Sampling Methods

Greg Mori - CMPT 419/726

Bishop PRML Ch. 11

Recall – Inference For General Graphs

- Junction tree algorithm is an exact inference method for arbitrary graphs
  - A particular tree structure defined over cliques of variables
  - Inference ends up being exponential in maximum clique size
  - Therefore slow in many cases
- Sampling methods: represent desired distribution with a set of samples, as more samples are used, obtain more accurate representation

Outline

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Sampling

- The fundamental problem we address in this lecture is how to obtain samples from a probability distribution $p(\mathbf{z})$
  - This could be a conditional distribution $p(\mathbf{z}|\mathbf{e})$
- We often wish to evaluate expectations such as

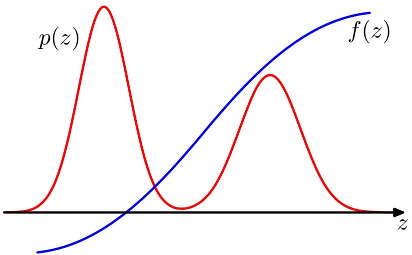
$$\mathbb{E}[f] = \int f(\mathbf{z})p(\mathbf{z})d\mathbf{z}$$

  - e.g. mean when $f(\mathbf{z}) = \mathbf{z}$
- For complicated $p(\mathbf{z})$, this is difficult to do exactly, approximate as

$$\hat{f} = \frac{1}{L}\sum_{l=1}^{L} f(\mathbf{z}^{(l)})$$

where $\{\mathbf{z}^{(l)}|l = 1, \ldots, L\}$ are independent samples from $p(\mathbf{z})$

Sampling



- Approximate

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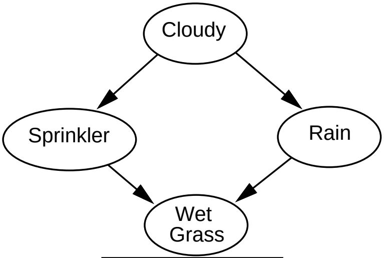
Bayesian Networks - Generating Fair Samples

P(C)
.50



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F	.50

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S	R	P(W|S,R)
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- How can we generate a fair set of samples from this BN?

from Russell and Norvig, AIMA

Sampling from Bayesian Networks

- Sampling from discrete Bayesian networks with no observations is straight-forward, using ancestral sampling
- Bayesian network specifies factorization of joint distribution

$$P(z_1, \ldots, z_n) = \prod_{i=1}^{n} P(z_i | pa(z_i))$$

- Sample in-order, sample parents before children
  - Possible because graph is a DAG
- Choose value for z_i from $p(z_i | pa(z_i))$

Sampling From Empty Network – Example

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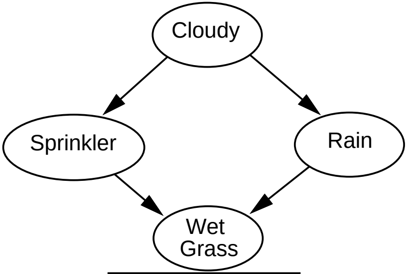

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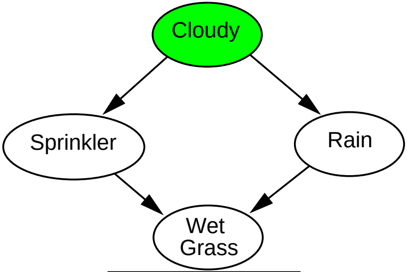

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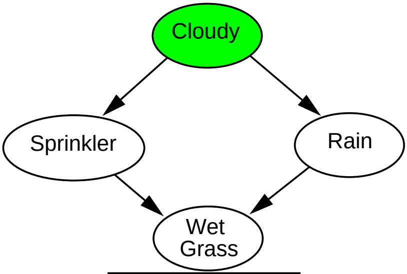

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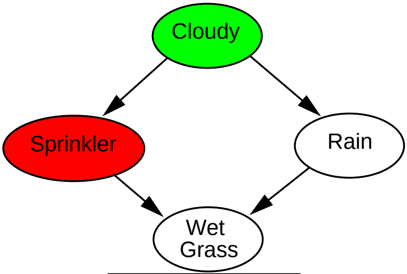

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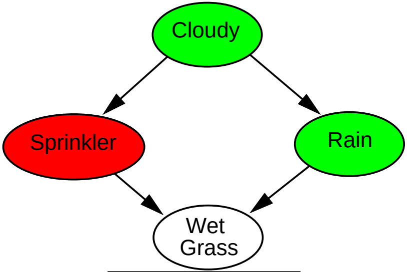

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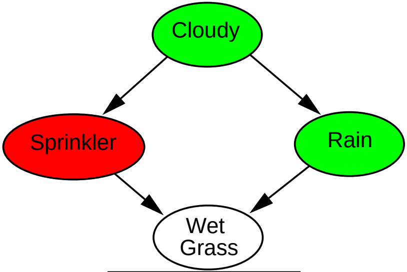

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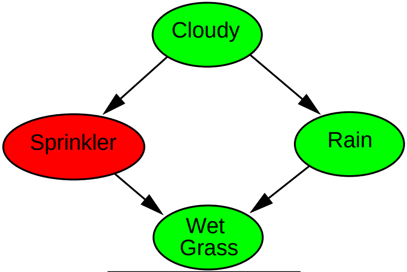

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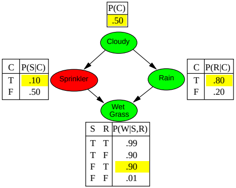
Ancestral Sampling

- This sampling procedure is fair, the fraction of samples with a particular value tends towards the joint probability of that value
- Define $S_{PS}(z_1, \ldots, z_n)$ to be the probability of generating the event $(z_1, \ldots, z_n)$
  - This is equal to $p(z_1, \ldots, z_n)$ due to the semantics of the Bayesian network
- Define $N_{PS}(z_1, \ldots, z_n)$ to be the number of times we generate the event $(z_1, \ldots, z_n)$

$$\lim_{N \to \infty} \frac{N_{PS}(z_1, \ldots, z_n)}{N} = S_{PS}(z_1, \ldots, z_n) = p(z_1, \ldots, z_n)$$

Sampling Marginals



- Note that this procedure can be applied to generate samples for marginals as well
- Simply discard portions of sample which are not needed
- e.g. For marginal $p(rain)$, sample $(cloudy = t, sprinkler = f, rain = t, wg = t)$ just becomes $(rain = t)$
- Still a fair sampling procedure

Sampling with Evidence

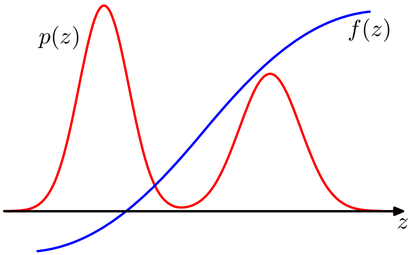
- What if we observe some values and want samples from $p(\mathbf{z}|\mathbf{e})$?
- Naive method, logic sampling:
  - Generate N samples from $p(\mathbf{z})$ using ancestral sampling
  - Discard those samples that do not have correct evidence values
- e.g. For $p(rain|cloudy = t, spr = t, wg = t)$, sample $(cloudy = t, spr = f, rain = t, wg = t)$ discarded
- Generates fair samples, but wastes time
  - Many samples will be discarded for low $p(\mathbf{e})$

Other Problems

- Continuous variables?
  - Gaussian okay, Box-Muller and other methods
  - More complex distributions?
- Undirected graphs (MRFs)?

Outline

Rejection Sampling

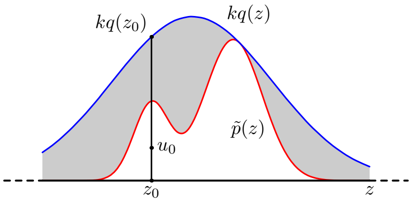


- Consider the case of an arbitrary, continuous $p(z)$
- How can we draw samples from it?
- Assume we can evaluate $p(z)$, up to some normalization constant

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

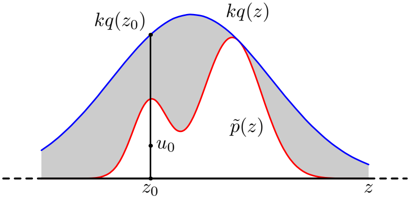
where $\tilde{p}(z)$ can be efficiently evaluated (e.g. MRF)

Proposal Distribution



- Let's also assume that we have some simpler distribution $q(z)$ called a proposal distribution from which we can easily draw samples
  - e.g. $q(z)$ is a Gaussian
- We can then draw samples from $q(z)$ and use these
- But these wouldn't be fair samples from $p(z)$?!

Comparison Function and Rejection



- Introduce constant k such that $kq(z) \geq \tilde{p}(z)$ for all z
- Rejection sampling procedure:
  - Generate z_0 from $q(z)$
  - Generate u_0 from $[0, kq(z_0)]$ uniformly
  - If $u_0 > \tilde{p}(z)$ reject sample z_0, otherwise keep it
- Original samples are uniform in grey region
- Kept samples uniform in white region – hence samples from $p(z)$

Rejection Sampling Analysis

- How likely are we to keep samples?
- Probability a sample is accepted is:

$$\begin{aligned} p(accept) &= \int \{\tilde{p}(z)/kq(z)\}q(z)dz \\ &= \frac{1}{k}\int \tilde{p}(z)dz \end{aligned}$$

- Smaller k is better subject to $kq(z) \geq \tilde{p}(z)$ for all z
  - If $q(z)$ is similar to $\tilde{p}(z)$, this is easier
- In high-dim spaces, acceptance ratio falls off exponentially
- Finding a suitable k challenging

Outline

Discretization

- Importance sampling is a sampling technique for computing expectations:

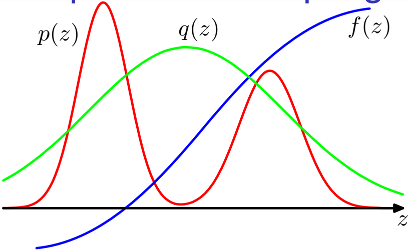
$$\mathbb{E}[f] = \int f(z)p(z)dz$$

- Could approximate using discretization over a uniform grid:

$$\mathbb{E}[f] \approx \sum_{l=1}^{L} f(z^{(l)})p(z^{(l)})$$

  - c.f. Riemannian sum
- Much wasted computation, exponential scaling in dimension
- Instead, again use a proposal distribution instead of a uniform grid

Importance sampling



- Approximate expectation

$$
\begin{aligned}
\mathbb{E}[f] &= \int f(\mathbf{z}) p(\mathbf{z}) d\mathbf{z} = \int f(\mathbf{z}) \frac{p(\mathbf{z})}{q(\mathbf{z})} q(\mathbf{z}) d\mathbf{z} \\
&\approx \frac{1}{L} \sum_{l=1}^{L} f(\mathbf{z}^{(l)}) \frac{p(\mathbf{z}^{(l)})}{q(\mathbf{z}^{(l)})}
\end{aligned}
$$

- Quantities $p(\mathbf{z}^{(l)})/q(\mathbf{z}^{(l)})$ are known as importance weights
    - Correct for use of wrong distribution $q(\mathbf{z})$ in sampling

Likelihood Weighted Sampling

- Consider the case where we have evidence $\boldsymbol{e}$ and again desire an expectation over $p(\boldsymbol{x}|\boldsymbol{e})$
- If we have a Bayesian network, we can use a particular type of importance sampling called likelihood weighted sampling:
  - Perform ancestral sampling
  - If a variable z_i is in the evidence set, set its value rather than sampling
- Importance weights are: ??

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$$\frac{p(\boldsymbol{z}^{(l)})}{q(\boldsymbol{z}^{(l)})} = ?$$

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$$\frac{p(\boldsymbol{z}^{(l)})}{q(\boldsymbol{z}^{(l)})} = \frac{p(\boldsymbol{x},\boldsymbol{e})}{p(\boldsymbol{e})} \frac{1}{\prod_{z_i \notin \boldsymbol{e}} p(z_i|pa_i)} \propto \prod_{z_i \in e} p(z_i|pa_i)$$

Likelihood Weighted Sampling Example

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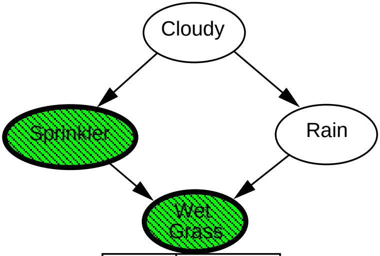

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$$w = 1.0$$

from Russell and Norvig, AIMA

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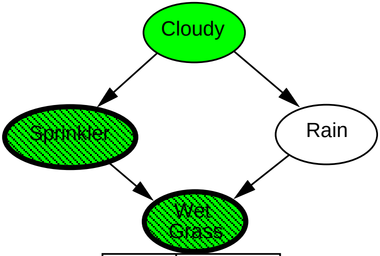

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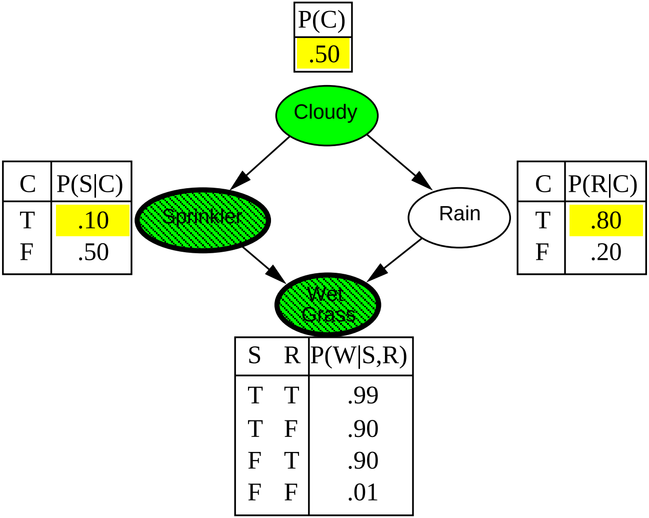

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$$w = 1.0 \times 0.1$$

from Russell and Norvig, AIMA

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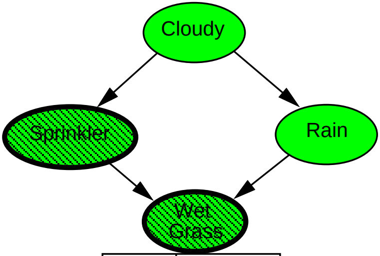

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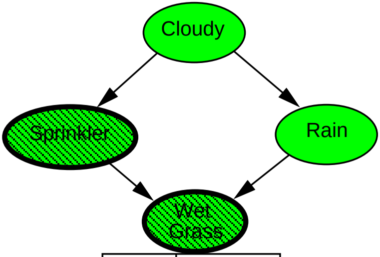

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$$w = 1.0 \times 0.1 \times 0.99 = 0.099$$

from Russell and Norvig, AIMA

Sampling Importance Resampling

- Note that importance sampling, e.g. likelihood weighted sampling, gives approximation to expectation, not samples
- But samples can be obtained using these ideas
- Sampling-importance-resampling uses a proposal distribution $q(z)$ to generate samples
    - Unlike rejection sampling, no parameter k is needed

SIR - Algorithm

- Sampling-importance-resampling algorithm has two stages
- Sampling:
  - Draw samples $z^{(1)}, \dots, z^{(L)}$ from proposal distribution $q(z)$
- Importance resampling:
  - Put weights on samples

$$w_l = \frac{\tilde{p}(z^{(l)})/q(z^{(l)})}{\sum_m \tilde{p}(z^{(m)})/q(z^{(m)})}$$

  - Draw samples from the discrete set $z^{(1)}, \dots, z^{(L)}$ according to weights w_l (uniform distribution)
- This two stage process is correct in the limit as $L \to \infty$

Outline

Sampling

Rejection Sampling

Importance Sampling

Markov Chain Monte Carlo

Markov Chain Monte Carlo

- Markov chain Monte Carlo (MCMC) methods also use a proposal distribution to generate samples from another distribution
- Unlike the previous methods, we keep track of the samples generated $z^{(1)}, \dots, z^{(\tau)}$
- The proposal distribution depends on the current state: $q(z|z^{(\tau)})$
  - Intuitively, walking around in state space, each step depends only on the current state

Metropolis Algorithm

- Simple algorithm for walking around in state space:
  - Draw sample $z^* \sim q(z|z^{(\tau)})$
  - Accept sample with probability

$$A(z^*, z^{(\tau)}) = \min\left(1, \frac{\tilde{p}(z^*)}{\tilde{p}(z^{(\tau)})}\right)$$

  - If accepted $z^{(\tau+1)} = z^*$, else $z^{(\tau+1)} = z^{(\tau)}$
- Note that if z^* is better than $z^{(\tau)}$, it is always accepted
- Every iteration produces a sample
  - Though sometimes it's the same as previous
  - Contrast with rejection sampling
- The basic Metropolis algorithm assumes the proposal distribution is symmetric $q(z_A|z_B) = q(z_B|z_A)$

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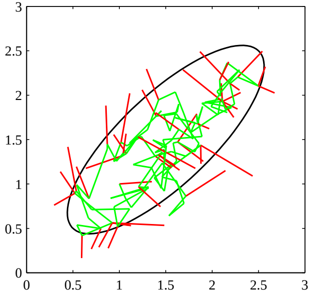
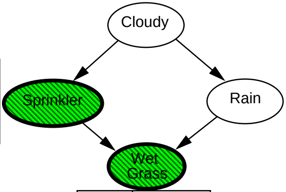
Metropolis Example



- $p(z)$ is anisotropic Gaussian, proposal distribution $q(z)$ is isotropic Gaussian
  - Red lines show rejected moves, green lines show accepted moves
- As $\tau \to \infty$, distribution of $z^{(\tau)}$ tends to $p(z)$
  - True if $q(z_A|z_B) > 0$
  - In practice, burn-in the chain, collect samples after some iterations
  - Only keep every M^{th} sample

Metropolis Example - Graphical Model

P(C)
.50



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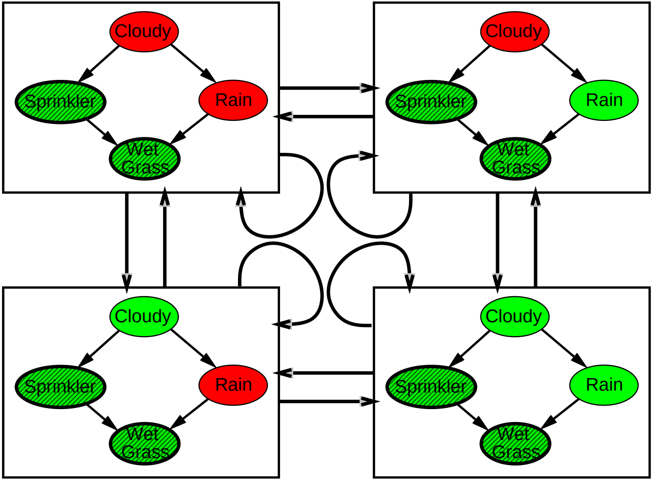
- Consider running Metropolis algorithm to draw samples from $p(cloudy, rain|spr = t, wg = t)$
- Define $q(z|z^{\tau})$ to be uniformly pick from $cloudy$, $rain$, uniformly reset its value

Metropolis Example



- Walk around in this state space, keep track of how many times each state occurs

Metropolis-Hastings Algorithm

- A generalization of the previous algorithm for asymmetric proposal distributions known as the Metropolis-Hastings algorithm
- Accept a step with probability

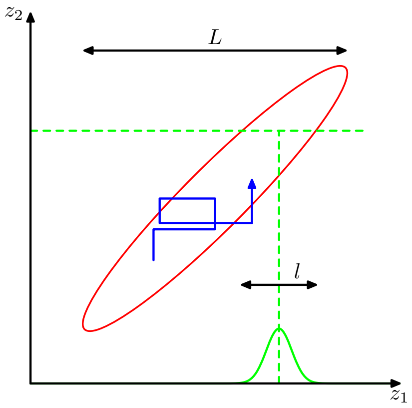
$$A(z^*, z^{(\tau)}) = \min\left(1, \frac{\tilde{p}(z^*)q(z^{(\tau)}|z^*)}{\tilde{p}(z^{(\tau)})q(z^*|z^{(\tau)})}\right)$$

- A sufficient condition for this algorithm to produce the correct distribution is detailed balance

Gibbs Sampling

- A simple coordinate-wise MCMC method
- Given distribution $p(\mathbf{z}) = p(z_1, \ldots, z_M)$, sample each variable (either in pre-defined or random order)
  - Sample $z_1^{(\tau+1)} \sim p(z_1 | z_2^{(\tau)}, z_3^{(\tau)}, \ldots, z_M^{(\tau)})$
  - Sample $z_2^{(\tau+1)} \sim p(z_2 | z_1^{(\tau+1)}, z_3^{(\tau)}, \ldots, z_M^{(\tau)})$
  - $\ldots$
  - Sample $z_M^{(\tau+1)} \sim p(z_M | z_1^{(\tau+1)}, z_2^{(\tau+1)}, \ldots, z_{M-1}^{(\tau+1)})$
- These are easy if Markov blanket is small, e.g. in MRF with small cliques, and forms amenable to sampling

Gibbs Sampling - Example



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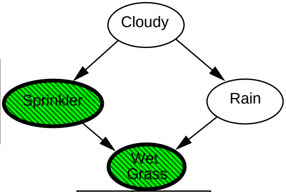
P(C)
.50



C	P(S|C)
T	.10
F	.50

C	P(R|C)
T	.80
F	.20

S	R	P(W|S,R)
T	T	.99
T	F	.90
F	T	.90
F	F	.01

- Consider running Gibbs sampling on $p(cloudy, rain|spr = t, wg = t)$
- $q(z|z^\tau)$: pick from $cloudy$, $rain$, reset its value according to $p(cloudy|rain, spr, wg)$ (or $p(rain|cloudy, spr, wg)$)
- This is often easy – only need to look at Markov blanket

Conclusion

- Readings: Ch. 11.1-11.3 (we skipped much of it)
- Sampling methods use proposal distributions to obtain samples from complicated distributions
- Different methods, different methods of correcting for proposal distribution not matching desired distribution
- In practice, effectiveness relies on having good proposal distribution, which matches desired distribution well