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Statistical methods in Data Science and AI

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Module 4.1: Resampling methods and MCMC

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Bayesian network inference

- Approximate inference, simulation or ***sampling*** is a hot topic in machine learning
- Basic idea:
  - Draw N samples from some sampling distribution $\hat{F}$
  - Compute an approximate posterior probability
  - Show that this converges to the true distribution F
- Why sample?
  - Learning: get samples from an unknonw distribution
  - Inference: faster than exact methods (if even possible)

Sampling basics

- We want to make inference about about a population that is too large to observe completely.
- Or a distribution that is too complex to observe directly.
- We draw a representative sample (*i.i.d.* observations) and assume that the conclusions approximate those of the population/distribution.
- ***But what if the distribution is too complex to even sample from?***

Sampling statistics

Given a *sample* $X_1, X_2, \dots, X_n$ from some distribution a *statistic* is a function $f(X_1, \dots, X_n)$ of the sample.

Common exampels

- **Sample mean:** $\bar{X} = \frac{1}{n}\sum_{i=1}^{n} X_i$
- **Sample variance:** $s^2 = \frac{1}{n-1}\sum_{i=1}^{n}(X_i - \bar{X})^2$
- **Sample range:** $r(X_1 \dots, X_n) = \max\{X_1, \dots, X_n\} - \min\{X_1, \dots X_n\}$

Simple sampling from a distribution

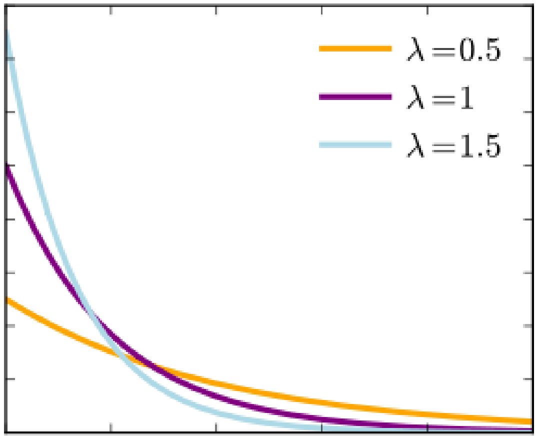
Inverse probability transformation

For a cumulative distribution function (cdf) F

- Generate uniform $U(0,1)$ sample $u_1, \ldots, u_n$
- Compute the inverse F^{-1}
- Sample from desired distribution is given by

$$x_i = F^{-1}(u_i), i = 1, \ldots, n$$

Example: sample from $\mathrm{Exp}(\lambda)$



We want to generate a sample for $X \sim \mathrm{Exp}(\lambda)$.
Distribution function

$$F(x) = 1 - e^{-\lambda x}$$

Inverse

$$y = 1 - e^{-\lambda x} \Leftrightarrow x = -\ln(1-x)/\lambda$$
$$\Leftrightarrow F^{-1}(x) = -\ln(1-x)/\lambda$$

Compute

$$x_i = -\ln(u_i)/\lambda$$

$$\boxed{U \sim U(0,1) \Rightarrow 1 - U \sim U(0,1)}$$

Resampling methods

Due to cheap rapid computing and new software ***resampling methods*** have become practical.

Common resampling methods

- **Permutation**: sampling without replacement to test hypotheses on the form ”no effect”
- **Bootstrap**: sampling with replacement to establish more precise confidence intervals
- **Monte Carlo**: repeated sampling from populations with known characteristics to determine the sensitivity to those characteristics

Resampling methods

Advantages over both nonparametric and parametric methods:

- Simpler
- More accurate
- Fewer assumptions
- Greater generalizability
- Answer questions not possible with traditional methods
- Conceptually simple

Empirical bootstrap

Example

Given a sample $X_1, \ldots, X_n$ we estimate the mean μ and variance σ^2 by the sample mean and variance

$$\hat{\mu} = \bar{X} = \frac{1}{n}\sum_{i=1}^{n} X_i$$

$$\hat{\sigma}^2 = s^2 = \frac{1}{n-1}\sum_{i=1}^{n}(X_i - \bar{X})\hat{\ }2$$

A $(1-\alpha)\%$ confidence interval for μ is then

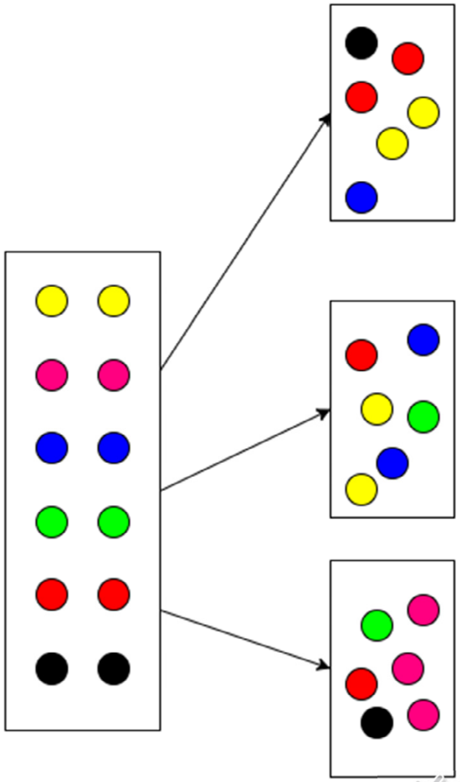
$$\mu = \bar{x} \pm z_{1-\alpha/2}\frac{s}{\sqrt{n}}$$

Can we construct a confidence interval for the sample *median* in a similar way?

Empirical bootstrap

- Given the sample $X_1, \dots, X_n$ we ***sample with replacement*** from these n points.
- Resampled sample: $X_1^{*(1)}, \dots, X_n^{*(1)}$
- Repeat this, creating B ***bootstrap samples***

$$X_1^{*(1)}, \dots, X_n^{*(1)}$$
$$X_1^{*(2)}, \dots, X_n^{*(2)}$$
$$\dots$$
$$X_1^{*(B)}, \dots, X_n^{*(B)}$$



Empirical bootstrap

- For each sample, compute the **sample median**

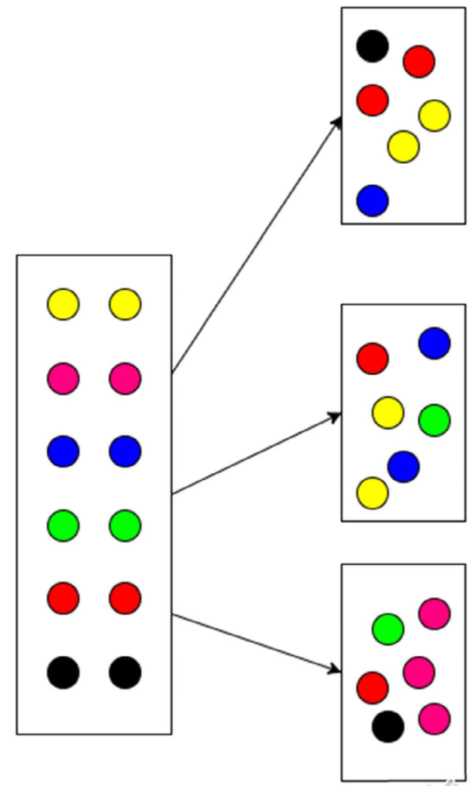
$$M_n^{*(1)}, M_n^{*(2)}, \dots, M_n^{*(B)}$$

- Estimate the median using: $\bar{M}_B = \frac{1}{B}\sum_{i=1}^{b} M_n^{*(i)}$
- Boostrap estimate of the **median variance**:

$$\widehat{\mathrm{Var}}_B(M_n) = \frac{1}{B-1}\sum_{i=1}^{B}\left(M_n^{*(i)} - \bar{M}_B^*\right)^2$$

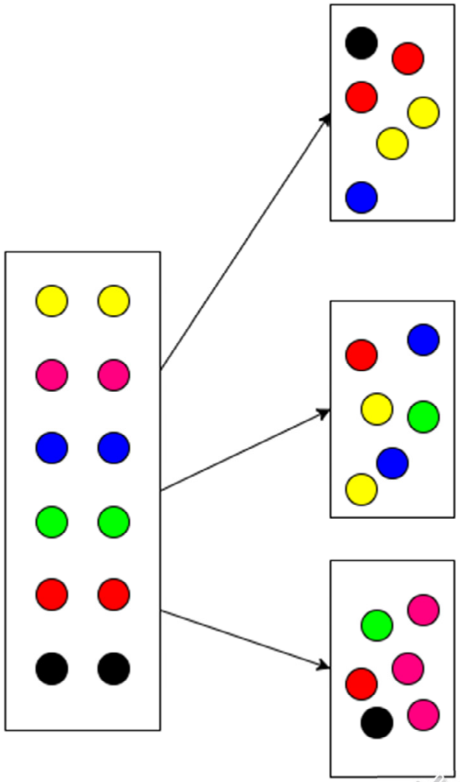
- Bootstrap **confidence interval** of the median

$$M_n \pm z_{1-\alpha/2} \cdot \sqrt{\widehat{\mathrm{Var}}_B(M_n)}$$



Empirical bootstrap

- Can be generalized to many other statistics
  - Sample quantiles
  - Interquartile range
  - Skewness (related to $E[X^3]$)
  - Kurtosis (related to $E[X^4]$)
  - …



Monte Carlo simulation

- We want to evaluate the integral

$$F(x) = \int_0^1 e^{-x^3} dx$$

No closed form solution!

- *Riemann integration*:
  Evaluate $f(x) = \exp(-x^3)$ in evenly spread points $0 \leq x_1 < x_x < \cdots < x_K \leq 1$, and compute

$$\sum_{i=1}^{K} f(x_i) / K$$

- Converges as $K \to \infty$.

Monte Carlo simulation

- **We want to evaluate an integral**

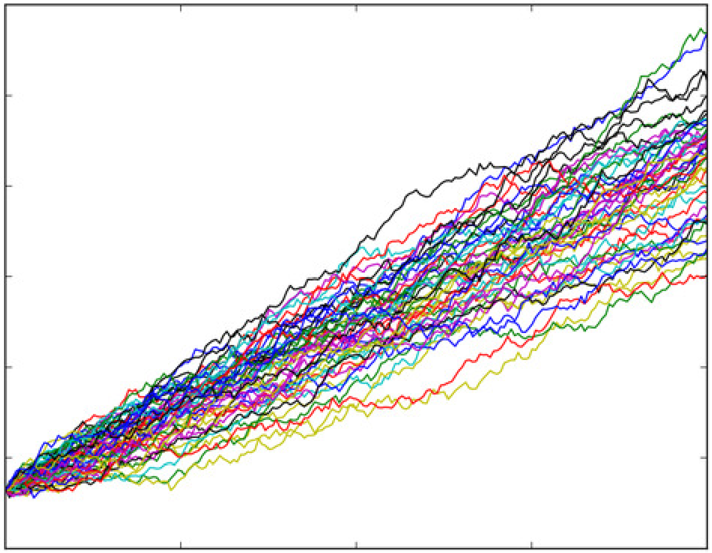
$$I = \int f(x)dx$$

- **We choose a pdf $p(x)$ of X and compute**

$$I = \int f(x)p(x)dx = E[f(X)]$$

- **Generate i.i.d. $X_1, \dots, X_n \sim p$ and compute**

$$\hat{I}_n = \frac{1}{n}\sum_{i=1}^{n} f(X_i)$$



Monte Carlo simulation – example

- We want to compute the integral

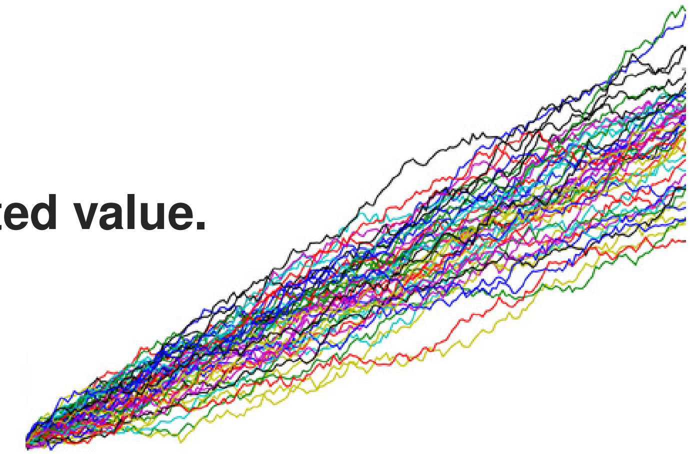
$$I = \int_0^1 e^{-x^3} dx$$

- Let $U \sim U[0,1]$ and write

$$I = \int_0^1 e^{-x^3} 1 dx = E\left[e^{-U^3}\right]$$

evaluating integral ⇔ estimating the expected value.

$$E\left[e^{-U^3}\right]$$

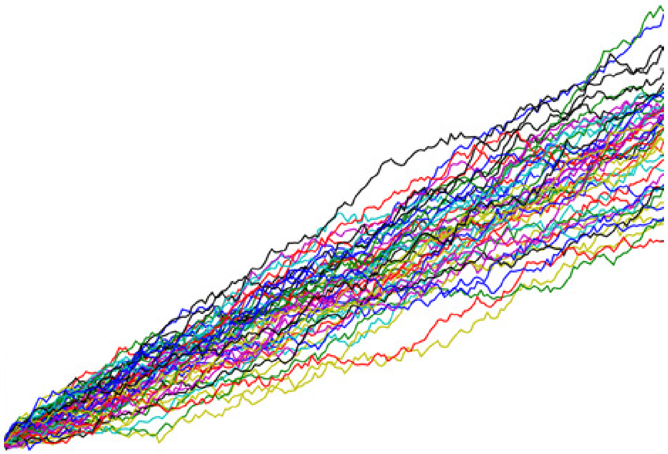


Monte Carlo simulation – example

- **Generate i.i.d. sample** $U_1, \dots, U_n \sim U[0,1]$**.**
- **Compute** $W_i = e^{-U_i^3}$ **and use**

$$\bar{W} = \frac{1}{n}\sum_{i=1}^{n} W_i = \frac{1}{n}\sum_{i=1}^{n} e^{-U_i^3}$$

- **Law of large numbers:** $\bar{W} \xrightarrow{P} E[W_i] = E\left[e^{-U^3}\right]$



Monte Carlo simulation – example

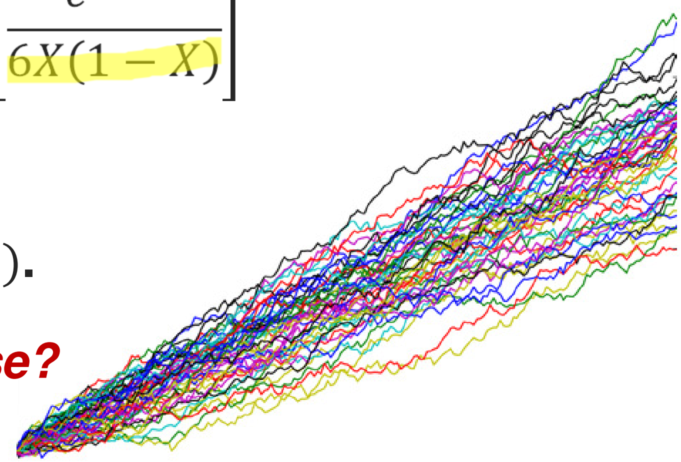
- **Note that the function f changes if the pdf p changes:**
- **Since $\mathrm{Beta}(2,2)$ has pdf $p(x) = 6x(1-x)$ we could write**

$$\int_0^1 e^{-x^3} dx = \int_0^1 \frac{e^{-x^3}}{6x(1-x)} \cdot 6x(1-x) dx = E\left[\frac{e^{-X^3}}{6X(1-X)}\right]$$

where now $X \sim \mathrm{Beta}(2,2)$.

- **Thus we can sample i.i.d. $X_1, \ldots, X_n \sim \mathrm{Beta}(2,2)$.**

So which sampling distribution p should we use?



Monte Carlo simulation: bias and variance

- **Bias:**

$$E[\hat{I}_n] = I \Rightarrow \mathbf{bias} = 0$$

Unbiased!

- **Variance**

$$\begin{aligned}\mathrm{Var}(\hat{I}_n) &= \frac{1}{n}\mathrm{Var}(f(X_1)) \\ &= \frac{1}{n}(E[f^2(X_1)] - (E[f(X_1)])^2) \\ &= \frac{1}{n}(\int f^2(x)p(x)dx - I^2)\end{aligned}$$

The variance depends on the sample size n and sampling distribution p.

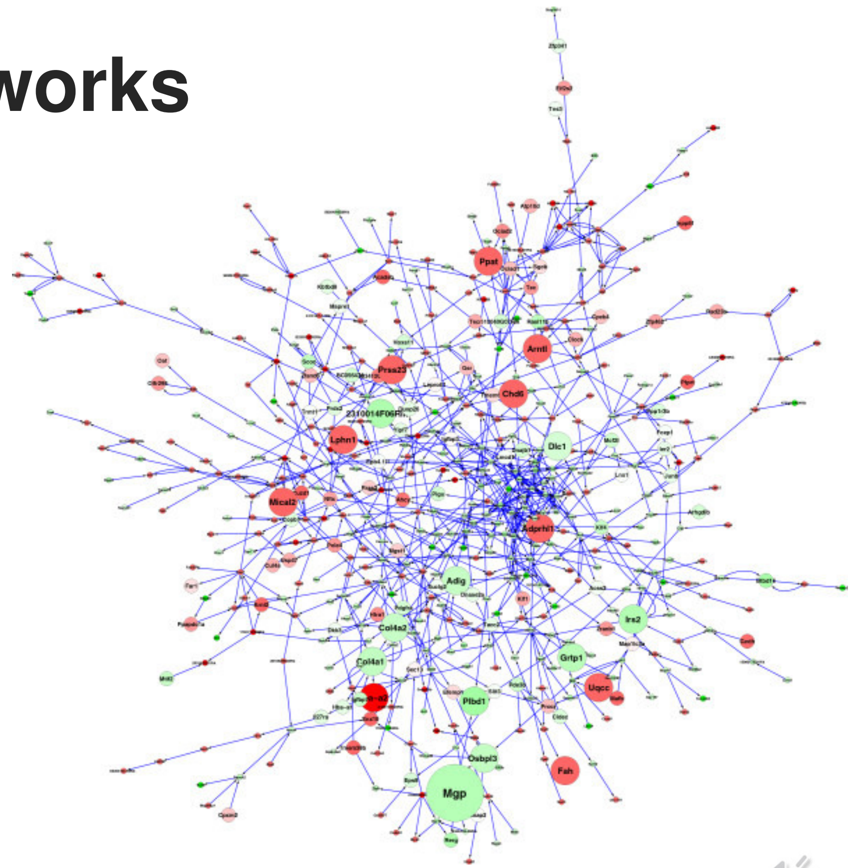
The quantity I^2 is fixed.

We choose a density p and a function f that minimizes the variance.

How?

Sampling in Bayesian networks

- Prior sampling
- Rejection sampling
- Likelihood weighting
- Gibbs sampling



Prior sampling

- **In a network of n nodes $X_1, \dots, X_n$ a sample is generated by drawing in hierarchical order from**

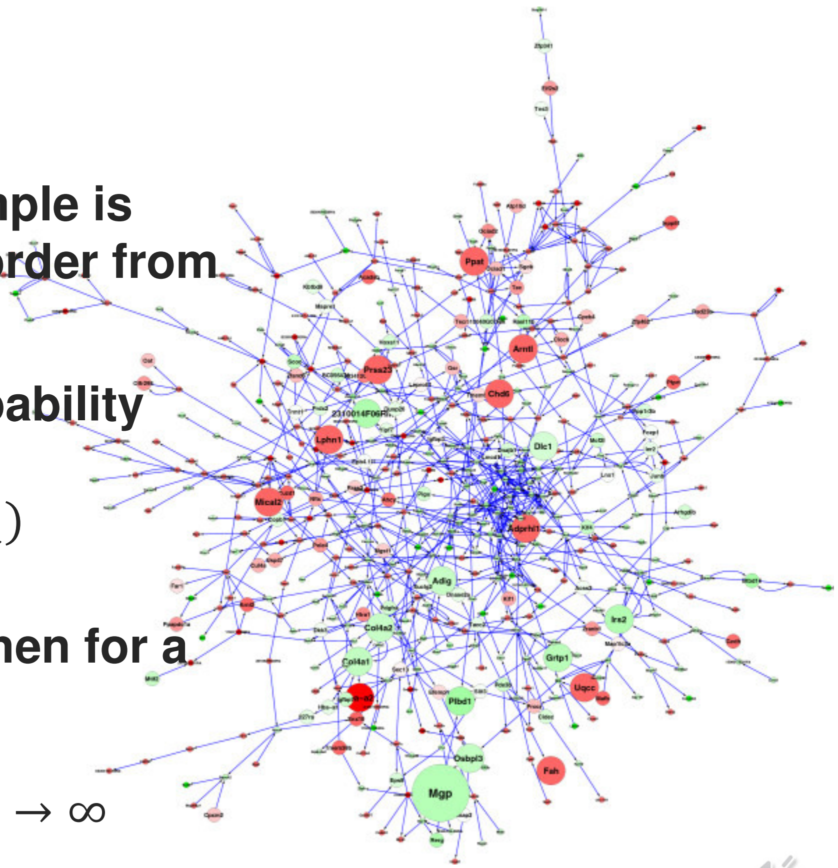
$$P(X_i|\text{pa}(X_i), i = 1, \dots, n$$

- **Then samples are generated with probability**

$$\prod_{i=1}^{n} P(X_i|\text{pa}(X_i)) = P(X_1, \dots, X_n)$$

- **Repeat the process many times (N). Then for a certain event $(x_1, \dots, x_n)$**

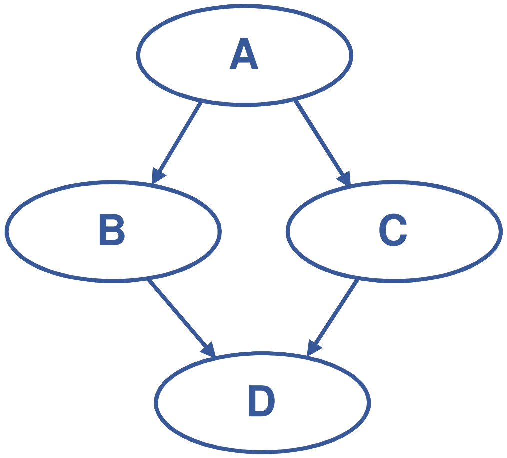
$$\frac{\#\{(x_1, \dots, x_n)\}}{N} \to P(x_1, \dots, x_n) \ \text{ as } \ N \to \infty$$



Prior sampling: example

- **Assume that we sample a Bayesian network with *true*/*false* variables A, B, C, D**

$$+a, -b, +c, +d$$
$$+a, +b, +c, +d$$
$$-a, +b, +c, -d$$
$$+a, -b, +c, +d$$
$$-a, -b, -c, +d$$



- **To compute the probability $P(D)$ we see**

$$\#\{+d\} = 4, \#\{-d\} = 1$$

- **Thus: $\widehat{P}(D = +d) = 4/5 = 0.80 = 1 - \widehat{P}(D = -d)$**

Rejection sampling (rejection/acceptance)

Assume we want to sample from some distribution $p(x)$

1. **Create a rejection distribution $q(x)$ that is easy to sample from and which satisfies**

$$Mq(x) \geq \tilde{p}(x)$$

envelope

constant M, $\tilde{p}(x)$ = unnormalized $p(x)$

$$p(x) = \tilde{p}(x)/Z_p \Leftrightarrow \tilde{p}(x) = p(x)Z_p$$

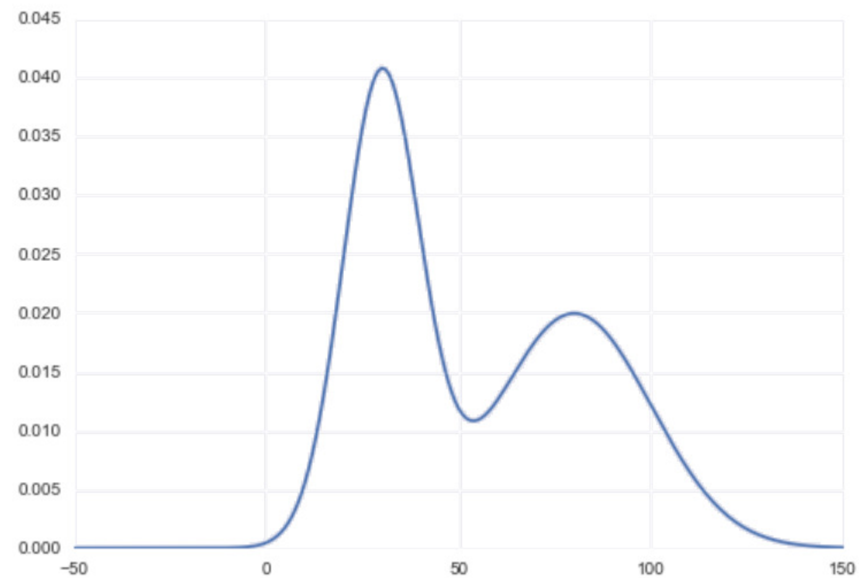
2. **Sample a random location $x \sim q(x)$ and a random height $u \sim U(0,1)$.**

3. **If $u \leq \frac{\tilde{p}(x)}{Mq(x)}$ keep the observation in sample.**

Example: rejection sampling

We want to sample from a Gaussian mixture

$$X + Y \sim N(30,10) + N(80,20)$$



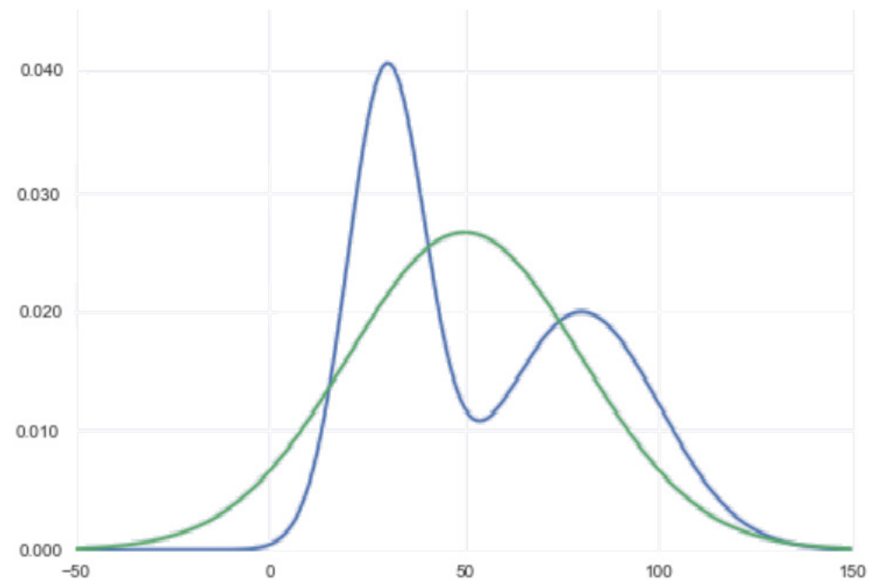
Example: rejection sampling

We want to sample from a Gaussian mixture

$$X + Y \sim N(30,10) + N(80,20)$$

Use $q(x) = N(50,30)$ **as proposal distribution. (Unnormalized)**

Bad choice since $q(x)$ **is *not* enveloping** $p(x)$**.**



Example: rejection sampling

We want to sample from a Gaussian mixture

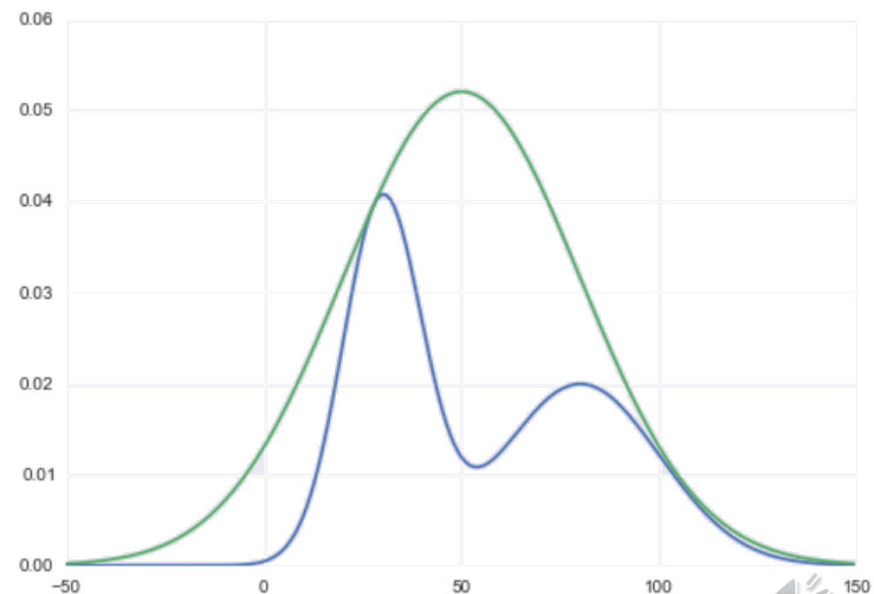
$$X + Y \sim N(30,10) + N(80,20)$$

Use $q(x) = N(50,30)$ as proposal distribution. (Unnormalized)

Bad choice since $q(x)$ is ***not*** enveloping $p(x)$.

Add on a scaling factor

$$k = \max\left(p(x)/q(x)\right) \text{ for all } x$$



Example: rejection sampling

- **Produce a large sample from**

$$Z \sim q(x)$$

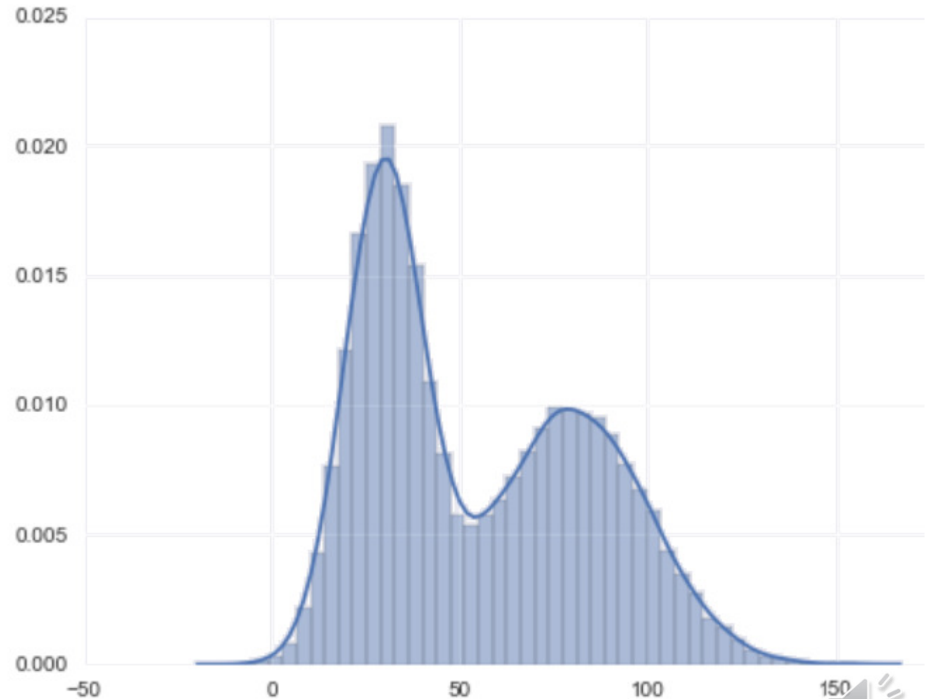
- **Uniformly pick the height**

$$u \sim U\big(0, kq(z)\big)$$

Now (z, u) is uniform under

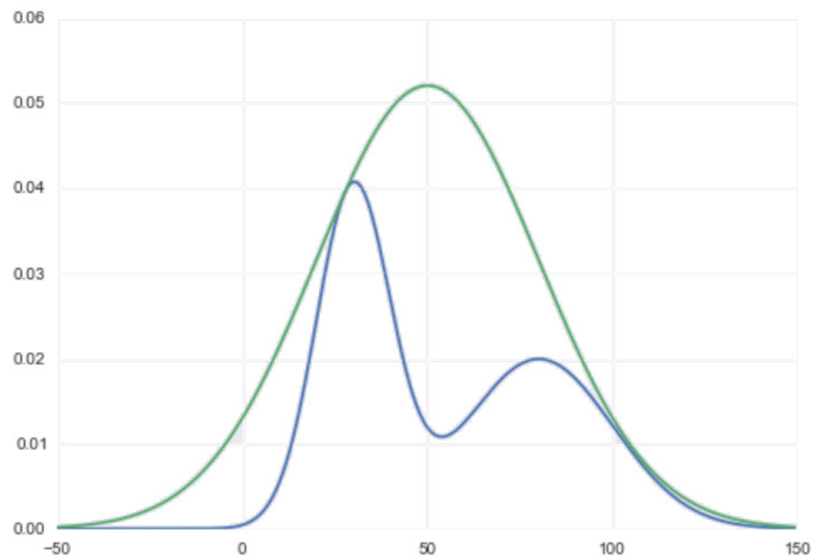
$$kq(x)$$

- **Accept points (z, u) under the $p(x)$ curve.**



Rejection sampling

- **Unnormalized target distribution – no problem.**
- **Drawbacks:**
  - **Need a closed form for q.**
  - **$q(x)$ has to envelope $p(x)$.**
  - **Need to know shape of $p(x)$.**
  - **Large M is time consuming.**



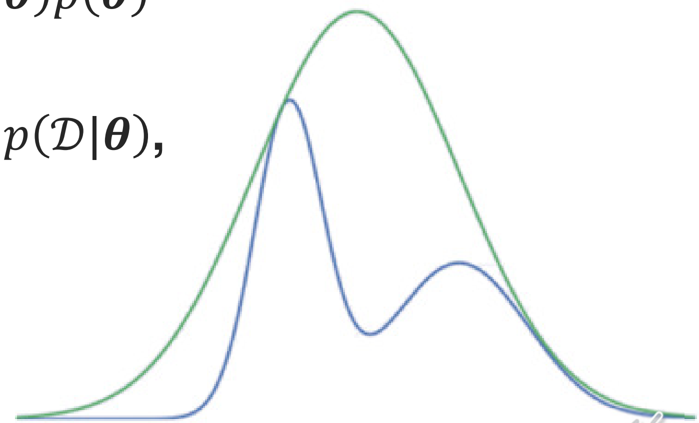
Rejection sampling in Bayesian statistics

- **Data set $\mathcal{D}$ and target distribution with parameter $\boldsymbol{\theta}$.**
- **We want to sample from the posterior**

$$p(\boldsymbol{\theta}|\mathcal{D}) = p(\mathcal{D}|\boldsymbol{\theta})p(\boldsymbol{\theta})/p(\mathcal{D})$$

- **We can use unnormalized target $\tilde{p}(\boldsymbol{\theta}) = p(\mathcal{D}|\boldsymbol{\theta})p(\boldsymbol{\theta})$**
  proposal distribution $q(\boldsymbol{\theta}) = p(\boldsymbol{\theta})$
  and envelope $M = p(\mathcal{D}|\widehat{\boldsymbol{\theta}})$ where $\widehat{\boldsymbol{\theta}} = \arg\max p(\mathcal{D}|\boldsymbol{\theta})$,
  i.e. the MLE
- **Accept sampled points with probability**

$$P = \frac{p(\boldsymbol{\theta}|\mathcal{D})}{Mq(\boldsymbol{\theta})}$$

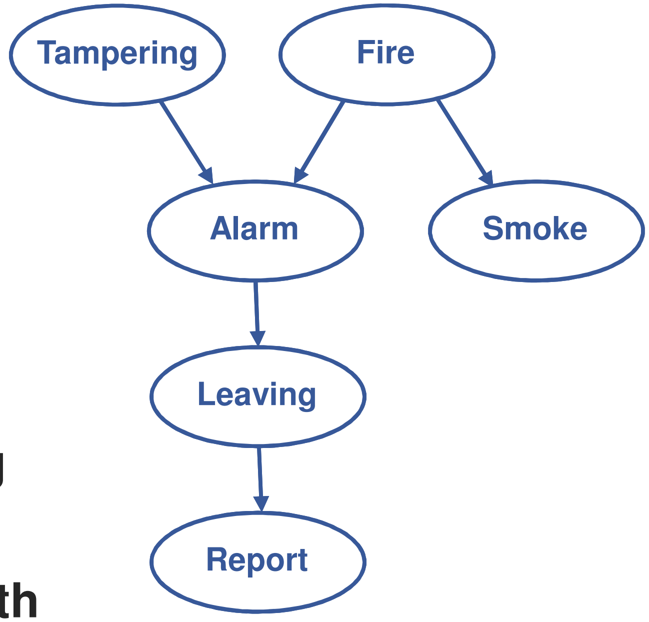


Sampling in Bayesian networks: example

We use an AI to diagnose the true cause of a fire alarm.

Variabels (all true/false):

- *Fire*: true when there is a fire
- *Alarm*: true when the alarm sounds
- *Smoke*: true when there is smoke
- *Leaving*: true if many people leave the building
- *Report*: true if reports of people leaving
- *Tampering*: true when alarm were tampered with

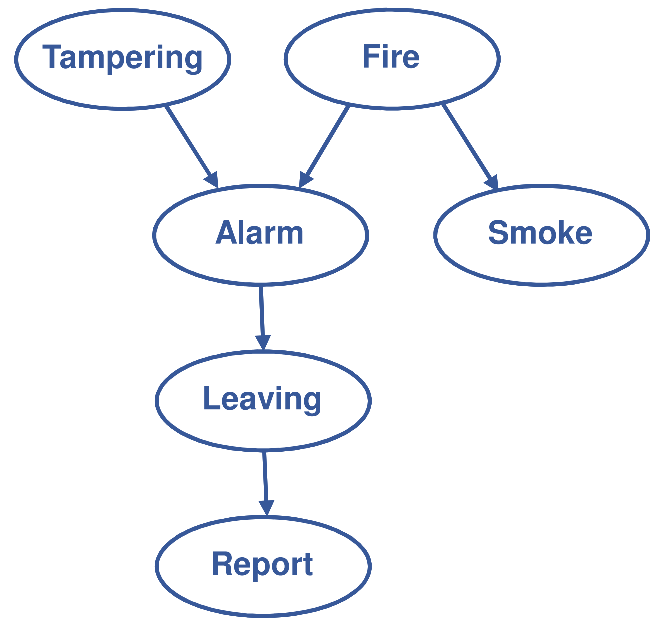


Conditional dependencies are given by the DAG.

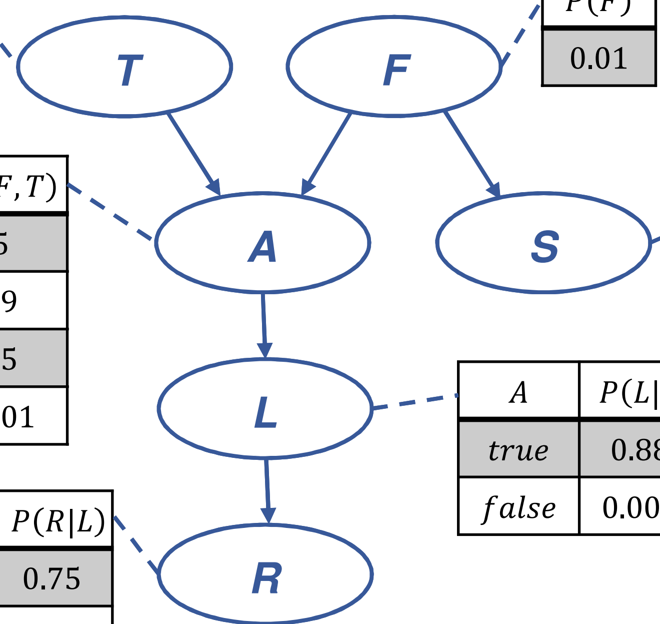
Sampling in Bayesian networks: example

Factorization

$$
\begin{aligned}
&\boldsymbol{P}(\text{tampering, fire, alarm, smoke, leaving, report}) = \\
&\quad = \boldsymbol{P}(\text{tampering}) \\
&\qquad \cdot \boldsymbol{P}(\text{fire}) \\
&\qquad \cdot \boldsymbol{P}(\text{alarm} \mid \text{tampering, fire}) \\
&\qquad \cdot \boldsymbol{P}(\text{smoke} \mid \text{fire}) \\
&\qquad \cdot \boldsymbol{P}(\text{leaving} \mid \text{alarm}) \cdot \\
&\qquad \cdot \boldsymbol{P}(\text{report} \mid \text{leaving})
\end{aligned}
$$



Sampling in Bayesian networks: example



$P(T)$
0.02

$P(F)$
0.01

F	T	$P(A\|F,T)$
$true$	$true$	0.5
$true$	$false$	0.99
$false$	$true$	0.85
$false$	$false$	0.0001

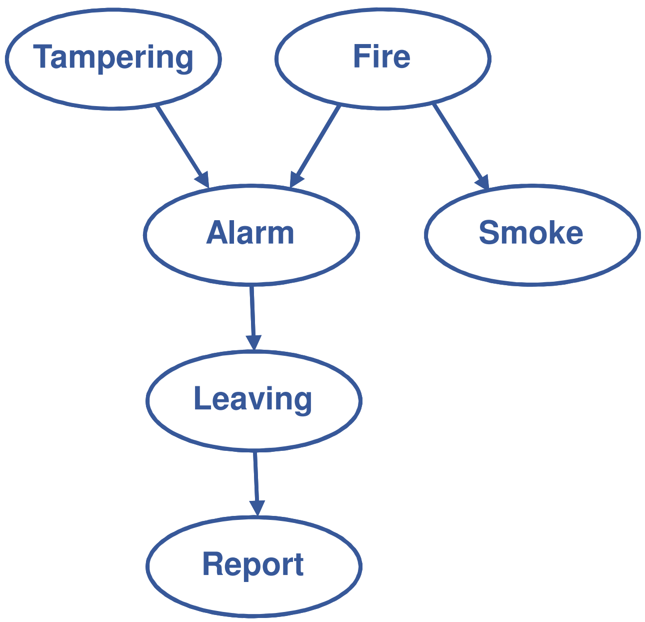
F	$P(S\|F)$
$true$	0.9
$false$	0.01

A	$P(L\|A)$
$true$	0.88
$false$	0.001

L	$P(R\|L)$
$true$	0.75
$false$	0.01

Forward sampling in Bayesian networks

A method to generate a sample of every variable so that each sample is generated in proportion to its probability.



Forward sampling

Assume variables $X_1, X_2, \dots, X_n$ are network variables ordered so parents come before children.

1. Sample X_1 using its CDF
2. Sample X_2 given the value of X_1
3. …

Forward sampling in Bayesian networks

Sampling from a single variable

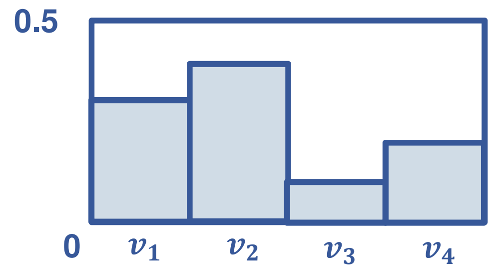
Assume variable X takes values $\{v_1, v_2, v_3, v_4\}$.
Assume

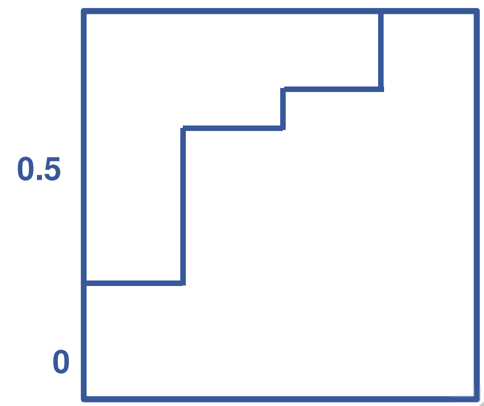
$$P(X = v_1) = 0.3$$
$$P(X = v_2) = 0.4$$
$$P(X = v_3) = 0.1$$
$$P(X = v_4) = 0.2$$

Order the values, say $v_1 < v_2 < v_3 < v_4$.

Generate numbers from $u \sim U(0,1)$:

If $v_2 < u < v_3$, then v_3 etc.





Sampling in Bayesian networks: example

Forward sampling:

Sample	T	F	A	S	L	R
s_1	*false*	*false*	*true*	*false*	*false*	*true*
s_2	*false*	*true*	*false*	*true*	*false*	*false*
s_3	*false*	*true*	*true*	*false*	*true*	*true*
s_4	*false*	*true*	*false*	*true*	*false*	*false*
s_5	*false*	*true*	*true*	*true*	*true*	*true*
s_6	*false*	*false*	*false*	*true*	*false*	*false*
s_7	*true*	*false*	*false*	*false*	*true*	*false*
s_8	*true*	*true*	*true*	*true*	*true*	*true*
…						
s_{1000}	*true*	*false*	*true*	*false*	*true*	*false*

Sample from Tampering:

$P(T) = 0.02, P(T^c) = 0.98$

Draw from $U(0,1) \Rightarrow u = 0.37$

$\Rightarrow T = false$

Sample from Fire:

$P(F) = 0.01, P(F^c) = 0.99$

$\Rightarrow F = true$

Sample from Alarm given parents

$P(A|T^c, F) = 0.99,$

$P(A^c|T^c, F) = 0.01$

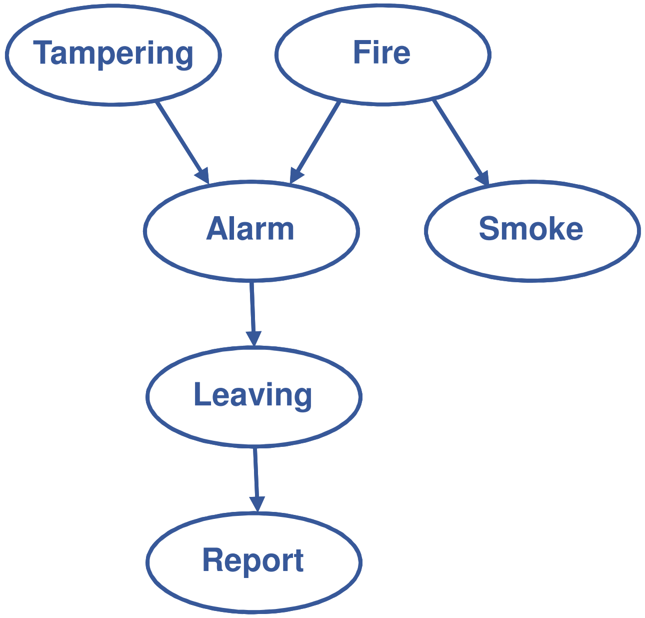
$\Rightarrow A = true$

etc.

Rejection sampling in Bayesian networks

Given some data D rejection sampling estimates the posterior

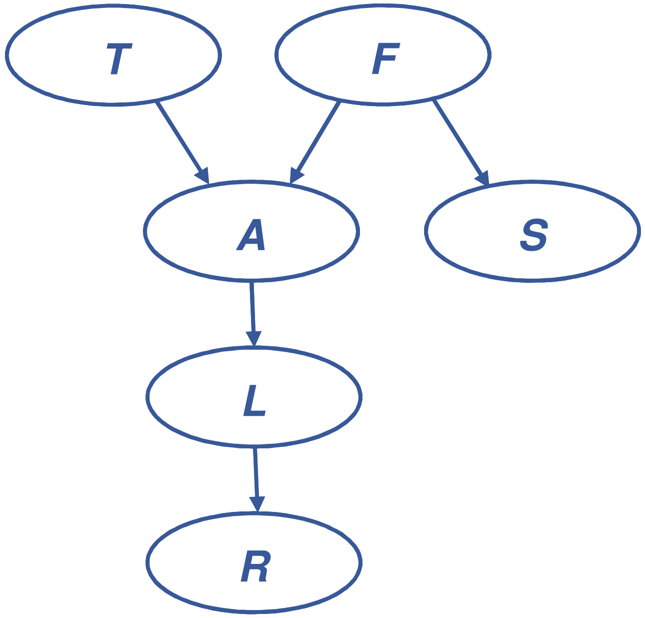
$$P(Y|D) = \frac{P(D|Y)P(Y)}{P(D)}$$



Sampling in Bayesian networks: example

Rejection sampling for $P(T|S, R^c)$

Sample	T	F	A	S	L	R	
s_1	*false*	*false*	*true*	*false*	**X**		
s_2	*false*	*true*	*false*	*true*	*false*	*false*	✓
s_3	*false*	*true*	*true*	*false*	**X**		
s_4	*false*	*true*	*false*	*true*	*false*	*false*	✓
s_5	*false*	*true*	*true*	*true*	*true*	*true*	**X**
s_6	*false*	*false*	*false*	*true*	*false*	*false*	✓
s_7	*true*	*false*	*false*	*false*	**X**		
s_8	*true*	*true*	*true*	*true*	*true*	*true*	**X**
…							
s_{1000}	*true*	*false*	*true*	*false*	**X**		



Sampling in Bayesian networks: example

Rejection sampling for $P(T|S, R^c)$

Sample	T	F	A	S	L	R	
s_1	*false*	*false*	*true*	*false*	**X**		
s_2	*false*	*true*	*false*	*true*	*false*	*false*	✓
s_3	*false*	*true*	*true*	*false*	**X**		
s_4	*false*	*true*	*false*	*true*	*false*	*false*	✓
s_5	*false*	*true*	*true*	*true*	*true*	*true*	**X**
s_6	*false*	*false*	*false*	*true*	*false*	*false*	✓
s_7	*true*	*false*	*false*	*false*	**X**		
s_8	*true*	*true*	*true*	*true*	*true*	*true*	**X**
…							
s_{1000}	*true*	*false*	*true*	*false*	**X**		

The probability $P(T|S, R^c)$ is estimated using observed proportions:

$$\hat{P}(T|S, R^c) = \frac{\#\{\text{accepted}, T\}}{\#\{\text{accepted}\}}$$

Sampling in Bayesian networks: example

Downside: Rejection sampling requires MANY samples

Sample	T	F	A	S	L	R
s_1	*false*	*false*	*true*	*false*	*false*	*true*
s_2	*false*	*true*	*false*	*true*	*false*	*false*
s_3	*false*	*true*	*true*	*false*	*true*	*true*
s_4	*false*	*true*	*false*	*true*	*false*	*false*
s_5	*false*	*true*	*true*	*true*	*true*	*true*
s_6	*false*	*false*	*false*	*true*	*false*	*false*
s_7	*true*	*false*	*false*	*false*	*true*	*false*
s_8	*true*	*true*	*true*	*true*	*true*	*true*
…						
s_{1000}	*true*	*false*	*true*	*false*	*true*	*false*

Example: estimate $P(T|S,F)$

Recall:

$$P(F) = 0.01$$
$$P(S|F) = 0.9$$
$$P(S|F^c) = 0.01$$

Out of 1000 samples:

≈ **990** $F = false$

Of these 990

≈ **1% = 10** $S = true$

⇒ **remaining 980 (98%) rejected**

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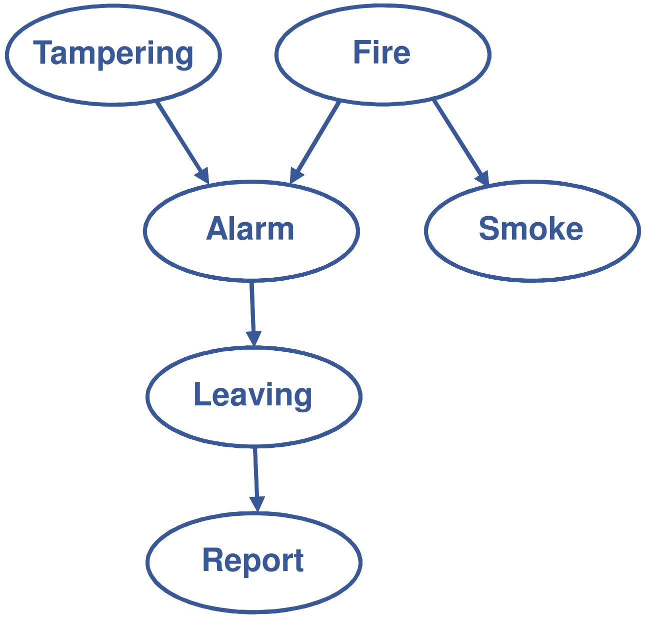
Likelihood weighting in Bayesian networks

- A kind of importance sampling where instead of accepting/rejecting a sample, we **weigh** its contribution to the sample.
- Instead of generating samples until enough many has been accepted:
  - Generate only samples that agree with **evidence** (what we condition on)
  - **Weigh** samples by their likelihood
  - Combine the corresponding weights in the final probability estimates.



Likelihood weighting in Bayesian networks

If we wanted to estimate $P(\mathbf{X}|\mathbf{Y})$:

- Compute the sampling distribution of $\mathbf{X}$ with $\mathbf{Y}$ fixed

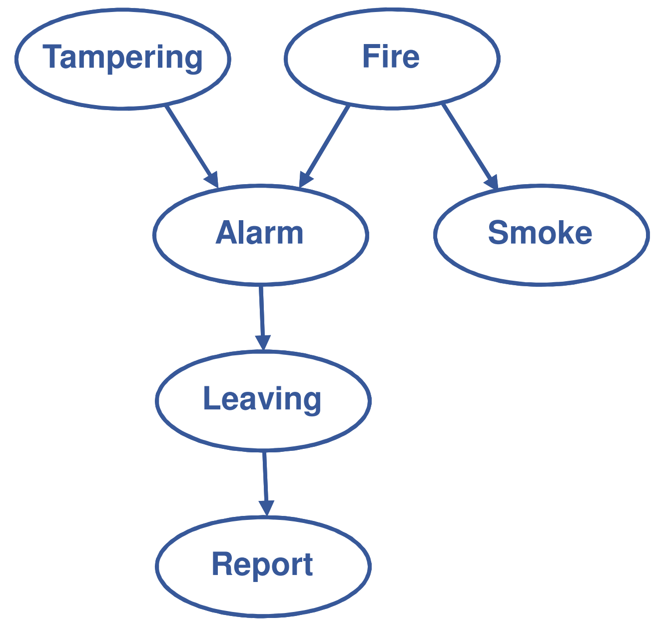
$$S_{LW}(\mathbf{x}, \mathbf{y}) = \prod_{X_i \in \mathbf{X}} P(X_i | \mathrm{pa}(X_i))$$

- Compute sample weights

$$w(\mathbf{x}, \mathbf{y}) = \prod_{Y_i \in \mathbf{Y}} P(Y_i | \mathrm{pa}(Y_i))$$

- We get

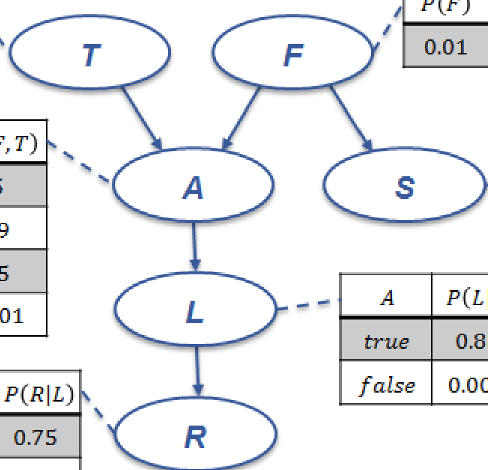
$$\hat{P}(\mathbf{X} = \mathbf{x}, \mathbf{Y} = \mathbf{y}) = S_{LW}(\mathbf{x}, \mathbf{y}) w(\mathbf{x}, \mathbf{y})$$



Likelihood weighting in Bayesian networks

$P(T)$
0.02

$P(F)$
0.01



F	T	$P(A\|F,T)$
$true$	$true$	0.5
$true$	$false$	0.99
$false$	$true$	0.85
$false$	$false$	0.0001

F	$P(S\|F)$
$true$	0.9
$false$	0.01

A	$P(L\|A)$
$true$	0.88
$false$	0.001

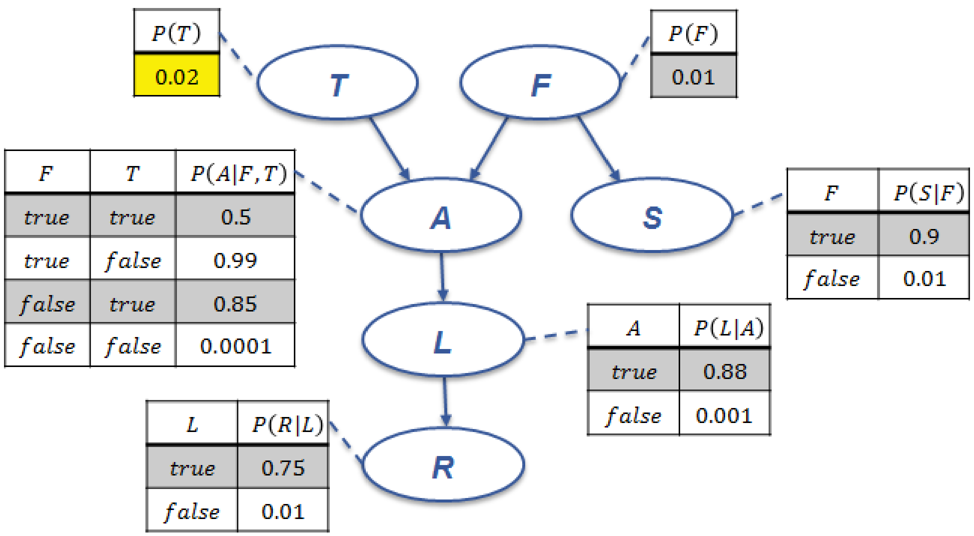
L	$P(R\|L)$
$true$	0.75
$false$	0.01

Example: estimate $P(T|S,R^c)$

Variables $S = true$ **and** $R = false$ **are fixed** ***evidence***

Generate sample:

Likelihood weighting in Bayesian networks



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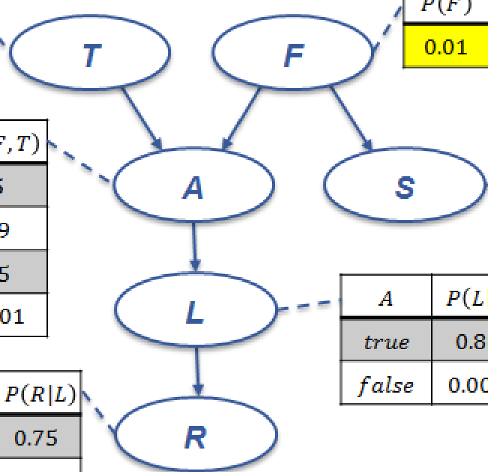
Example: estimate $P(T|S,R^c)$

Variables $S = true$ and $R = false$ are fixed *evidence*

Generate sample:

1. **Sample T: e.g $T = false$**

Likelihood weighting in Bayesian networks



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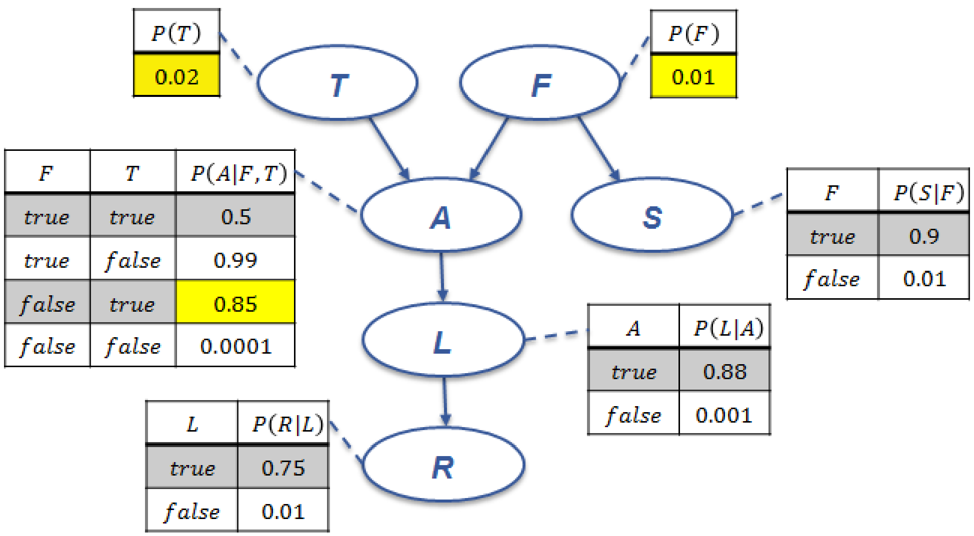
Example: estimate $P(T|S,R^c)$

Variables $S = true$ **and** $R = false$ **are fixed** ***evidence***

Generate sample:

1. **Sample** T**: e.g** $T = false$
2. **Sample** F**: e.g.** $F = true$

Likelihood weighting in Bayesian networks



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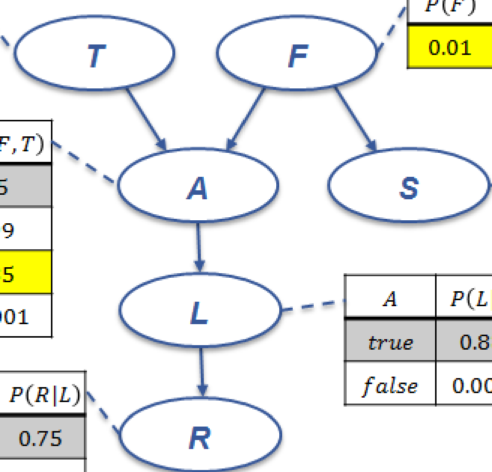
Example: estimate $P(T|S,R^c)$

Variables $S = true$ and $R = false$ are fixed *evidence*

Generate sample:

1. **Sample T: e.g $T = false$**
2. **Sample F: e.g. $F = true$**
3. **Sample $A|F,T^c$: e.g. $A = true$**

Likelihood weighting in Bayesian networks



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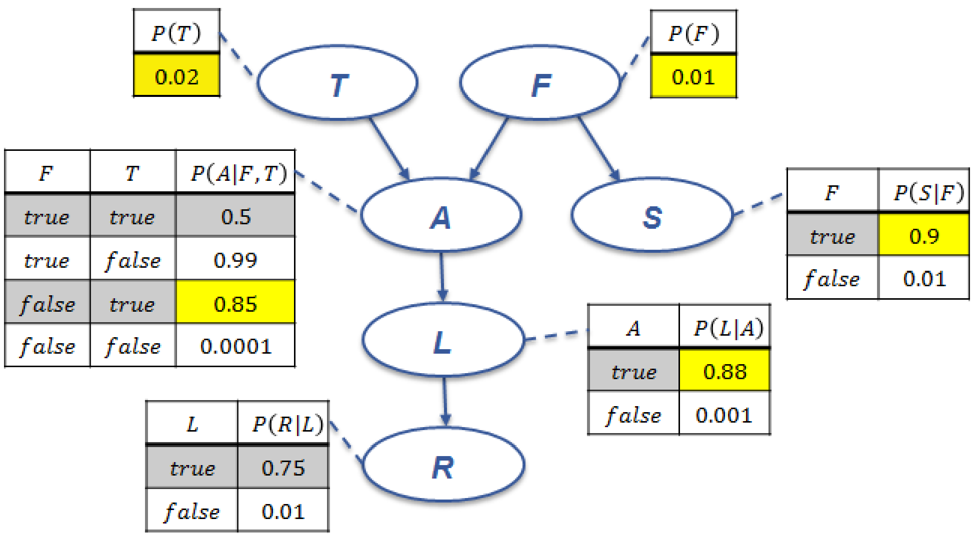
Example: estimate $P(T|S,R^c)$

Variables $S = true$ and $R = false$ are fixed *evidence*

Generate sample:

1. **Sample T: e.g $T = false$**
2. **Sample F: e.g. $F = true$**
3. **Sample $A|F,T^c$: e.g. $A = true$**
4. **Now: $S = true$ is evidence**
   weight $w = P(S|F) = 0.9$

Likelihood weighting in Bayesian networks



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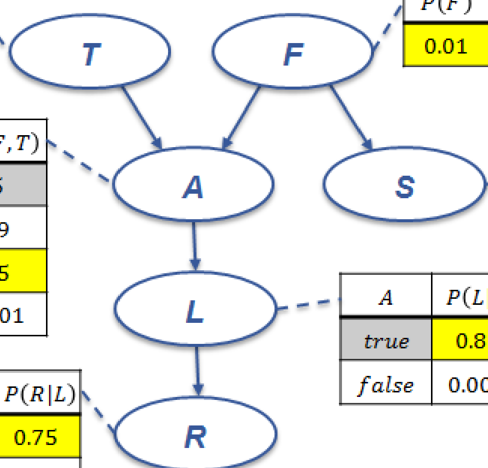
Example: estimate $P(T|S,R^c)$

Variables $S = true$ **and** $R = false$ **are fixed** ***evidence***

Generate sample:

1. **Sample** T**: e.g** $T = false$
2. **Sample** F**: e.g.** $F = true$
3. **Sample** $A|F,T^c$**: e.g.** $A = true$
4. **Now:** $S = true$ **is evidence**
   weight $w = P(S|F) = 0.9$
5. **Sample** $L|A$**: e.g.** $L = true$

Likelihood weighting in Bayesian networks



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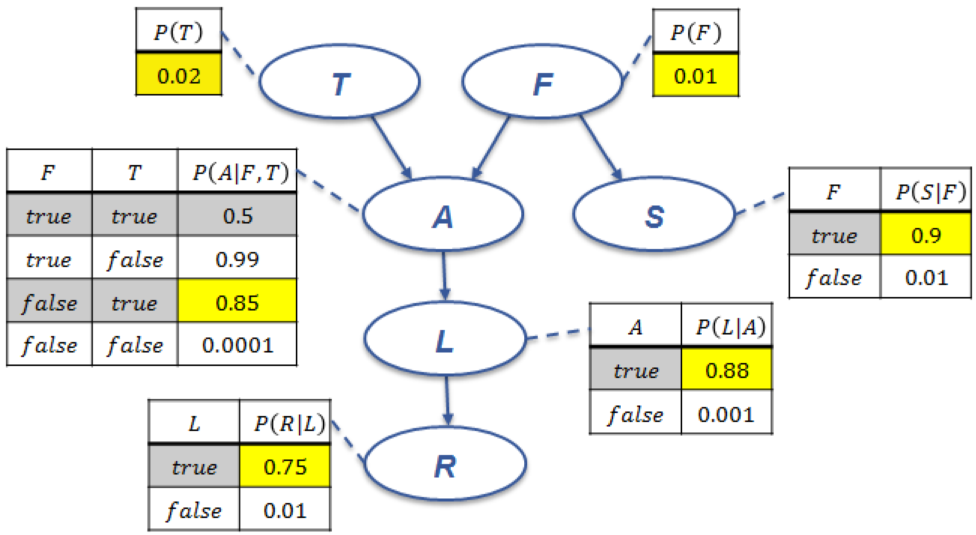
Example: estimate $P(T|S,R^c)$

Variables $S = true$ **and** $R = false$ **are fixed *evidence***

Generate sample:

1. **Sample** T**: e.g** $T = true$
2. **Sample** F**: e.g.** $F = true$
3. **Sample** $A|F,T$**: e.g.** $A = false$
4. **Now:** $S = true$ **is evidence**
   weight $w = P(S|F) = 0.9$
5. **Sample** $L|A^c$**: e.g.** $L = true$
6. **Now:** $R = false$ **is evidence**
   $w = 0.9 \cdot P(R^c|L) = 0.9 \cdot 0.25 = 0.225$

Likelihood weighting in Bayesian networks



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$true$	0.75
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Example: estimate $P(T|S,R^c)$

$$w = 0.9 \cdot P(R^c|L) = 0.9 \cdot 0.25 = 0.225$$

Sample $\{T, F, A^c, S, L, R^c\}$ **gets weight** $w = 0.225$

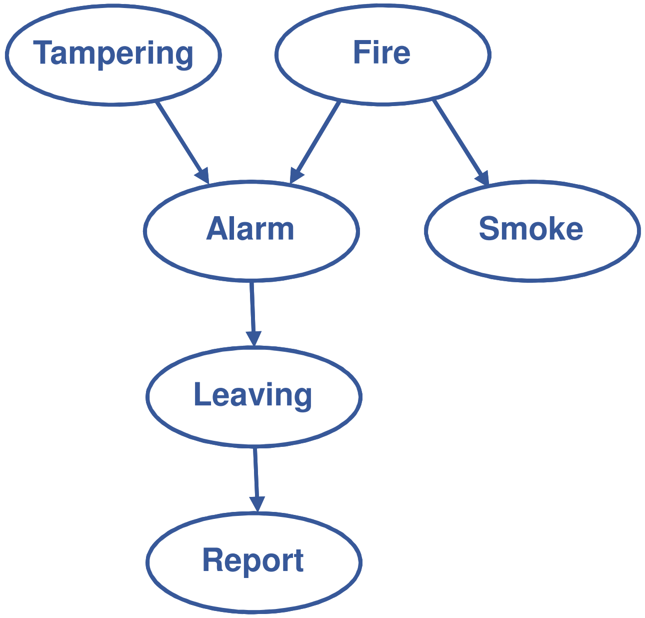
Draw new samples and add the weights for each specific state. E.g. if state $\{T, F, A^c, S, L, R^c\}$ **occurs** n **times the total weight for that state is** $n \cdot 0.225$**.**

To compute $P(T|S,R^c)$

$$P(T|S,R^c) = \frac{\text{sum of weights where } T = true}{\text{sum of all weights}}$$

Likelihood weighting: algorithm

1. Initiate the weight of the sample: $w = 1$
2. Initiate the state of the sample $x = \{\}$
3. Initiate total weights: $W(x) = 0$
4. Sample node by node:
   a) If current node is evidence (conditioned on)
      $w = w \cdot P(currentNode|parents)$
      Add state of node to x.
   b) If not, sample from distribution to determine its state.
      Add state of node to x.
5. Add weight to total weight: $W(x) = W(x) + w$



Compute estimate for specific probabilities

$$\hat{P}(X|Y) = \left(\sum_{x:X|Y} W(x)\right) / \left(\sum_{x} W(x)\right)$$

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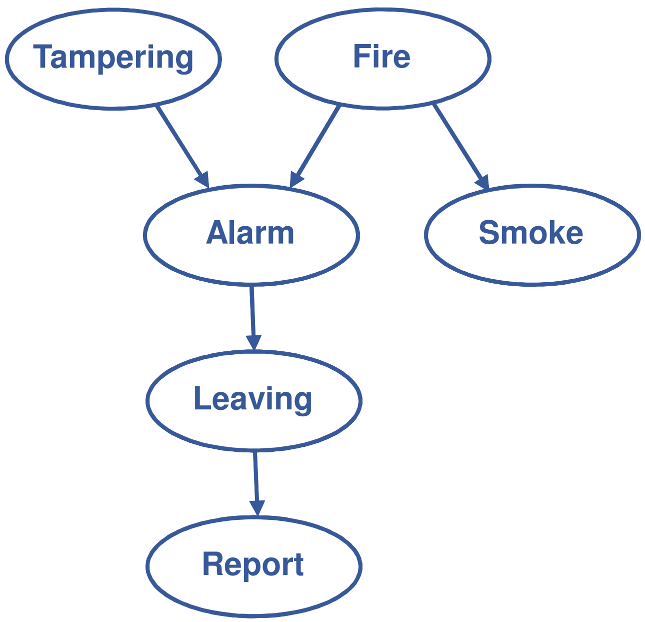
Likelihood weighting in Bayesian networks

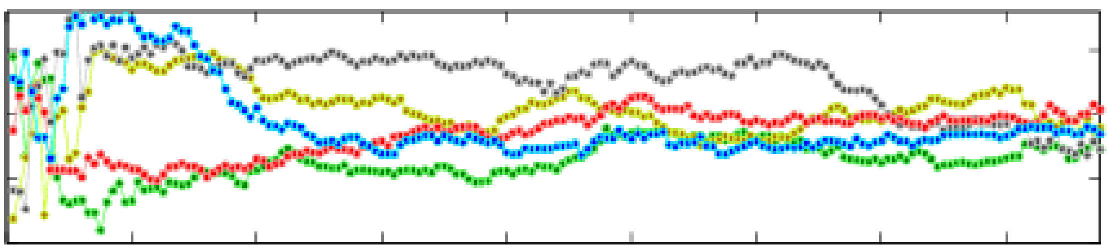
- **More efficient than rejection sampling.**
- **But doesn't solve all our problems:**
  - **By fixing the evidence nodes, we influence the sampling of the downstream variables, not the upstream ones.**



We would like to consider the evidence when we sample every node!

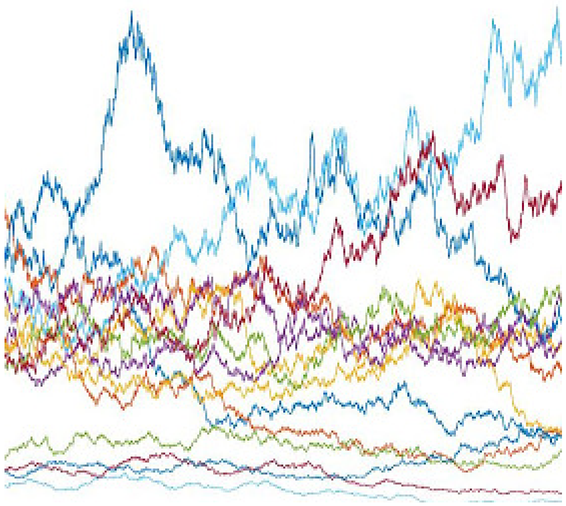
Markov chain Monte Carlo (MCMC)

- **MCMC combines Monte Carlo simulation and Markov chains.**
- **Idea: Instead of generating every sample from scratch, we create samples that are similar to the previous one**
- **We construct a Markov chain that has the desired distribution as stationary distribution.**



Markov processes

- A **random process** is a set of random variables $\{X(t)\}_{t \in T}$ developing over time t.
  - The time can be continuous or discrete
  - It can be actual time or some kind of spatial enumeration (e.g. characters in a text)
- A **Markov process** is a random process were conditioning on the current state, future states are independent of the past.



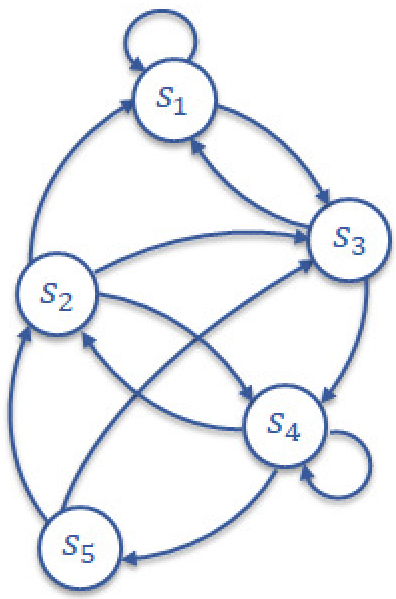
Markov chains

- A **Markov chain** is a discrete realization $X_1, X_2, X_3, \dots$ of a Markov process, where the process jumps between states in some state space

$$S = \{s_1, \dots, s_N\}$$

and where the next jump only depends on the current state

$$P(X_{n+1} = j | X_1 = x_1, \dots, X_{n-1} = x_{n-1}, X_n = i)$$
$$= P(X_{n+1} = j | X_n = i)$$



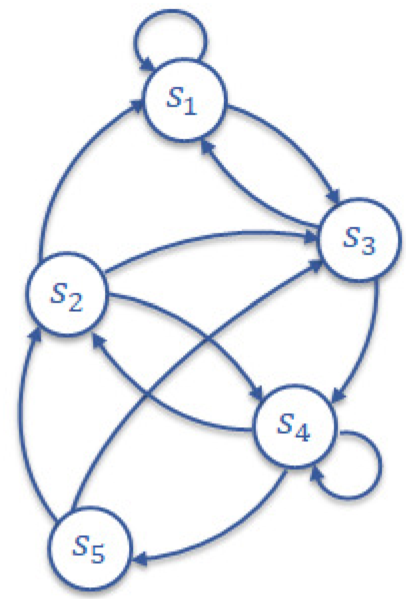
Markov chains

- A Markov chain is defined by its
  - state space $S = \{s_1, \dots, s_N\}$
  - initial state distribution

    $$\pi_i = P(X_1 = s_i), i = 1, \dots, n$$

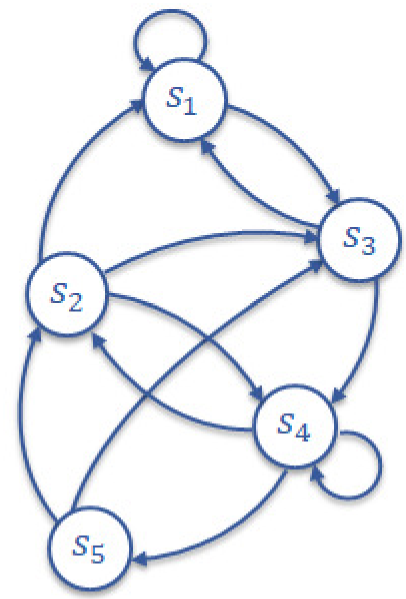
  - transition probabilities

    $$p_{ij} = P(X_{n+1} = j | X_n = i)$$



Markov chains

- A Markov chain is said be be ***stationary*** if its distribution of the state is independent of its starting condition.
- This means that we can start the chain in any initial state and if we run it long enough (burn-in period) we approach stationarity.
- Key idea of MCMCs: construct a Markov chain whose stationary distribution is the distribution we want to sample from.



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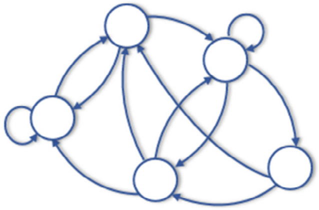
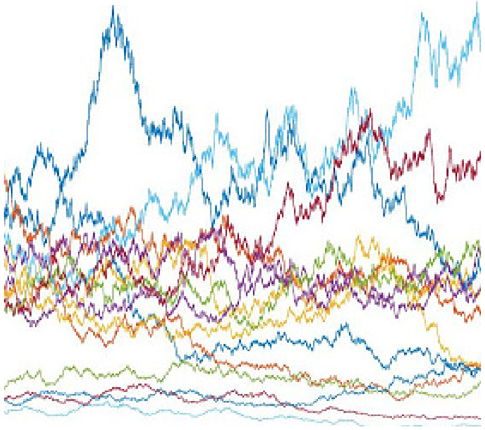
The Metropolis-Hastings algorithm





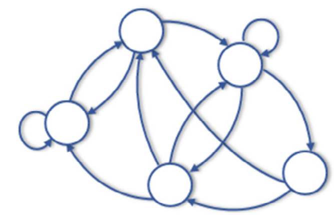
Assume that we want to sample from

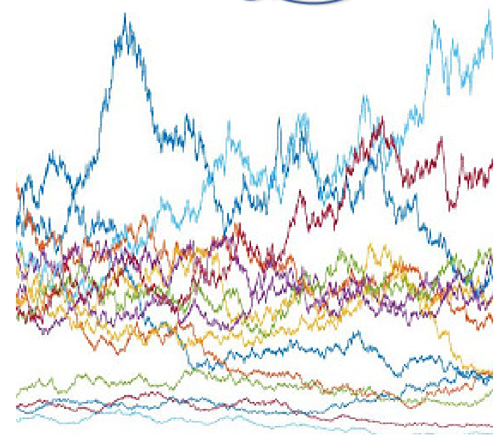
$$p(\theta) = f(\theta)/K$$

where K is a normalizing constant that may be difficult to compute.

The idea is choose generate random numbers from some *proposal* distribution, which will be accepted or rejected according to some *acceptance* probability.

The Metropolis-Hastings algorithm





1. **Choose an initial value $\theta^{(0)}$ where $f(\theta^{(0)}) > 0$.**
2. **Use current value $\theta^{(k)}$, sample a candidate point θ^{*} according to some proposal prob $q\left(\theta^{*}\middle|\theta^{(k)}\right)$ (symmetric $q(x|y) = q(y|x)$.)**
3. **Compute the ratio**

$$\alpha = \frac{f(\theta^{*})q(\theta^{*}|\theta^{(k)})}{f(\theta^{(k)})q\left(\theta^{(k)}\middle|\theta^{*}\right)}$$

4. **If the jump increases the density ($\alpha > 1$), accept the point: $\theta^{(k+1)} = \theta^{*}$. If the jump decreases the density ($\alpha < 1$), accept the point with probability α. Else reject it. Return to step 2.**

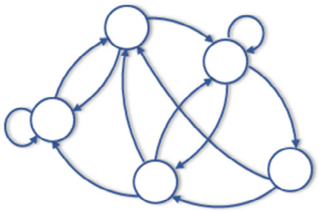
The Metropolis-Hastings algorithm

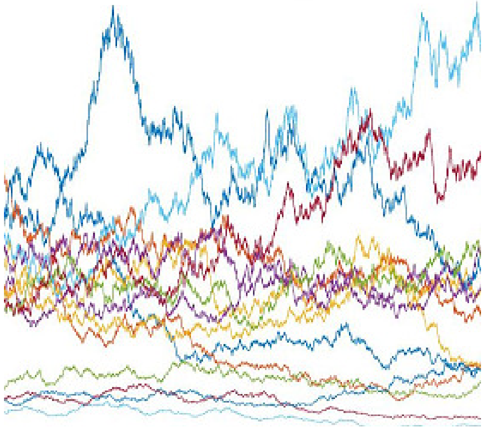
- **Generates a Markov chain**

$$\left(\theta^{(0)}, \theta^{(1)}, \dots, \theta^{(k)}, \dots\right)$$

as the transition probability from $\theta^{(k)}$ to $\theta^{(k+1)}$ depends only on $\theta^{(k)}$.

- **After a burn-in period T samples from the vector $(\theta_{T+1}, \theta_{T+2}, \dots, \theta_{T+n})$ are samples from $p(x)$.**





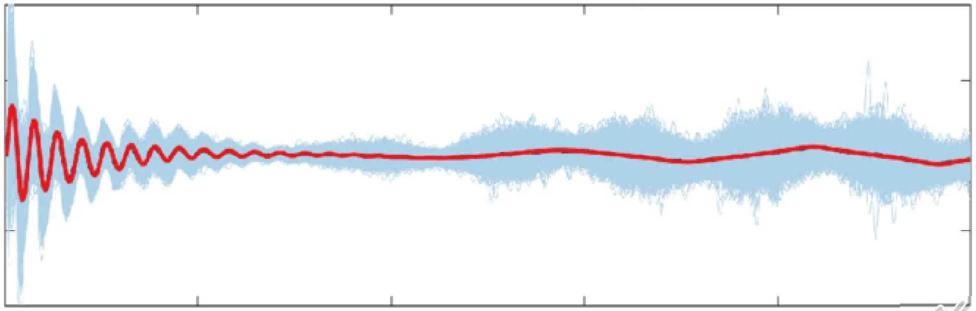
Burn-in period

A key issue in Metropolis-Hastings and MCMC is the number of steps until the chain reaches stationarity

- this is called the **burn-in period**.
- typically the 1000-5000 first points are tossed.

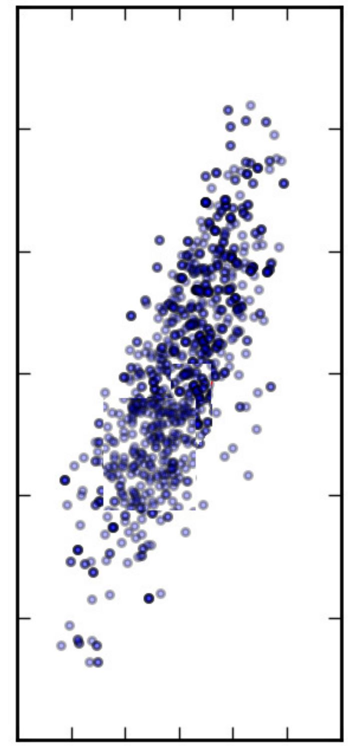
A poor choice of initial values can greatly increase the burn-in period.

- Initiate in the centre of the distribution



Gibbs sampling

- The Gibbs sampler is a version of the Metropolis-Hastings algorithm that accepts all generated samples
- Key: all conditional distributions must have a nice form (conditionally conjugate likelihoods)
- Idea: resample one variable at a time, conditioned on the rest, but keep evidence fixed.
- Now samples are not independent, but sample averages are still consistent estimators.



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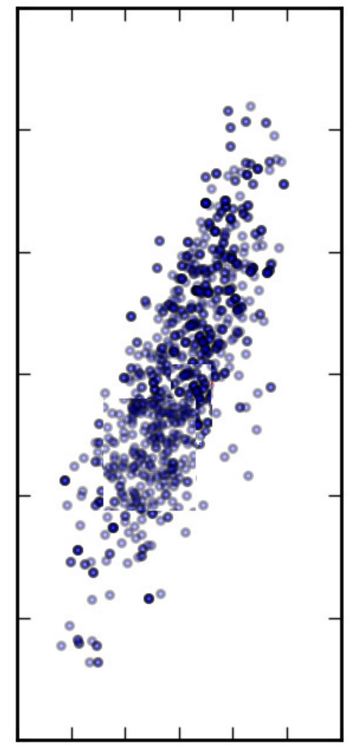
Example: Gibbs sampling

Assume we have a joint distribution of a discrete random variable $X \in \{0,1,\ldots n\}$ and a continuous random variable Y, $0 \leq Y \leq 1$, with joint density function

$$p(x,y) = \frac{n!}{(n-x)!\,x!} y^{x+\alpha-1}(1-y)^{n-x+\beta-1}$$

Complex joint distribution, but simple conditionals:

$$X|Y \sim \mathrm{Bin}(n,y)$$
$$Y|X \sim \mathrm{Beta}(x+\alpha, n-x+\beta)$$

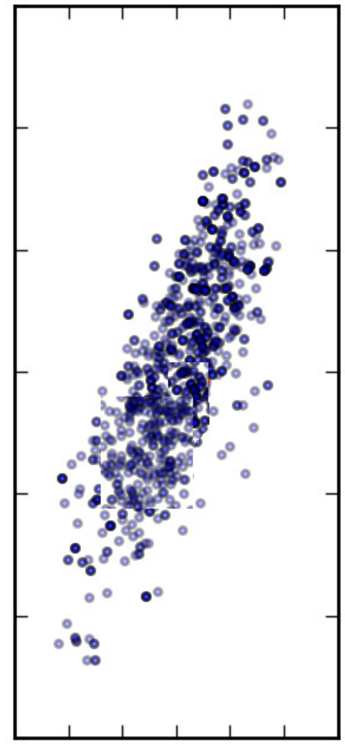


Example: Gibbs sampling

Let $n = 10$ **and** $\alpha = 1, \beta = 2$**. Initiate with** $y_0 = 1/2$**.**

1. **Generate** x_0 **from** $\mathrm{Bin}(n, y_0) = \mathrm{Bin}(10,1/2)$**. Say we get** $x_0 = 5$**.**
2. **Generate** y_1 **from** $\mathrm{Beta}(x_0 + \alpha, n - x_0 + \beta) = \mathrm{Beta}(6,7)$**, giving** $y_1 = 0.33$.
3. **Generate** x_1 **from** $\mathrm{Bin}(10,0.33)$ **giving** $x_1 = 3$**.**

And so on. The x_i **are samples from the marginal posterior of** X_i**, and** y_i **from that of** Y_i**.**



Gibbs sampling in a Bayesian network

Assume again that we want to estimate a probability $P(T, A^c | S, R)$

1. **Initialization:**
   a. **Fix the evidence variables** $S = true, R = true$
   b. **Sample all other variables** T, F, A, L
2. **Repeat (as many times as wanted)**
   a. **Pick a non-evidence variable** X_i **uniformly**
   b. **Sample** x_i' **from** $P(X_i | x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_n)$
   c. **Keep all other variables** $x_j' = x_j, \forall j \neq i$
   d. **The new sample is** $x_1', \dots x_n'$
3. **Alternatively march through the variables in some predefined order.**