S_{PS}(x_1, \ldots, x_n) = \prod_i^n P(x_i | parents(X_i)) = P(x_1, \ldots, x_n)$$

i.e., the true prior probability.

E.g., $S_{PS}(t, f, t, t) = 0.5 \times 0.9 \times 0.8 \times 0.9 = 0.324 = P(t, f, t, t)$

Let $N_{PS}(x_1, \ldots, x_n)$ be the number of samples generated for event $x_1, \ldots, x_n$

Then we have

$$\begin{aligned} \lim_{N \to \infty} \hat{P}(x_1, \ldots, x_n) &= \lim_{N \to \infty} N_{PS}(x_1, \ldots, x_n)/N \\ &= S_{PS}(x_1, \ldots, x_n) \\ &= P(x_1, \ldots, x_n) \end{aligned}$$

That is, estimates derived from Ancestral Sampling are **consistent**.

Shorthand: $\hat{P}(x_1, \ldots, x_n) \approx P(x_1, \ldots, x_n)$

Rejection sampling in network with observed nodes

- We have a Bayesian Network with RVs $X_{1:n}$, some of which are observed: $X_{obs} = y_{obs}, obs \subset \{1 : n\}$
- The goal is to compute marginal posteriors $P(X|X_{obs} = y_{obs})$ conditioned on the observations
- Our strategy is to generate a set of K (joint) samples of all variables

$$\mathcal{S} = \left\{(x_1^k, x_2^k, \ldots, x_n^k)\right\}_{k=1}^{K}$$

Note: Each sample $x_{1:n}^k$ is a list of instantiations of all RVs.

Rejection sampling in network with observed nodes

To generate a single sample $x^k_{1:n}$

1. Sort all RVs in topological order; start with $i = 1$
2. Sample a value $x^k_i \sim P\left(X_i | x_{\text{Parents(i)}}\right)$ for the ith RV conditional to the previous samples $x^k_{1:i-1}$
3. If $i \in obs$ compare the sampled value x^k_i with the observation y_i. Reject and repeat from 1) if the sample is not equal to the observation.
4. Repeat with $i \leftarrow i + 1$ from 2.

Rejection sampling in network with observed nodes

- Since computers are fast, we can sample for large K
- The sample set

$$\mathcal{S} = \left\{(x_1^k, x_2^k, \ldots, x_n^k)\right\}_{k=1}^{K}$$

implies the necessary information:

- We can compute the marginal probabilities from these statistics:

$$P\left(X_i = x | X_{obs} = y_{obs}\right) \approx \frac{count_{\mathcal{S}}\left(X_i^k = x\right)}{K}$$

- or pair-wise marginals:

$$P\left(X_i = x, X_i = x' | X_{obs} = y_{obs}\right) \approx \frac{count_{\mathcal{S}}\left(X_i^k = x \wedge X_i^k = x'\right)}{K}$$

- etc.

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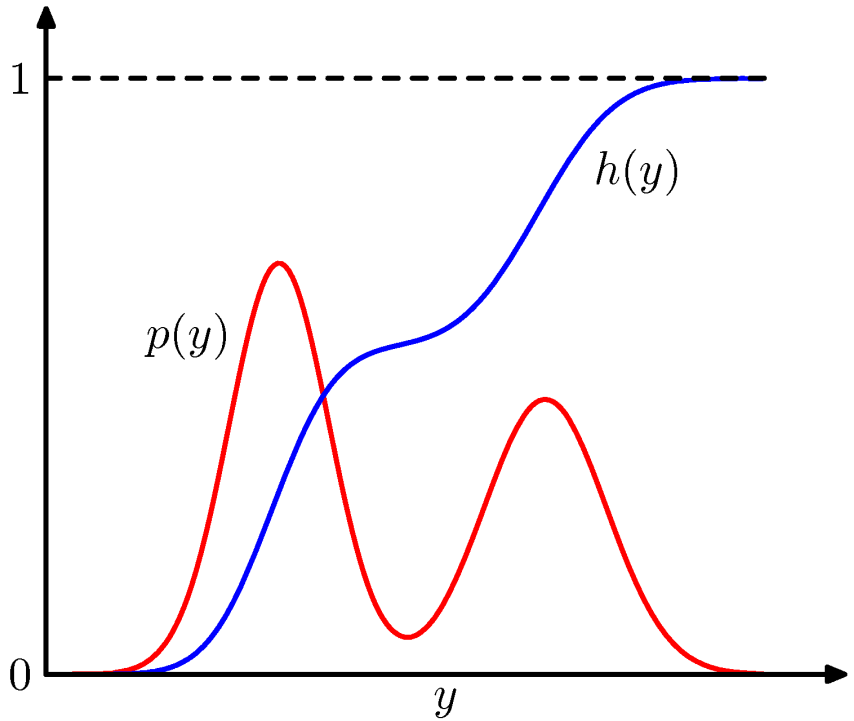
  - etc.

Sampling continuous distributions

Again, as in the discrete case, assume a uniform sample generator given.
Now, how can we convert samples from a Uniform $[0, 1]$ random number generator?



$$F(y) = \int_{-\infty}^{y} p(y')\, dy' \qquad (1)$$

Draw mass to left of point:
$u \approx$ Uniform $[0, 1]$
Sample, $y(u) = F^{-1}(u)$

Sampling continuous distributions

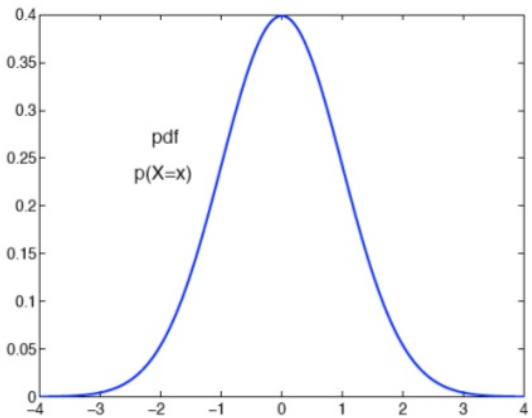
- **Given: 1-dim. Gaussian pdf (probability density function) $p(\mathbf{x}|\mu,\sigma^2)$ and the corresponding cumulative distribution:**

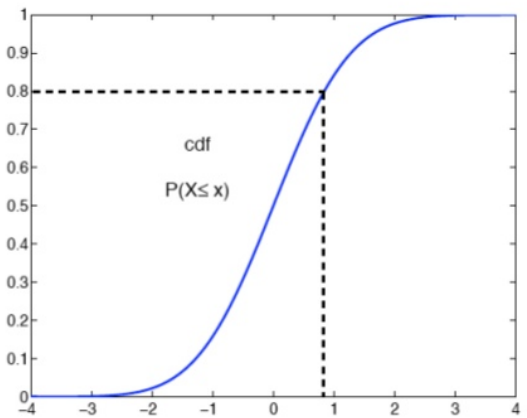
$$F_{\mu,\sigma^2}(x) = \int_{-\infty}^{x} p(x|\mu,\sigma^2)dx$$

- **To draw samples from a Gaussian, we can invert the cumulative distribution function:**

$$u \sim Uniform(0,1) \Rightarrow F^{-1}_{\mu,\sigma^2}(u) \sim p(x|\mu,\sigma^2)$$

$p(x|\mu,\sigma^2)$





$F_{\mu,\sigma^2}(x)$

Sampling continuous distributions

Parametric density model example

A simple multivariate (D-dimensional) Gaussian model

$$p(\mathbf{x}|\mu, \mathbf{\Sigma}) = \frac{1}{(2\pi)^{D/2}|\mathbf{\Sigma}|^{1/2}} \exp\left\{-\frac{1}{2}(\mathbf{x}-\mu)^T \mathbf{\Sigma}^{-1}(\mathbf{x}-\mu)\right\}$$

- This is a "generative" model in the sense that we can generate samples $\mathbf{x}$ according to the distribution.
- With a $\mathbf{C}$ fulfulling $\mathbf{\Sigma} = \mathbf{C}\mathbf{C}^T$ and $T : \mathbf{y} = \mathbf{C}^{-1}(\mathbf{x} - \mu)$ we can transform $p(\mathbf{x}|\mu, \mathbf{\Sigma}) \rightarrow p(\mathbf{y}|\mathbf{0}, \mathbf{I})$

We can now draw indepedent Gaussian samples y_i of $\mathbf{y}$, since $p(\mathbf{y}) = \mathcal{N}(\mathbf{y}|\mathbf{0}, \mathbf{I}) = \prod_i \mathcal{N}(y_i|0, 1) = \prod_i p(y_i)$ and transform them back $T^{-1} : \mathbf{x} = \mathbf{C}\mathbf{y} + \mu$ to generate data

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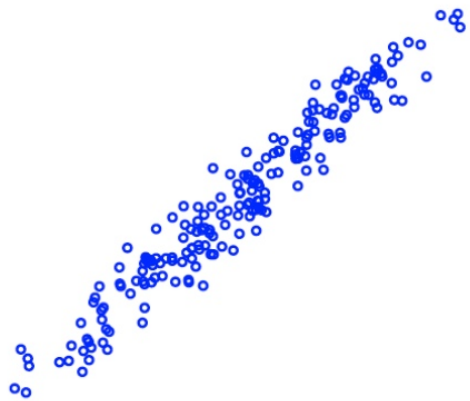

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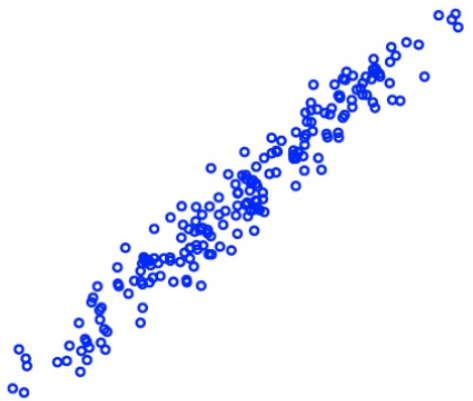

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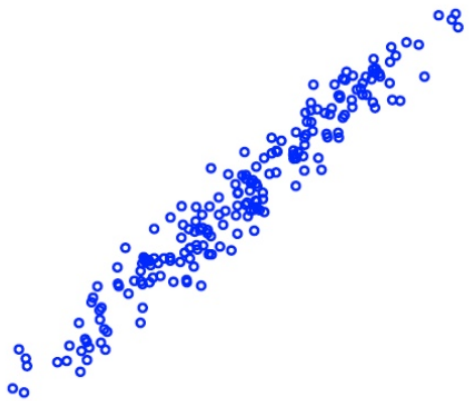

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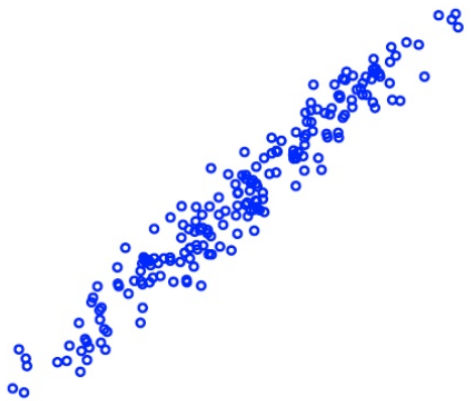

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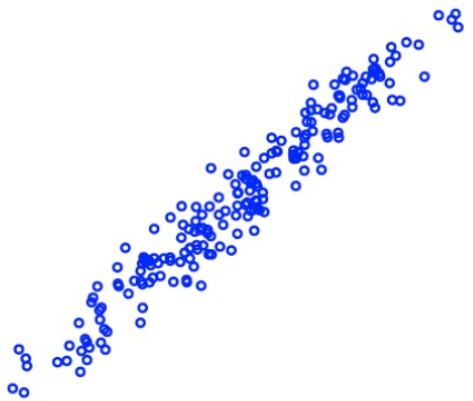

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Discussion

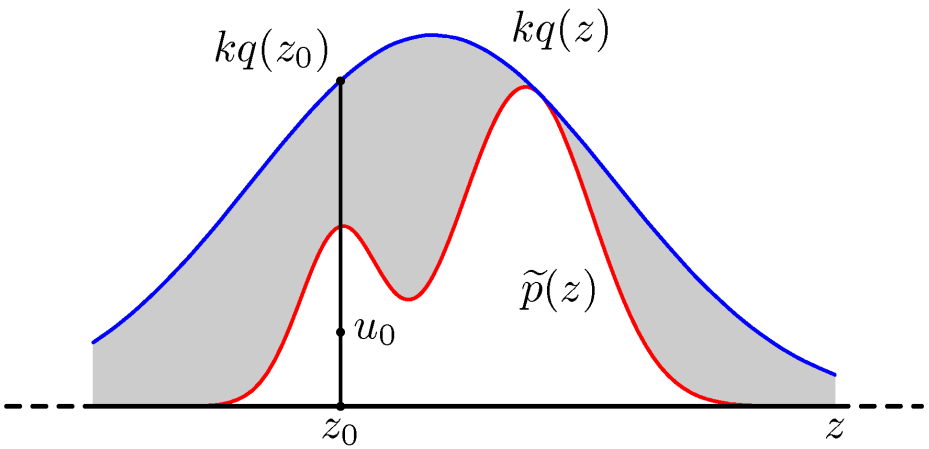
- Transformation method
  - Limited applicability, as we need to invert the indefinite integral of the required distribution $p(x)$
- More general
  - Rejection Sampling
  - Importance Sampling

Rejection Sampling

- Assumptions
  - Sampling directly from $p(\mathbf{z})$ is difficult
  - But we can easily evaluate $p(\mathbf{z})$ (up to some normalization factor Z_p):

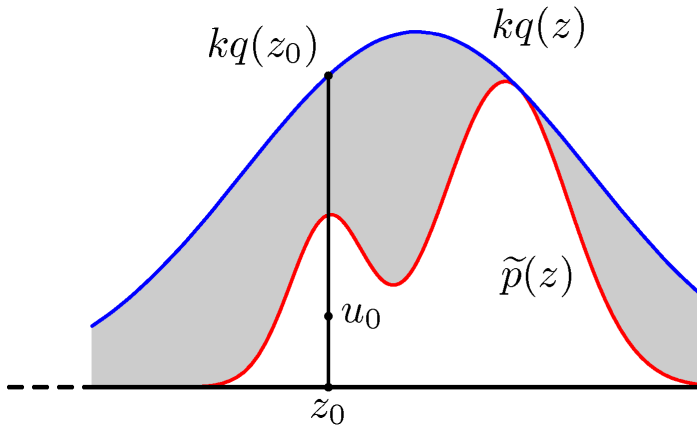
$$p(\mathbf{z}) = \frac{1}{Z_P}\tilde{p}(\mathbf{z})$$

- Idea
  - We need some simpler distribution $q(\mathbf{z})$ (called proposal distribution) from which we can draw samples.
  - Choose a constant k such that: $\forall z : kq(z) \geqslant \tilde{p}(z)$



Rejection Sampling

Sampling procedure



- Generate a number z_0 from $q(z)$
- Generate a number u_0 from the uniform distribution over $[0, kq(z_0)]$.
- If $u_0 > \tilde{p}(z_0)$ reject sample, otherwise accept.
  - Sample is rejected if it lies in the grey shaded area.
  - The remaining pairs (u_0, z_0) have uniform distribution under the curve $\tilde{p}(z)$.

Discussion

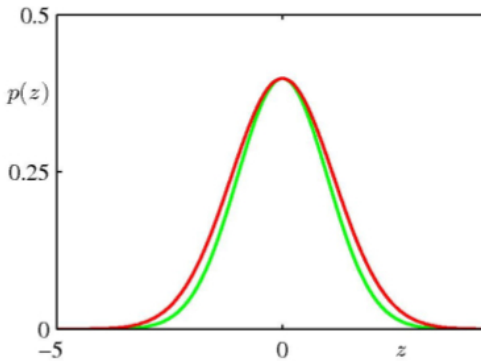
- Original values of z are generated from the distribution $q(z)$.
- Samples are accepted with probability $\tilde{p}(z)/kq(z)$

$$p(accept) = \int (\tilde{p}(z)/kq(z))\, q(z) dz = \frac{1}{k} \int \tilde{p}(z_0)\, dz$$

$\rightarrow$ k should be as small as possible!!!

Rejection Sampling - Discussion

- **Limitation: high-dimensional spaces**
  - For rejection sampling to be of practical value, we require that $kq(z)$ be close to the required distribution, so that the rate of rejection is minimal.
- **Artificial example**
  - Assume that $p(\mathbf{z})$ is Gaussian with covariance matrix $\sigma_p^2 I$
  - Assume that $q(\mathbf{z})$ is Gaussian with covariance matrix $\sigma_q^2 I$
  - Obviously: $\sigma_q^2 \geq \sigma_p^2$
  - In D dimensions: $k = (\sigma_q/\sigma_p)^D$.
    - Assume σ_q is just 1% larger than σ_p.
    - $D = 1000 \Rightarrow k = 1.01^{1000} \geq 20{,}000$
    - And $p(accept) \leq \frac{1}{20000}$



$\Rightarrow$ Often impractical to find good proposal distributions for high dimensions!

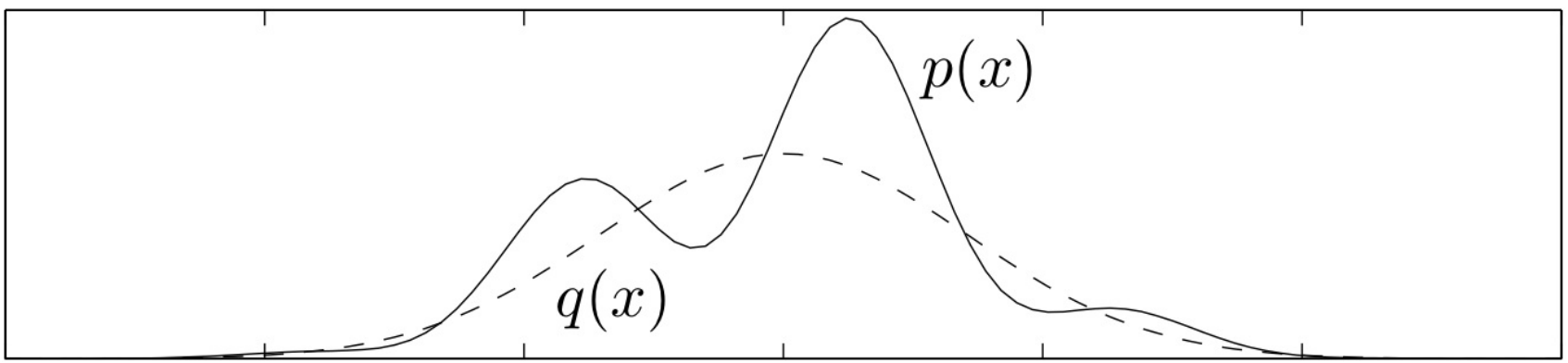
Idea importance sampling

Weighting scheme

Idea: Sample from a different distribution $q(x)$ and weight those samples by $p(x)/q(x)$
Sample $x^{(t)}$ from $q(x)$:

$$\int f(x)\, p(x)\, dx = \int f(x)\, \frac{p(x)}{q(x)} q(x) dx \simeq \frac{1}{T} \sum_{t=1}^{T} f\left(x^{(t)}\right) \frac{p\left(x^{(t)}\right)}{q\left(x^{(t)}\right)}$$

where $q(x)$ is non-zero wherever $p(x)$ is; $w^{(t)} \equiv p\left(x^{(t)}\right)/q\left(x^{(t)}\right)$.



Importance sampling (with likelihood weighting)

- Rejection whole sample (see Ancrestral/Rejection Sampling) may become very inefficient in large Bayes Nets!
- New strategy: We generate a **weighted** sample set

$$\mathcal{S} = \left\{(\omega^k, x_1^k, x_2^k, \ldots, x_n^k)\right\}_{k=1}^{K}$$

where each sample $x_{1:n}^k$ is associated with a weight ω^k.

- In our case, we will choose the weights proportional to the likelihood $P\left(X_{obs} = y_{obs} | X_{1:n} = x_{1:n}^k\right)$ of the observations conditional to the sample $x_{1:n}^k$

Importance sampling

To generate a single sample $(\omega^k, x^k_{1:n})$:

1. Sort all RVs in topological order; start with $i = 1$ and $\omega^k = 1$
2. a) If $i \notin obs$, sample a value $x^k_i \sim P\left(X_i | x^k_{\text{Parents}(i)}\right)$ for the ith RV conditional to the previous samples $x^k_{1:i-1}$
   b) If $i \in obs$, set the value $x^k_i = y_i$ and update the weight according to likelihood
   $$\omega^k \leftarrow \omega^k P\left(X_i = y_i | x^k_{1:i-1}\right)$$
3. Repeat with $i \leftarrow i + 1$ from 2.

Importance sampling (with likelihood weighting)

From a weighted sample set

$$\mathcal{S} = \left\{\left(\omega^k, x_1^k, x_2^k, \ldots, x_n^k\right)\right\}_{k=1}^{K}$$

- we can compute the marginal probabilities:

$$P\left(X_i = x | X_{obs} = y_{obs}\right) \approx \frac{\sum_{k=1}^{K} \omega^k [[x_i^k = x]]}{\sum_{k=1}^{K} \omega^k}$$

- and likewise pair-wise marginals, etc.

Notation: $[[expr]] = 1$ if *expr* is true and zero otherwise

Importance Sampling - Discussion

- Observations
  - Success of importance sampling depends crucially on how well the sampling distribution $q(x)$ matches the desired distribution $p(x)$.
  - Often, $p(x)f(x)$ is strongly varying and has a significant proportion of its mass concentrated over small regions of x-space.

  $\rightarrow$ Weights w may be dominated by a few weights having large values.
  - Practical issue: if none of the samples falls in the regions where $p(x)f(x)$ is large
    - The results may be arbitrary in error.
    - And there will be no diagnostic indication
- Key requirement for sampling distribution $q(x)$:
  - Should not be small or zero in regions where $p(x)$ is significant!

Summary so far

- Sums and integrals, often expectations, occur frequently in statistics
- Monte Carlo approximates expectations with a sample average
- Rejection sampling draws samples from complex distributions
- Importance sampling applies Monte Carlo to any sum/integral

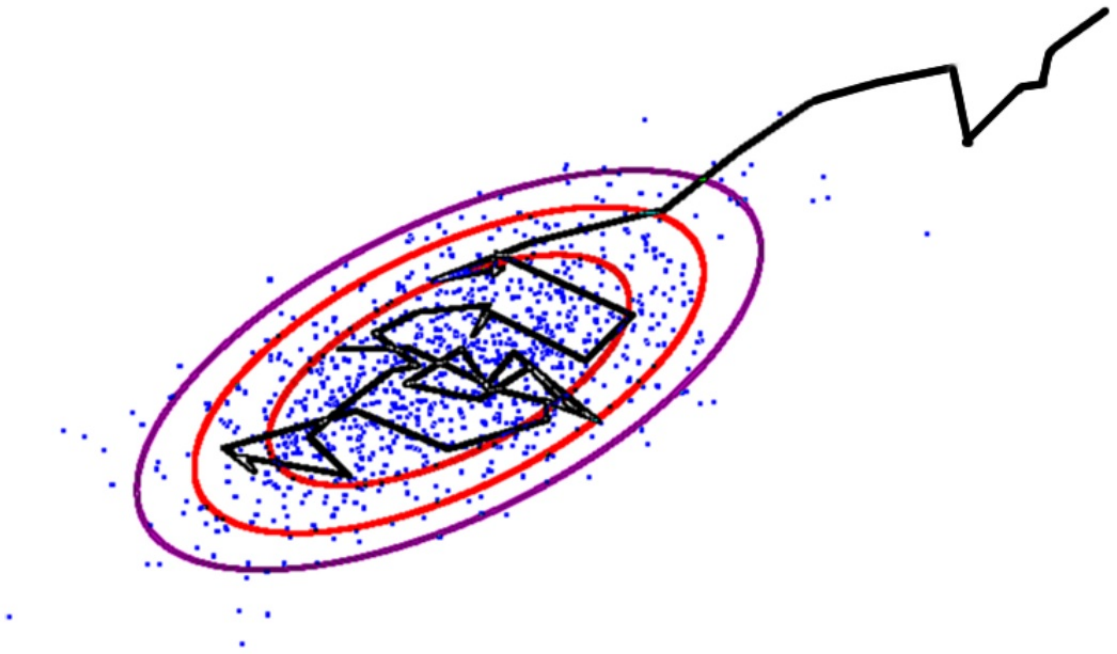
Independent Sampling vs. Markov Chains

- So far
  - We've considered two methods, Rejection Sampling and Importance Sampling, which were both based on independent samples from $q(x)$.
  - However, for many problems of practical interest, it is difficult or impososible to find $q(x)$ with the necessary properties.
- Different approach
  - We abandon the idea of independent sampling.
  - Instead, rely on Markov Chain to generate dependent samples from the target distribution.
  - Independence would be a nice thing, but it is not necessary for the Monte Carlo estimate to be valid.

Markov Chain Monte Carlo

Construct a biased random walk that explores target dist $P^{\star}(x)$

Markov steps, $x_t \sim T(x_{t-1} \to x_t)$



MCMC gives approximate, correlated samples of $P^{\star}$.

MCMC - Markov Chain Monte Carlo

- Overview
  - Allows to sample from a large class of distributions
  - Scales well with the dimensionality of the sample space.
- Idea
  - We maintain a record of the current state x_t
  - The proposal distribution depends on the current state : $q(x|x_t)$
  - The sequence of samples forms a Markov chain $x_1, x_2, \ldots$
- Setting
  - We can evaluate $p(z)$ (up to some normalization factor Z_P): $p(z) = \frac{\tilde{p}(z)}{Z_P}$
  - At each time step, we generate a candidate sample from the proposal distribution and accept the sample according to a criterion.

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Markov Chain Monte Carlo

What are the ingredients of a sampler

Design issues:

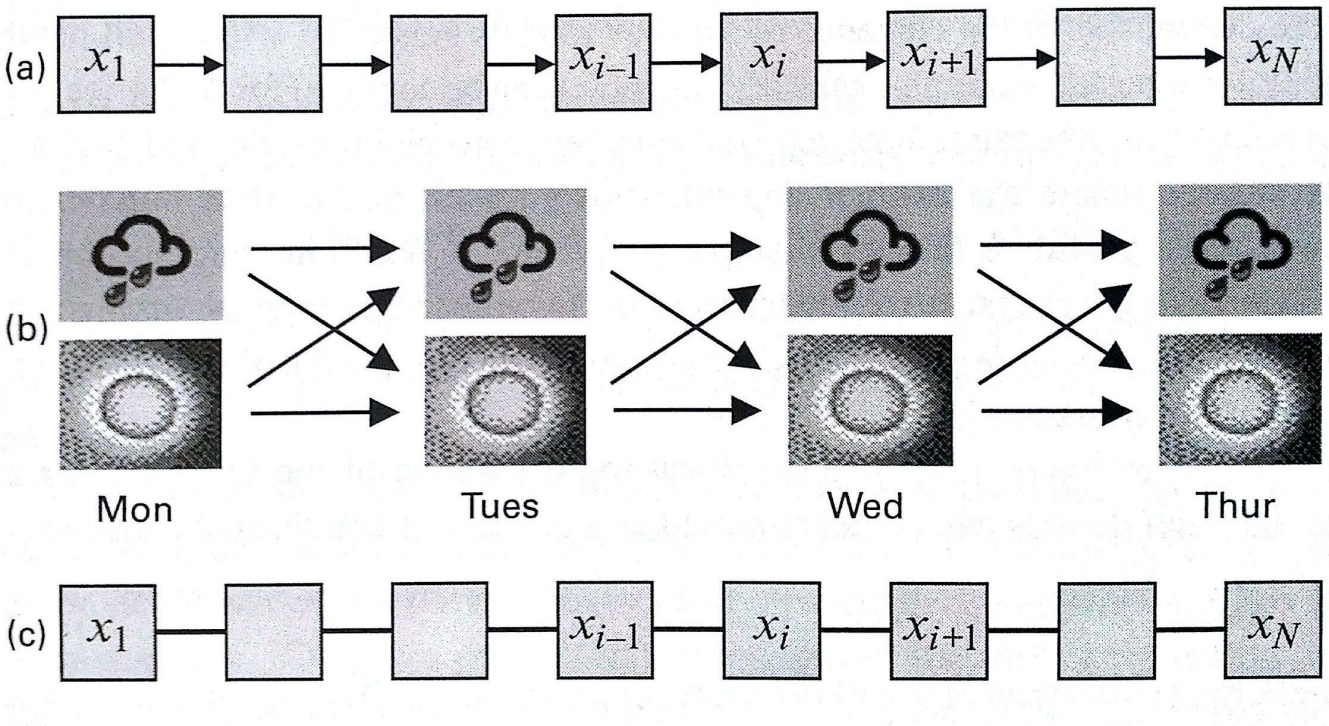
- to sample from a proposal density, conditioned on the previous sample, but which *does not need to match the target density closely*.
- and subsequently reject a certain amount of the samples according to the following rules.

Ingredient rules for MCMC samplers

- we need a proposal density $q(\mathbf{x}_t|\mathbf{x}_{t-1})$ from which we sample
- rule for rejecting or accepting samples from that density $A(\mathbf{x}_n, \mathbf{x}_{n-1})$

Together, these rules must ensure eventually, the samples will be drawn from the taget distribution $P^\star(\mathbf{x})$

Markov Chain



		Yesterday (X_{i-1})	
		Rain	Sun
Today (X_i)	Rain	0.4	0.8
	Sun	0.6	0.2

Markov Chain
Basics

Simple directed graph

We define a Markov Chain:

$$x_1 \to x_2 \to x_3 \to x_4 \to x_5 \to \ldots \to x_N \to$$

where $x_1 \sim p_1(x)$, $x_2 \sim p_2(x)$, etc., with the property that:

$$p_t(x') = \sum_x p_{t-1}(x)\, T(x \to x')$$

where $T(x \to x') = p(X_t = x' | X_{t-1} = x)$ is the Markov chain transition probability from x to x'.

We say that $p^\star(x)$ is an invariant (or stationary) distribution of the Markov chain defined by T if:

$$p^\star(x') = \sum_x p^\star(x)\, T(x \to x')\, \forall x'$$

Markov Chain Monte Carlo (MCMC) methods

Detailed balance

We have a Markov chain $x_1 \to x_2 \to x_3 \to\to \ldots x_N \to$ where $x_1 \sim p_1(x)$, $x_2 \sim p_2(x)$, etc., with the property

$$p_t(x') = \sum_x p_{t-1}(x)\, T(x \to x')$$

where $T(x \to x')$ is the Markov chain transition probability from x to x'.

A useful condition that implies invariance of $p^\star(x')$ is detailed balance:

$$p^\star(x')\, T(x' \to x) = p^\star(x)\, T(x \to x')$$

Stationary distribution of Markov Chain

Discrete example

$$P^\star = \begin{pmatrix} 3/5 \\ 1/5 \\ 1/5 \end{pmatrix} \qquad T = \begin{pmatrix} 2/3 & 1/2 & 1/2 \\ 1/6 & 0 & 1/2 \\ 1/6 & 1/2 & 0 \end{pmatrix} \qquad T_{ij} = T(x_i \leftarrow x_j)$$

$P^\star$ is an **invariant distribution** of T because $TP^\star = P^\star$, i.e.

$$\sum_x T(x' \leftarrow x) P^\star(x) = P^\star(x')$$

Also $P^\star$ is *the* **equilibrium distribution** of T:

To machine precision: $T^{100} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 3/5 \\ 1/5 \\ 1/5 \end{pmatrix} = P^\star$

Ergodicity requires: $T^K(x' \leftarrow x) > 0$ for all $x' : P^\star(x') > 0$, for some K

Outline

Markov Chain Monte Carlo Methods:

- Metropolis(-Hastings) Algorithm
- Gibbs Sampling
- not covered today Slice Sampling, Hybrid Monte Carlo

The Metropolis-Hastings algorithm

Transition operator

- Propose a move from the current state $Q(x';x)$, e.g. $\mathcal{N}(x, \sigma^2)$
- Accept with probability $\min\left(1,\ \frac{P(x')Q(x;x')}{P(x)Q(x';x)}\right)$
- Otherwise next state in chain is a copy of current state

Notes

- Can use $\tilde{P} \propto P(x)$; normalizer cancels in acceptance ratio
- Satisfies detailed balance (shown below)
- Q must be chosen to fulfill the other technical requirements

---

$$P(x) \cdot T(x' \leftarrow x) = P(x) \cdot Q(x';x) \min\left(1,\ \frac{P(x')Q(x;x')}{P(x)Q(x';x)}\right) = \min\Big(P(x)Q(x';x),\ P(x')Q(x;x')\Big)$$

$$= P(x') \cdot Q(x;x') \min\left(1,\ \frac{P(x)Q(x';x)}{P(x')Q(x;x')}\right) = P(x') \cdot T(x \leftarrow x')$$

The Metropolis-Hastings algorithm

Implementation

1: Choose a starting point x^1.
2: **for** $i = 2$ to L **do**
3: Draw a candidate sample x^{cand} from the proposal $\tilde{q}(x'|x^{l-1})$.
4: Let $a = \frac{\tilde{q}(x^{l-1}|x^{cand})p(x^{cand})}{\tilde{q}(x^{cand}|x^{l-1})p(x^{l-1})}$
5: **if** $a \geq 1$ **then** $x^l = x^{cand}$ ▷ Accept the candidate
6: **else**
7: draw a random value u uniformly from the unit interval $[0, 1]$.
8: **if** $u < a$ **then** $x^l = x^{cand}$ ▷ Accept the candidate
9: **else**
10: $x^l = x^{l-1}$ ▷ Reject the candidate
11: **end if**
12: **end if**
13: **end for**

MH-Algorithm example

2D-Gaussian target distribution $P^\star$

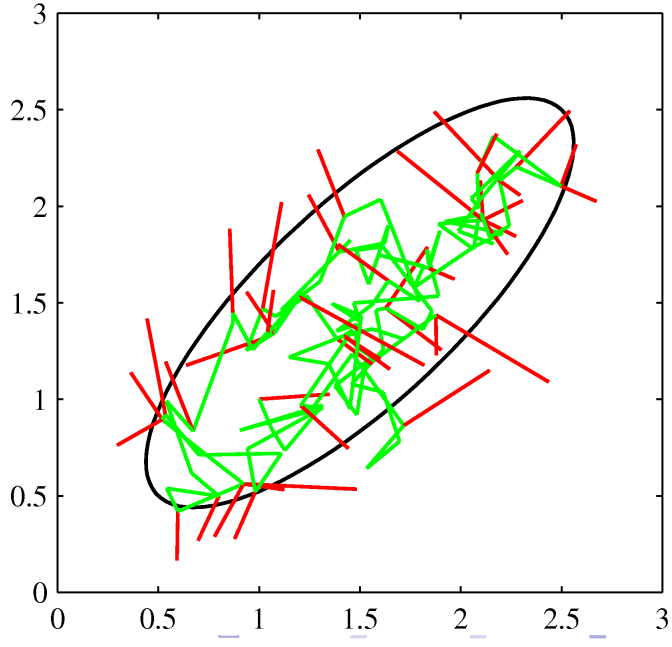
Property: when proposal $q(x, x') > 0$ for all x, the distribution of x_t tends to $p(x)$ as $t \to \infty$.

Note:

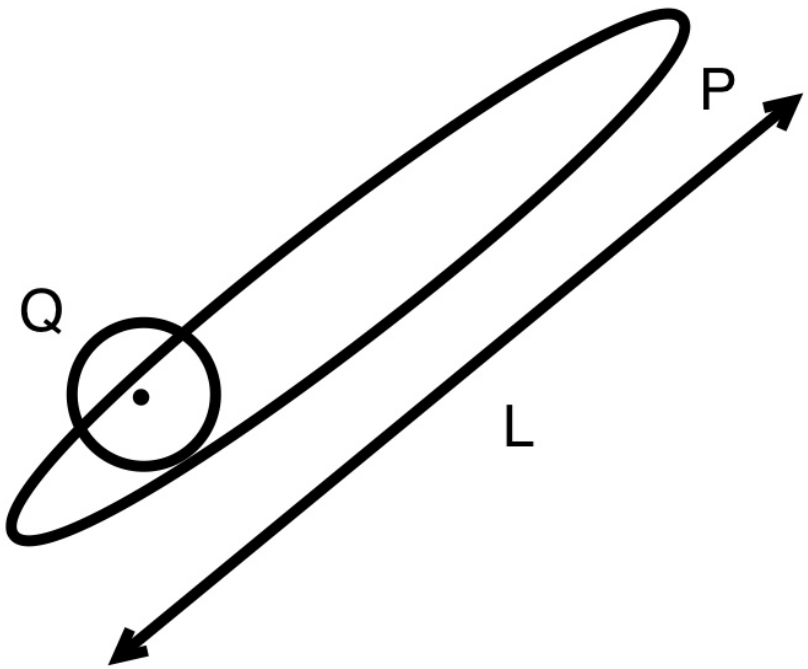
- Sequence $x_1, x_2, \ldots$ is not a set of independent samples from $p(x)$, as successive samples are highly correlated.
- We can obtain (largely) independent samples by just retaining every M^{th} sample (thinning).

Example: Sampling from a Gaussian

- Proposal: Gaussian with $\sigma = 0.2$
- Green: accepted samples
- Red: rejected samples



Example Metropolis-Hastings algorithm

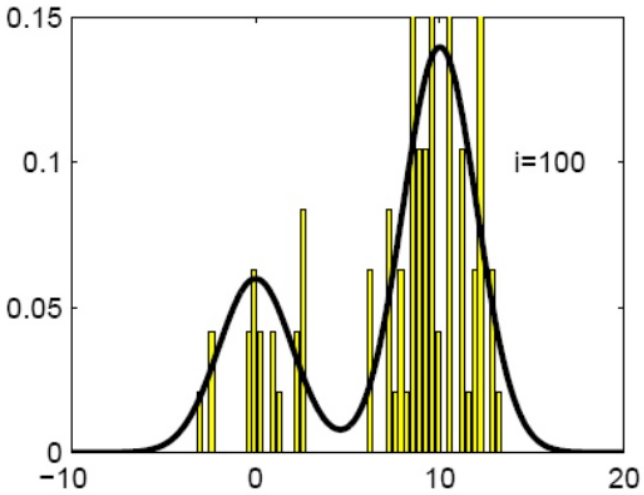


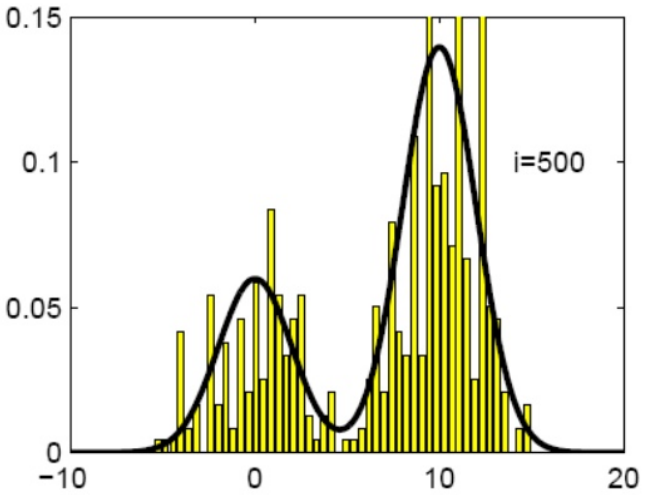
Generic proposals use
$Q(x';x) = \mathcal{N}(x, \sigma^2)$

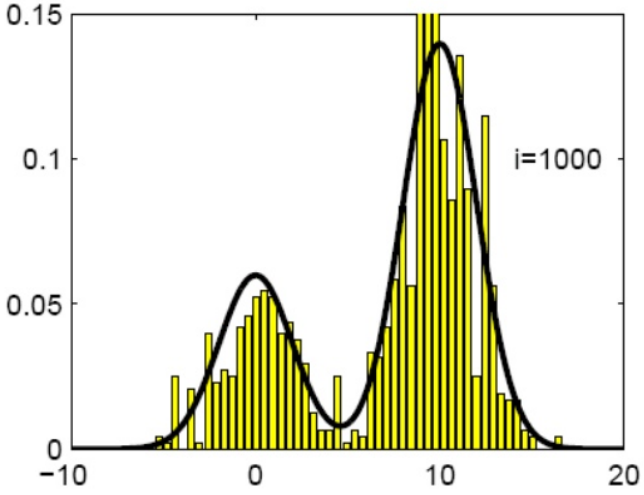
σ large $\rightarrow$ many rejections

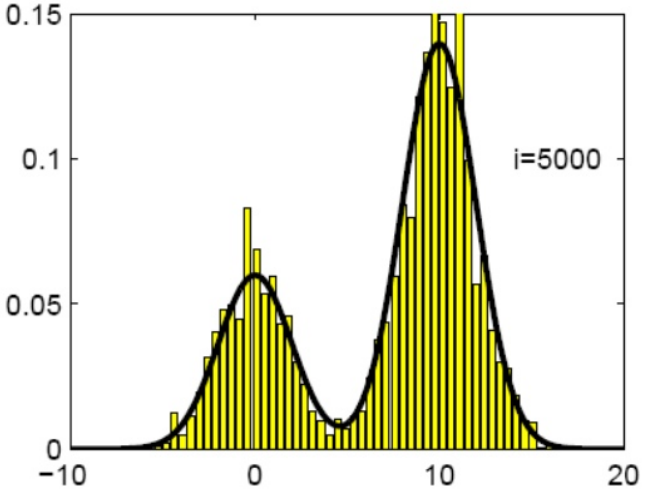
σ small $\rightarrow$ slow diffusion:
$\sim (L/\sigma)^2$ iterations required

Example Metropolis-Hastings algorithm

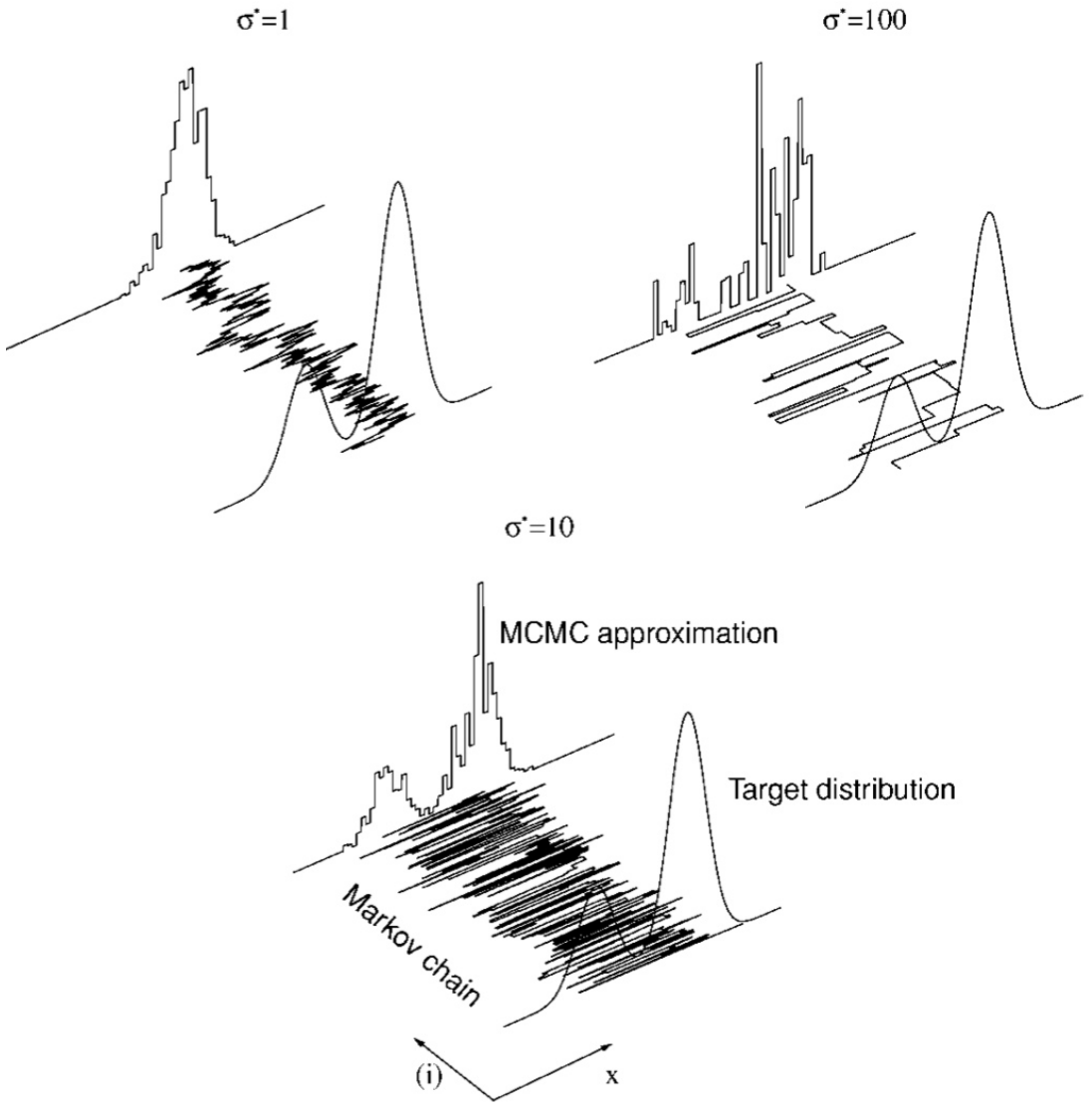








Example Metropolis-Hastings algorithm contd.



Gibbs Sampling

Method for sampling from a multivariate distribution $p(\mathbf{x})$

Idea: sample from a conditional of each variable given the settings of the other variables.
Repeatedly:

1. pick i (either at random or in turn)
2. replace x_i by a sample from the conditional distribution

$$p(x_i | x_1, \ldots, x_{i-1}, x_{i+1}, \ldots x_n)$$

This creates a Markov Chain

$$\mathbf{x}^1 \rightarrow \mathbf{x}^2 \rightarrow \mathbf{x}^3 \rightarrow \mathbf{x}^t$$

Under some (mild) conditions, the **equilibrium distribution**, i.e. $p(\mathbf{x}^\infty)$, of this Markov chain is $p(\mathbf{x})$

Gibbs Sampling contd.

Method for sampling from a multivariate distribution $p(\mathbf{x})$ of dimension D

- $x_1^{(t+1)} \sim P\left(x_1 | x_2^{(t)}, x_3^{(t)}, \ldots x_D^{(t)}\right)$
- $x_2^{(t+1)} \sim P\left(x_2 | x_1^{(t+1)}, x_3^{(t)}, \ldots x_D^{(t)}\right)$

  $\ldots$
- $x_D^{(t+1)} \sim P\left(x_D | x_1^{(t+1)}, x_2^{(t+1)}, \ldots x_{D-1}^{(t+1)}\right)$

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Gibbs Sampling contd.

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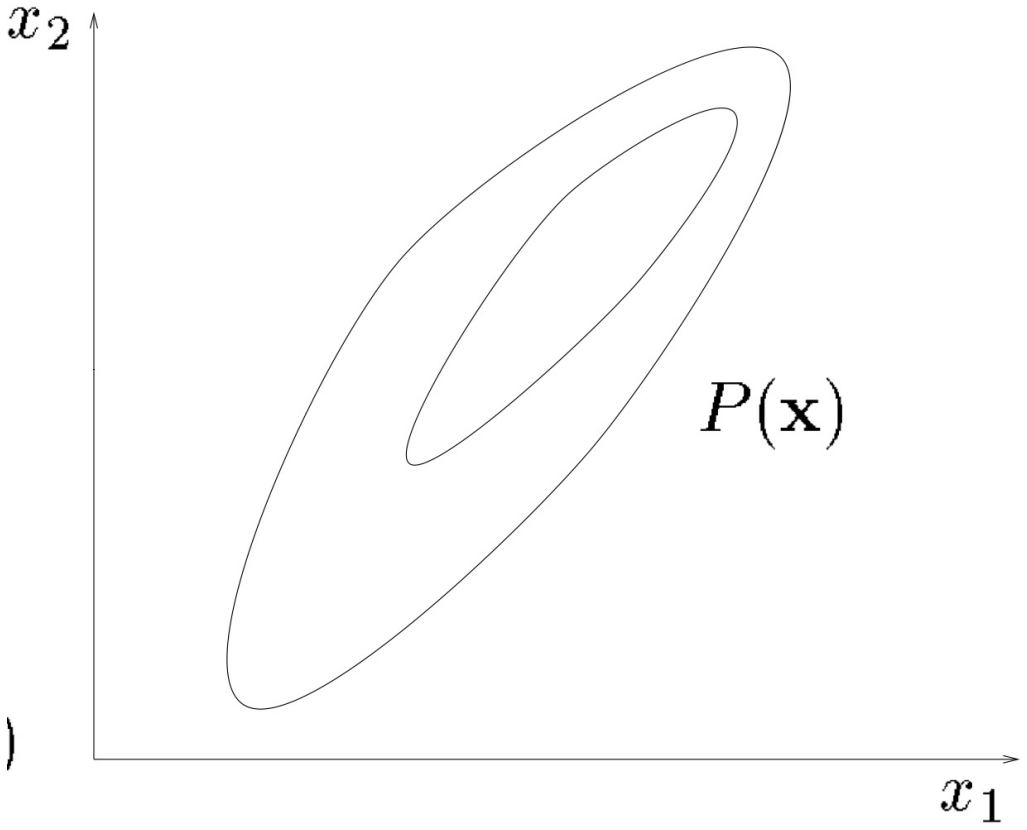
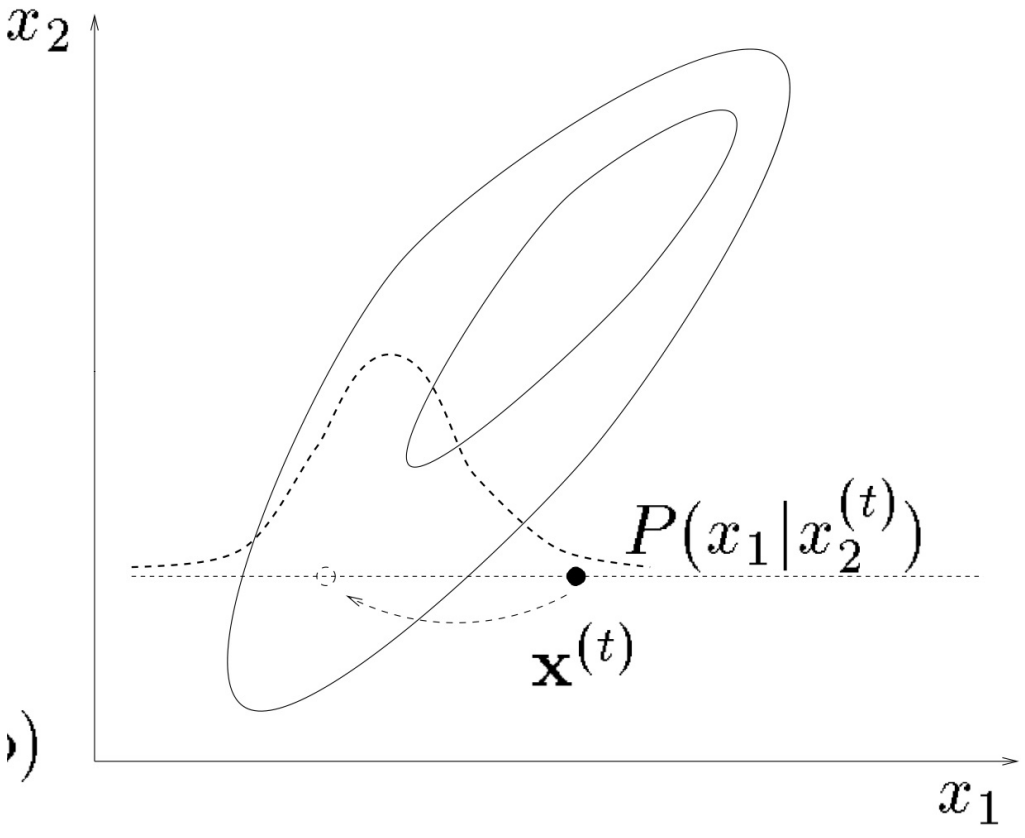


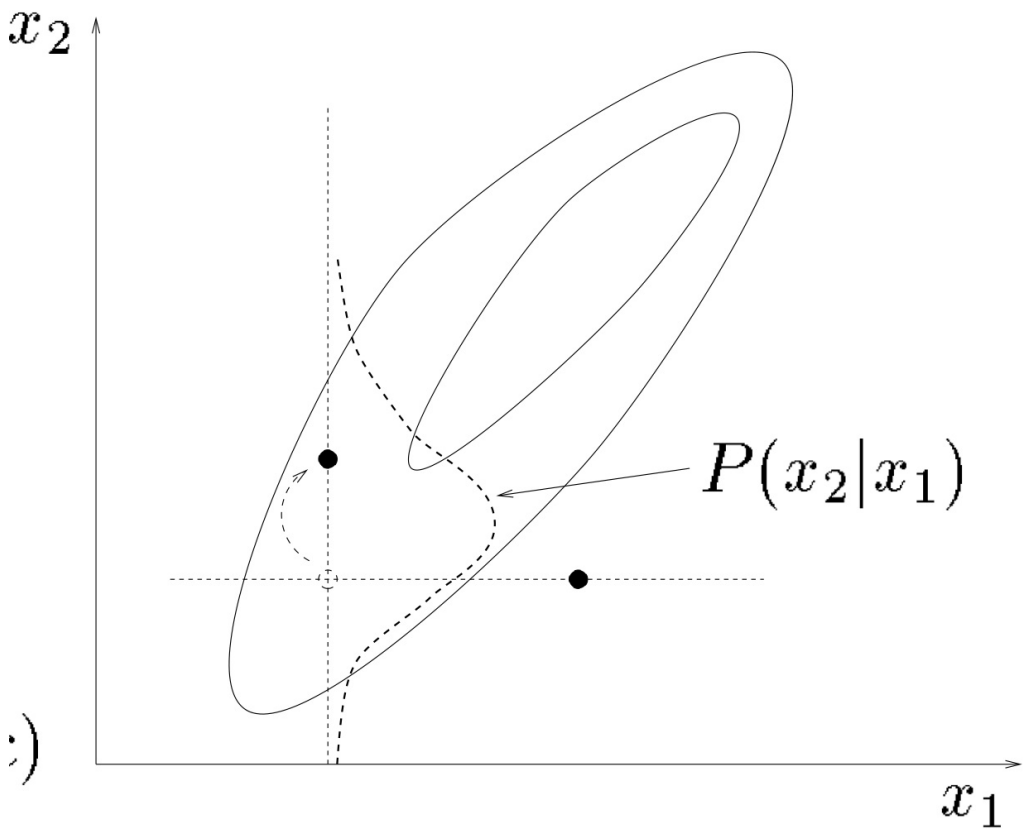
Gibbs Sampling contd.

Method for sampling from a multivariate distribution $p(\mathbf{x})$



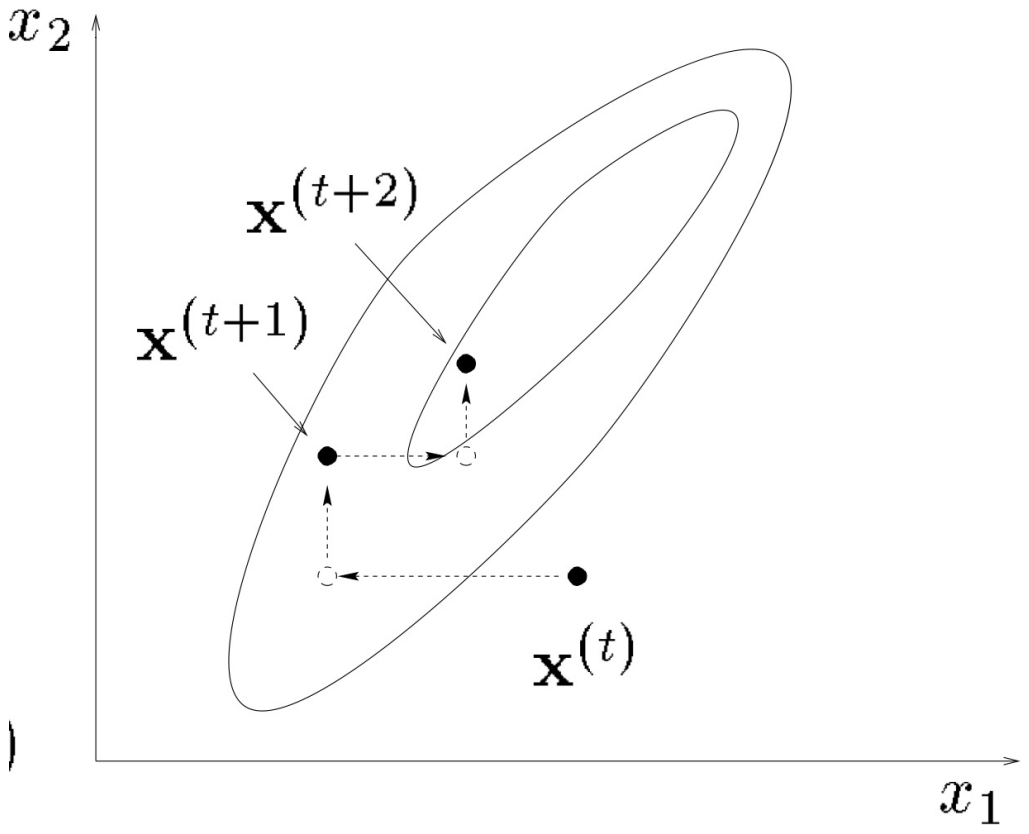
Gibbs Sampling contd.

Method for sampling from a multivariate distribution $p(\mathbf{x})$



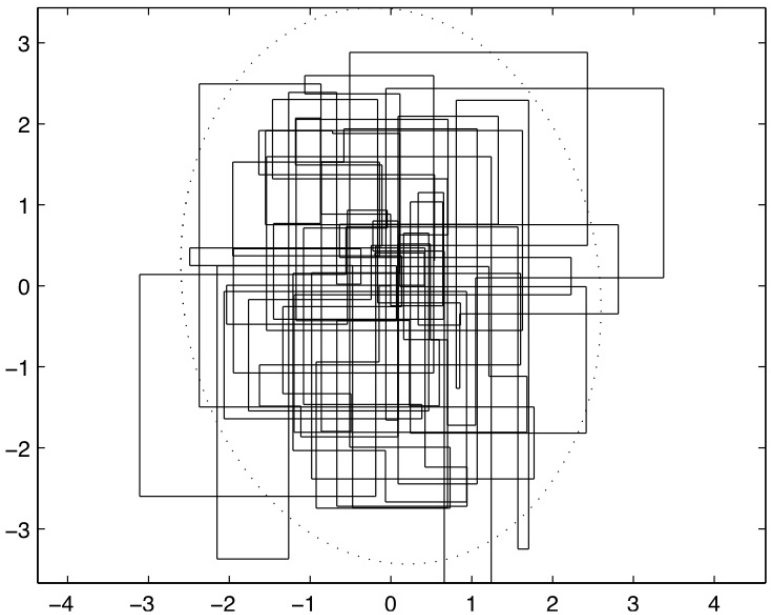
Gibbs Sampling contd.

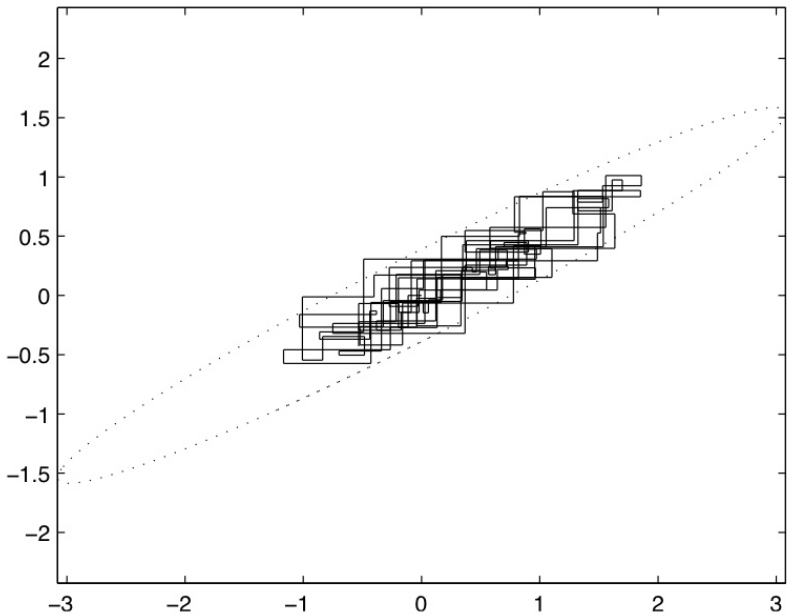
Method for sampling from a multivariate distribution $p(\mathbf{x})$



Slow convergence for correlated distributions

Sample from at least 2-Dimensional distributions

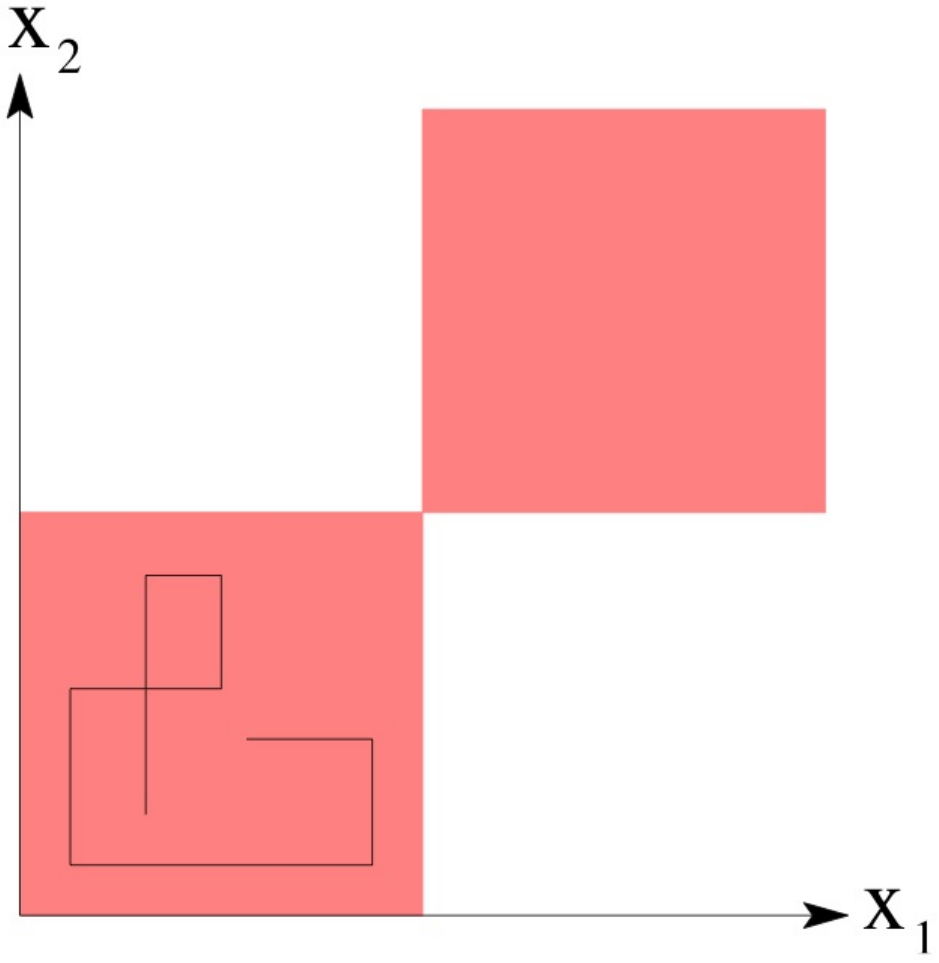




Left: Gibbs-Sampling from more uncorrelated distribution

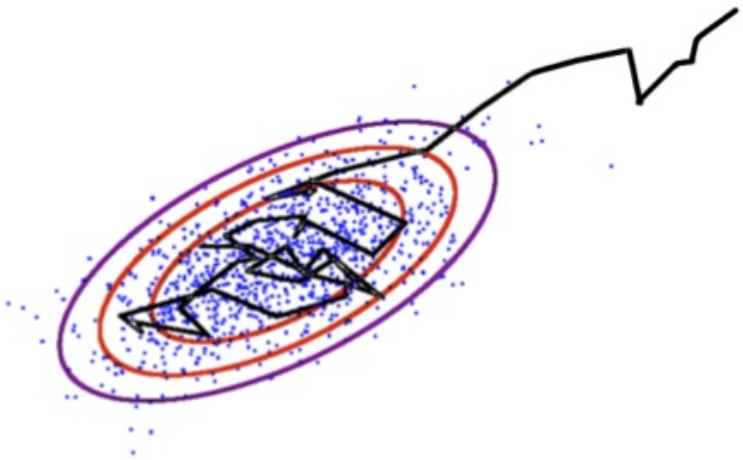
Right: Gibbs-Sampling from more correlated distribution

Ergodic/convergence behavior not guaranteed



Short review

Construct a biased random walk that explores a target dist.



Markov steps, $x^{(s)} \sim T\left(x^{(s)} \leftarrow x^{(s-1)}\right)$

MCMC gives approximate, correlated samples

$$\mathbb{E}_P[f] \approx \frac{1}{S}\sum_{s=1}^{S} f(x^{(s)})$$

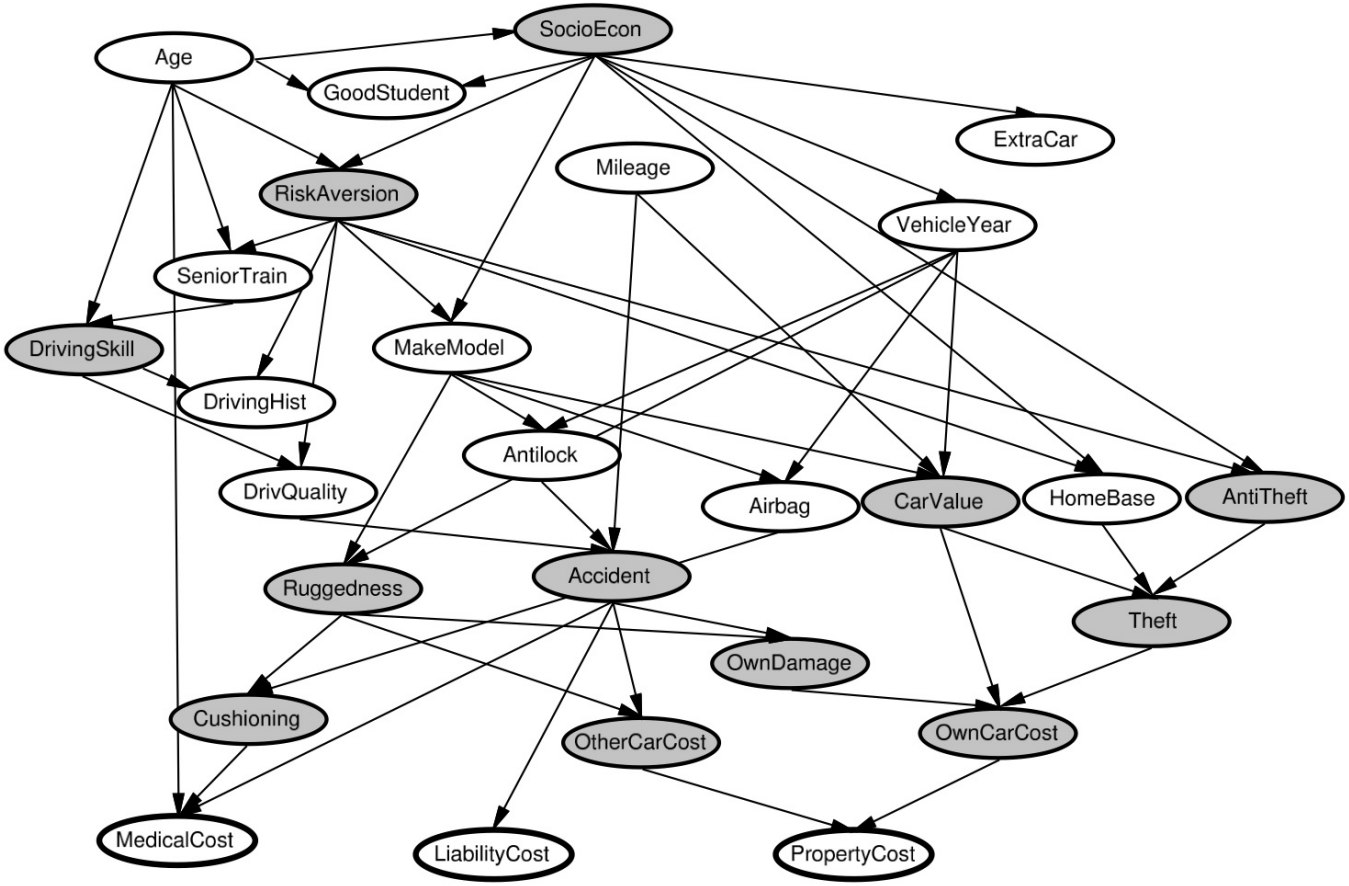
Example transitions:

Metropolis–Hastings: $T(x' \leftarrow x) = Q(x'; x)\, \min\left(1,\, \frac{P(x')\, Q(x; x')}{P(x)\, Q(x'; x)}\right)$

Gibbs sampling: $T_i(\mathbf{x}' \leftarrow \mathbf{x}) = P(x'_i \,|\, \mathbf{x}_{j\neq i})\, \delta(\mathbf{x}'_{j\neq i} - \mathbf{x}_{j\neq i})$

Gibbs Sampling

Gibbs Sampling for Graphical models



- Initialize all variables to some settings.
- Sample each variable conditioned on other variables.

Gibbs Sampling

Gibbs Sampling for Graphical models

A large-dimensional joint distribution is factored into a directed graph that encodes the conditional independencies in the model. In particular, if $x_{pa(j)}$ denotes the parent nodes of node x_j, we have

$$p(x) = \prod_j p\left(x_j | x_{pa(j)}\right) \tag{2}$$

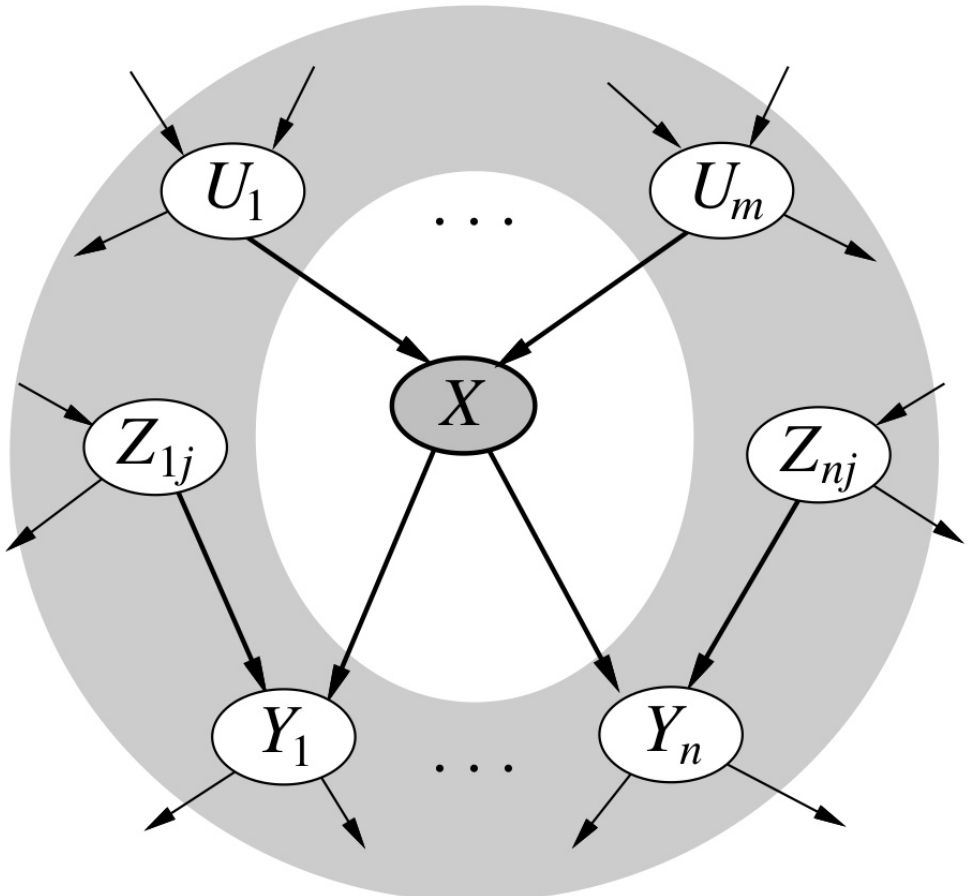
It follows that the full conditionals simplify as follows

$$p\left(x_j = |x_{-j}\right) = p\left(x_j | x_{pa(j)}\right) \prod_{k \in ch(j)} p\left(x_k | x_{pa(k)}\right) \tag{3}$$

where $ch(j)$ denotes the children nodes of x_j.

Gibbs Sampling in DAGs

- Recap: The Markov blanket of a node is the set that renders it independent of the rest of the graph
- This is the parents, children and co-parents.



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&= \frac{p\left(X_i, U_{1:n}, Y_{1:m}, Z_{1:m}, R\right)}{\sum_x p\left(X_i, U_{1:n}, Y_{1:m}, Z_{1:m}, R\right)} \\
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p\left(X_i|X_{-i}\right) &\propto p\left(X_i|Pa\left(X_i\right)\right) \prod_{Y_i \in ch(X_i)} p\left(Y_i|Pa\left(Y_i\right)\right)
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$$

Gibbs Sampling in DAGs

- Recap: The Markov blanket of a node is the set that renders it independent of the rest of the graph
- This is the parents, children and co-parents.

$$
\begin{aligned}
p\left(X_i|X_{-i}\right) &= \frac{p\left(X_i, X_{-i}\right)}{\sum_x p\left(X_i, X_{-i}\right)} \\
&= \frac{p\left(X_i, U_{1:n}, Y_{1:m}, Z_{1:m}, R\right)}{\sum_x p\left(X_i, U_{1:n}, Y_{1:m}, Z_{1:m}, R\right)} \\
&= \frac{p\left(X_i|U_{1:n}\right)\left[\prod_j p\left(Y_j|X_i, Z_j\right)\right] p\left(U_{1:n}, Z_{1:m}, R\right)}{\sum_x p\left(X_i = x|U_{1:n}\right)\left[\prod_j p\left(Y_j|X_i = x, Z_j\right)\right] p\left(U_{1:n}, Z_{1:m}, R\right)} \\
&= \frac{p\left(X_i|U_{1:n}\right)\left[\prod_j p\left(Y_j|X_i, Z_j\right)\right]}{\sum_x p\left(X_i = x|U_{1:n}\right)\left[\prod_j p\left(Y_j|X_i = x, Z_j\right)\right]}
\end{aligned}
$$

$$
p\left(X_i|X_{-i}\right) \propto p\left(X_i|Pa\left(X_i\right)\right) \prod_{Y_i \in ch(X_i)} p\left(Y_i|Pa\left(Y_i\right)\right)
$$

Gibbs Sampling scheme

- In Gibbs sampling we also generate a sample set S – but in this case the samples are not independent from each other anymore. The next sample "modifies" the previous one:
- First, all observed RVs are *clamped* to their fixed value $x_i^k = y_i$ for any k.
- To generate the $(k+1)$th sample, iterate through the latent variables $i \notin obs$, updating:

$$
\begin{aligned}
x_i^{k+1} &\sim P(X_i \mid x_{1:n\setminus i}^k) \\
&\sim P(X_i \mid x_1^k, x_2^k, .., x_{i\text{-}1}^k, x_{i+1}^k, .., x_n^k) \\
&\sim P(X_i \mid x_{\text{Parents}(i)}^k) \prod_{j:i\in\text{Parents}(j)} P(X_j = x_j^k \mid X_i, x_{\text{Parents}(j)\setminus i}^k)
\end{aligned}
$$

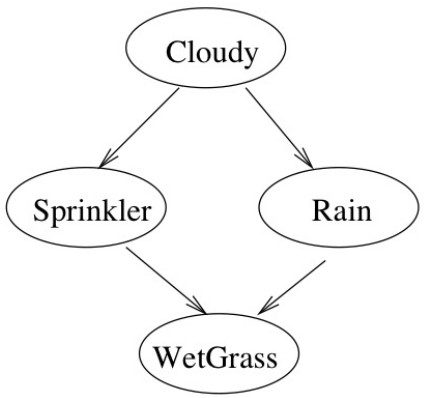
That is, each x_i^{k+1} is *resampled* conditional to the other (neighboring) current sample values.

Gibbs Sampling

Famous sprinkler DAG example

Binary nodes: (T & F)

P(C=F)	P(C=T)
0.5	0.5



C	P(S=F)	P(S=T)
F	0.5	0.5
T	0.9	0.1

C	P(R=F)	P(R=T)
F	0.8	0.2
T	0.2	0.8

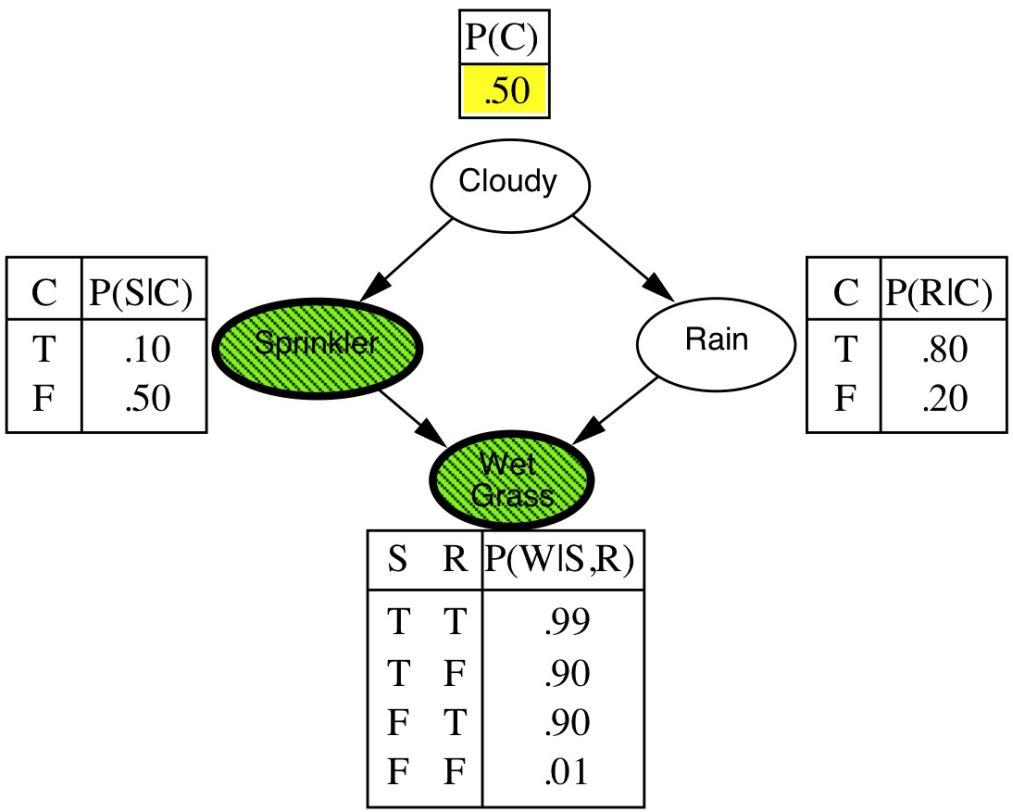
S	R	P(W=F)	P(W=T)
F	F	1.0	0.0
T	F	0.1	0.9
F	T	0.1	0.9
T	T	0.01	0.99

Gibbs Sampling for sprinkler DAG with evidence

1. Initialize:
   (a) Instantiate X_i to one of its possible values $x_i, 1 \leq i \leq n$.
   (b) Let $\mathbf{x}^{(0)} = (x_1, \ldots, x_n)$
2. For $t = 1, 2, \ldots$
   (a) Pick an index $i, 1 \leq i \leq n$ uniformly at random.[1]
   (b) Sample x_i from $P(X_i | \mathbf{x}_{(-i)}^{(t-1)}, \mathbf{e})$.
   (c) Let $\mathbf{x}^{(t)} = (\mathbf{x}_{(-i)}, x_i)$

Gibbs Sampling for sprinkler DAG

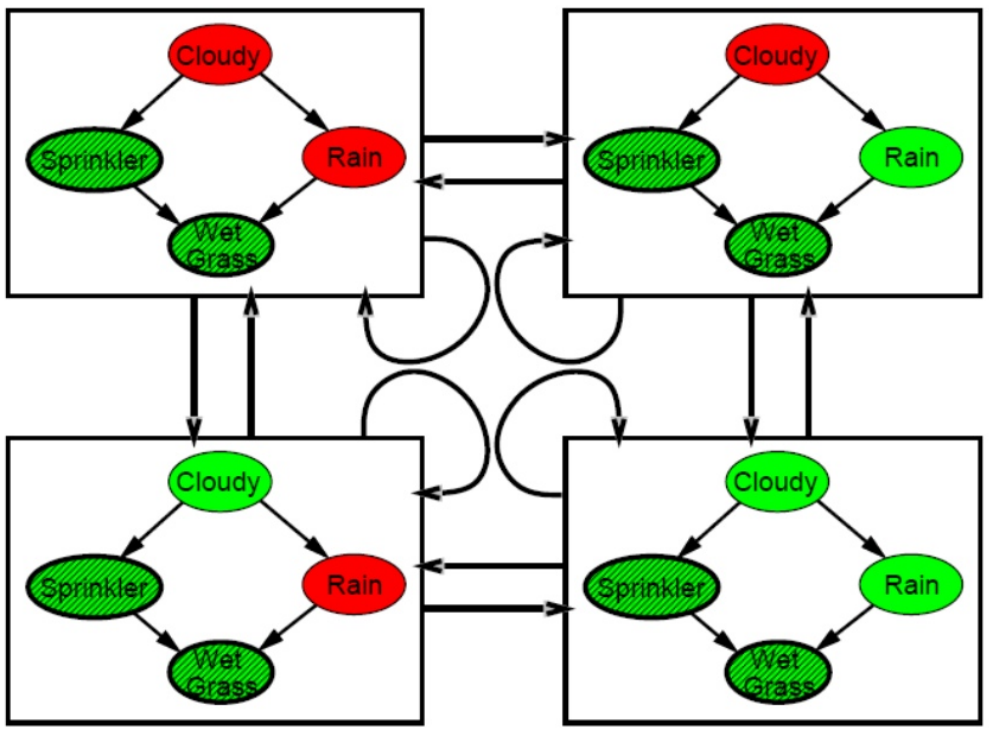
Question: $P(Rain|Sprinkler = true, WetGrass = true)$.
Since the observation/evidence *Sprinkler* and *WetGrass* is set to *true*, the Gibbs sampler draws samples from
$P(Rain, Cloudy|Sprinkler = true, WetGrass = true)$.



Markov Chain Gibbs Sampling for Sprinkler Problem

Question: $P(Rain|Sprinkler = true, WetGrass = true)$.
Since the observation/evidence *Sprinkler* and *WetGrass* is set to *true*, the Gibbs sampler draws samples from
$P(Rain, Cloudy|Sprinkler = true, WetGrass = true)$.

With $Sprinkler = true, WetGrass = true$, there are four states:

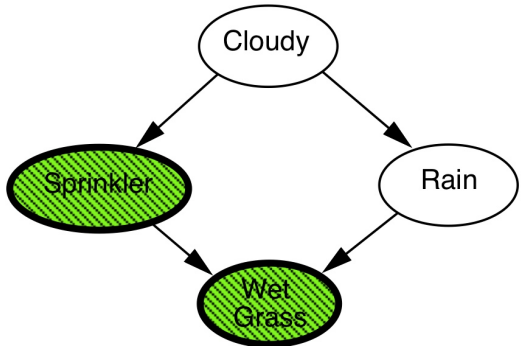


Wander about for a while, average what you see

Gibbs Sampling for sprinkler DAG

The Gibbs sampler for the rain network works as follows:

1. **Initialize**: (not.: $T = true$, $F = false$)
   1. Instantiate $Rain = T$, $Cloudy = T$
   2. Let $\mathbf{x}^{(0)} = (Rain = T, Cloudy = T)$
2. **For** $t = 1, 2, \ldots$:
   1. Pick variable to update from $\{Rain, Cloudy\}$ **uniformly** at random
   2. If *Rain* was picked
      1. Sample *Rain* from $P\left(Rain | Cloudy = [value]_{t-1}, Sprinkler = T, WetGrass = T\right)$
      2. Let $\mathbf{x}^{(t)} = \left(Rain = [value]_t, Cloudy = [value]_{t-1}\right)$
   3. Else
      1. Sample *Cloudy* from $P\left(Cloudy | Rain = [value]_{t-1}, Sprinkler = T, WetGrass = T\right)$
      2. Let $\mathbf{x}^{(t)} = \left(Rain = [value]_{t-1}, Cloudy = [value]_t\right)$



Gibbs Sampling for sprinkler DAG

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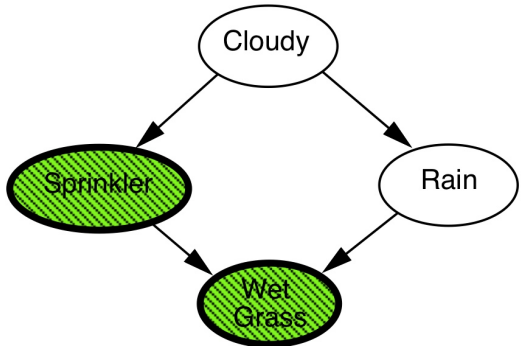

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Gibbs Sampling for sprinkler DAG

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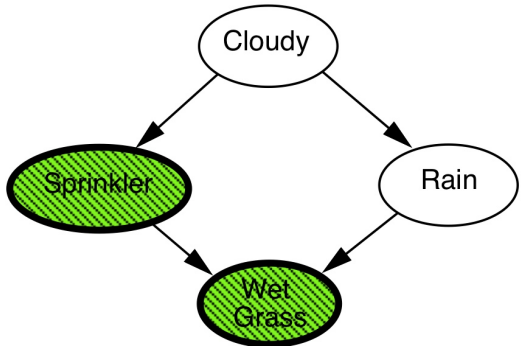

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Approximate inference by sampling

- Exact Bayesian Inference often intractable
- Rejection and Importance Sampling
  - Generate independent samples.
  - Impractical in high-dimensional state spaces.
- Markov Chain Monte Carlo (MCMC)
  - Simple & effective (even though typically computationally expensive).
  - Scales well with the dimensionality of the state space.
  - Issues of convergence have to be considered carefully.
- Gibbs Sampling
  - Used extensively in practice.
  - Parameter free.
  - Requires sampling conditional distributions.