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Statistical methods in Data Science and AI

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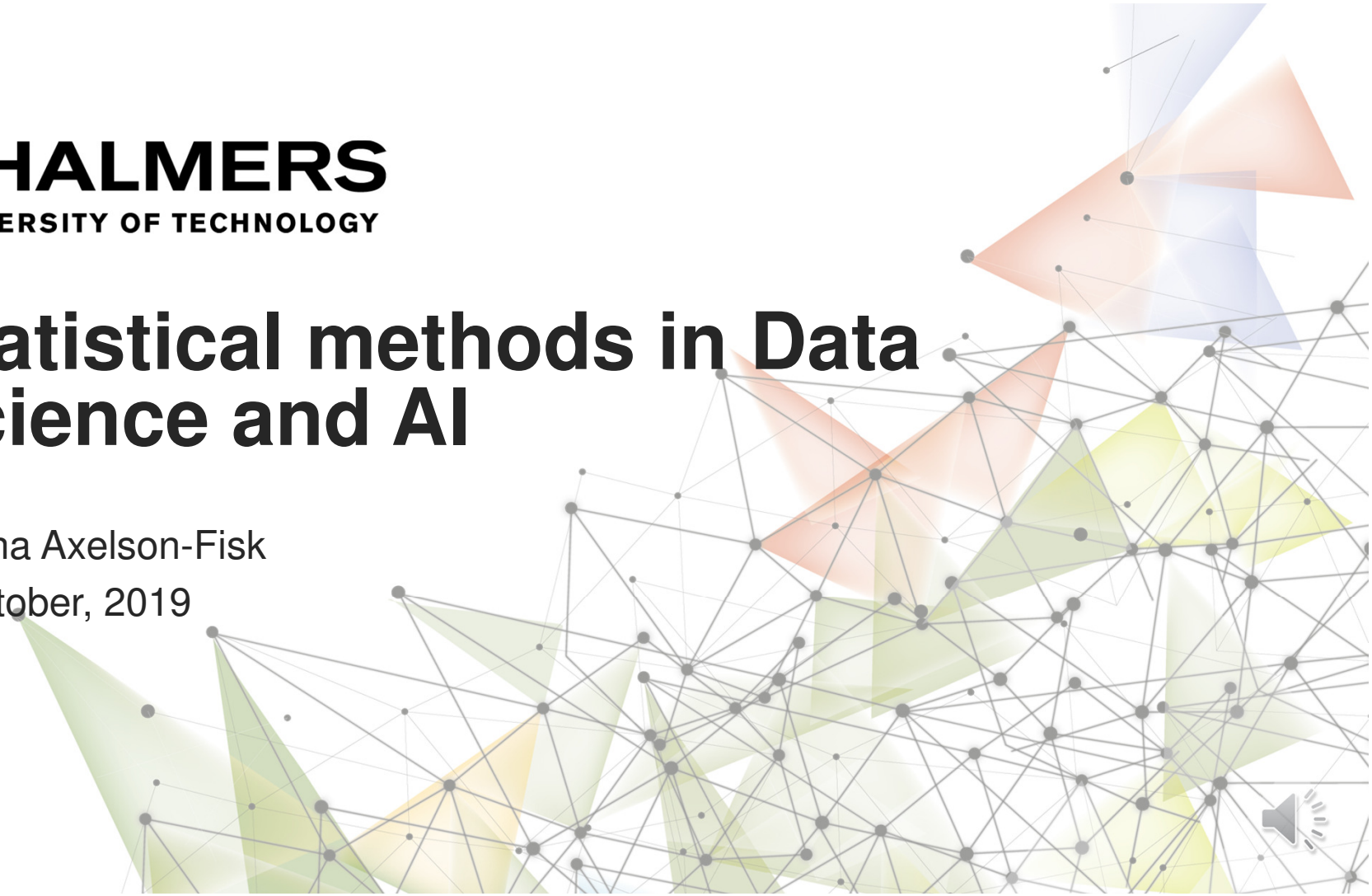

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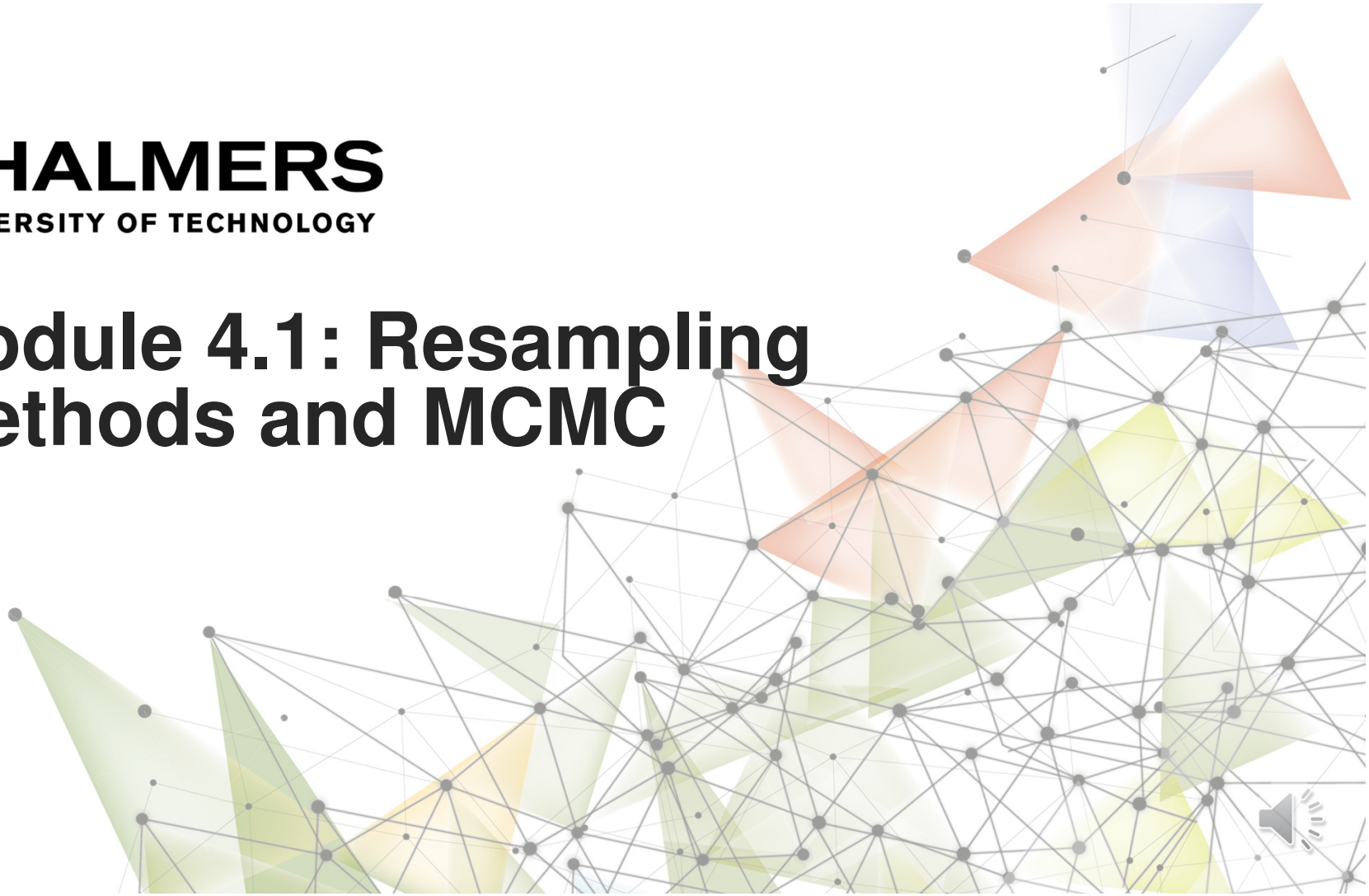
Module 4.1: Resampling methods and MCMC



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 $u_1, \dots, u_n$**
- **Compute the inverse F^{-1}**
- **Sample from desired distribution is given by**

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

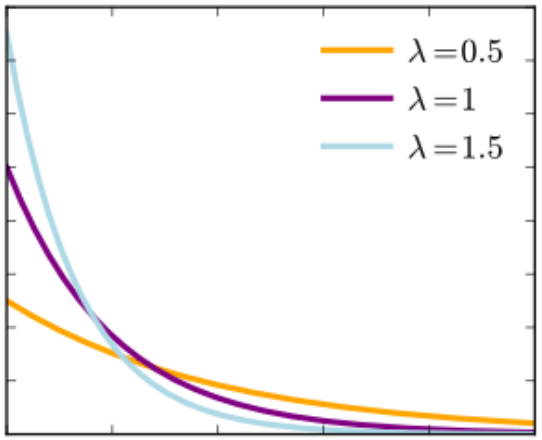
Example: sample from $\mathrm{Exp}(\lambda)$

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

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

$$U \sim U(0,1) \Rightarrow 1 - U \sim U(0,1)$$

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

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

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

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

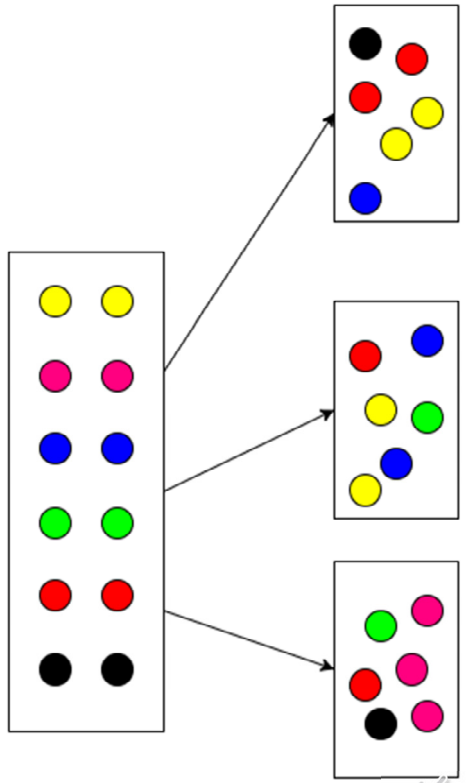
$$\mu = \bar{x} \pm z_{1-\alpha/2}\frac{s}{\sqrt{n}}$$

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

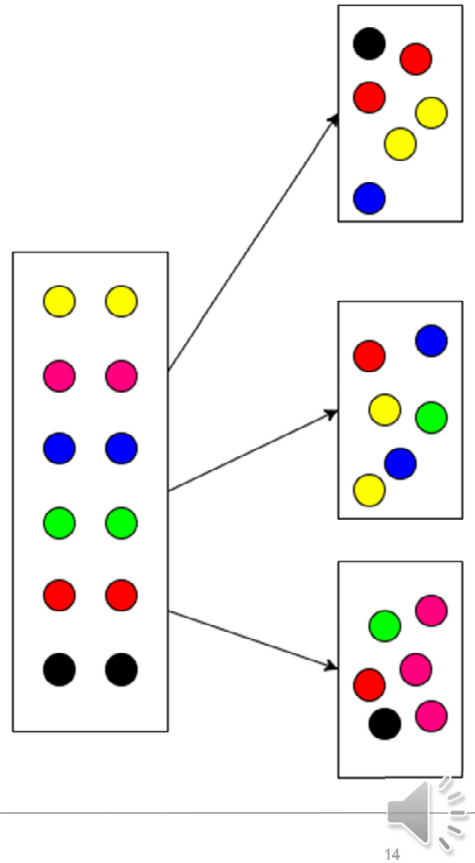
$$M_n^{*(1)}, M_n^{*(2)}, \ldots, M_n^{*(B)}$$

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

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

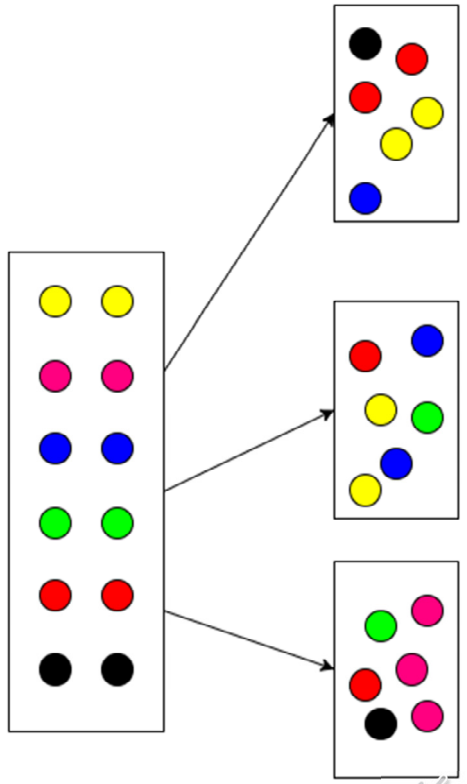
- Bootstrap confidence interval of the median

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



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**

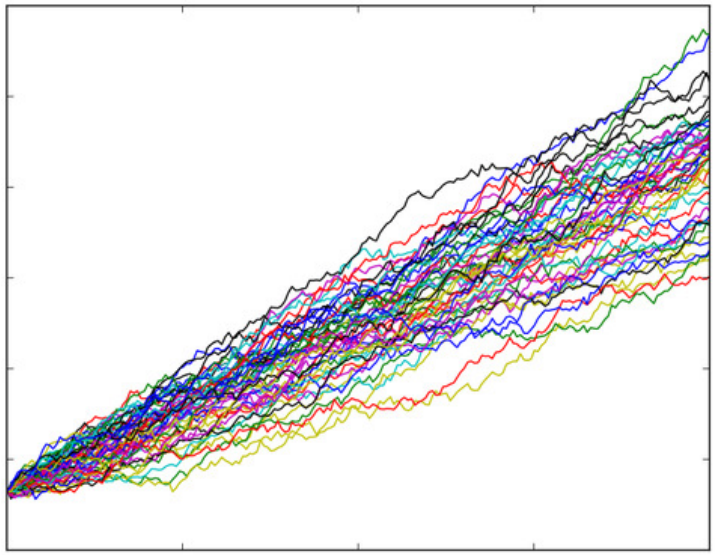
$$I = \int f(x)dx$$

- **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**

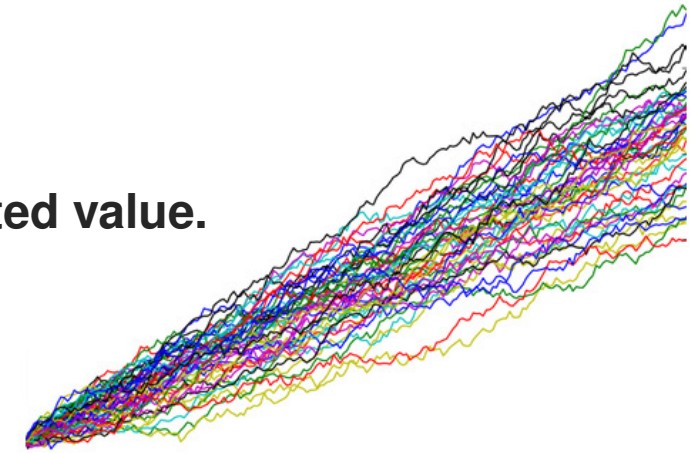
$$I = \int_0^1 e^{-x^3} dx$$

- **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.

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

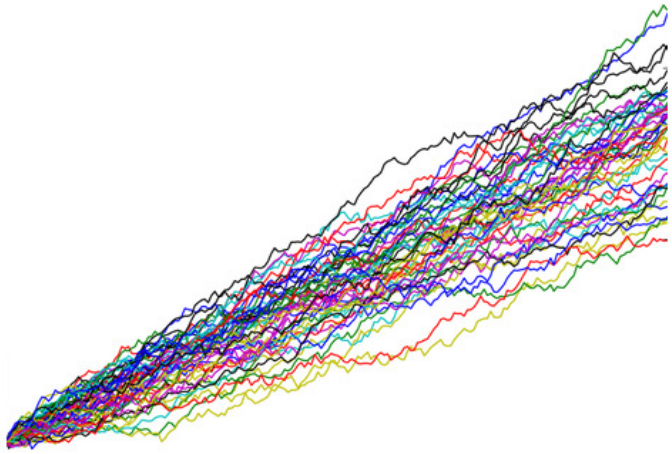


Monte Carlo simulation – example

- **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

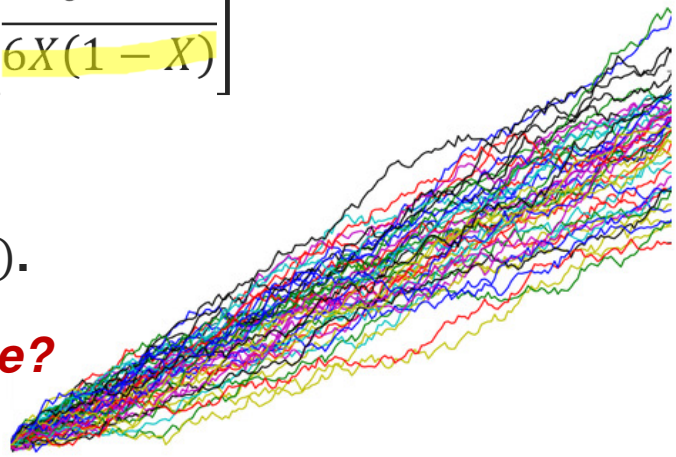
- **Note that the function f changes if the pdf p changes:**
- **Since** $\mathrm{Beta}(2,2)$ **has pdf** $p(x) = 6x(1-x)$ **we could write**

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

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:**

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

Unbiased!

- **Variance**

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

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

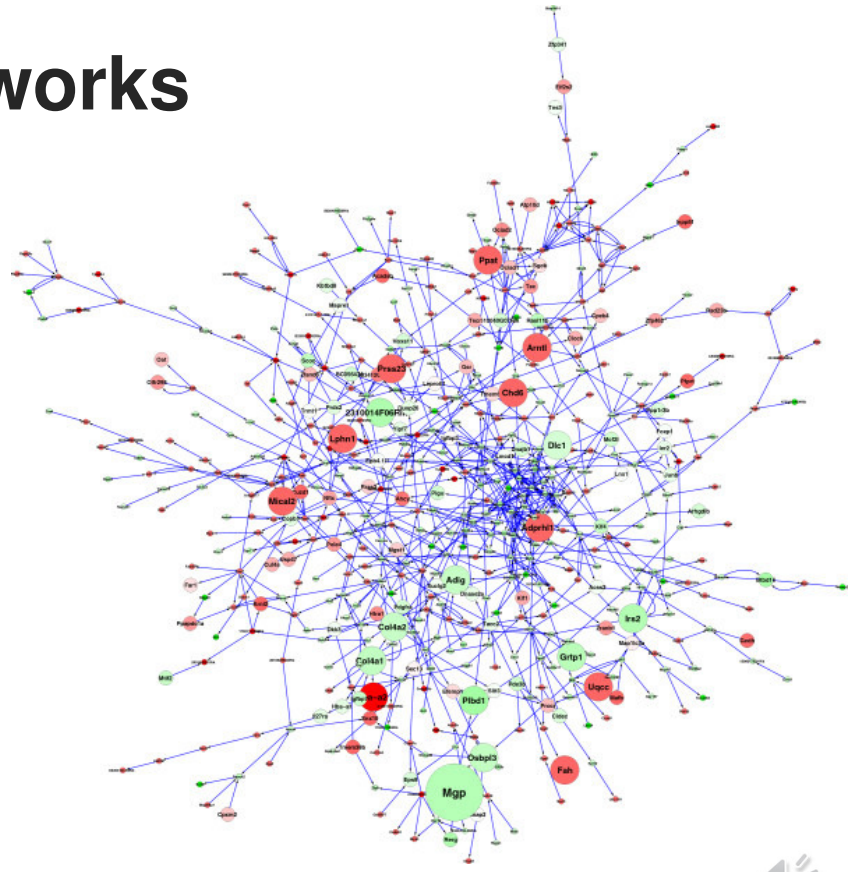
The quantity I^2 is fixed.

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**

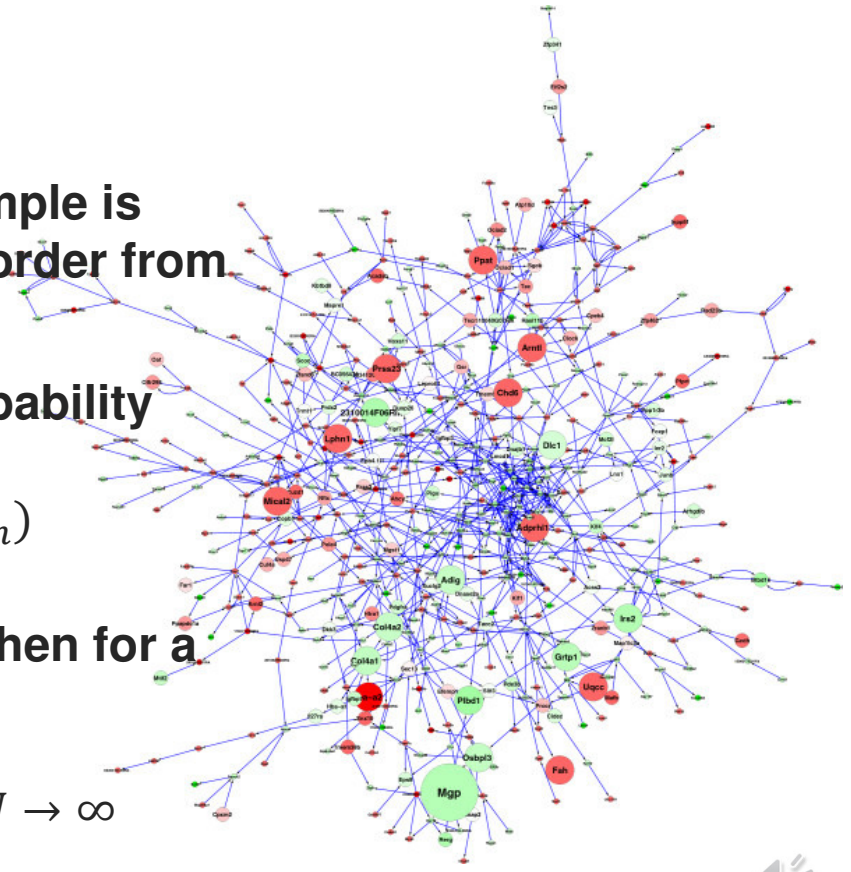
$$P(X_i|\mathrm{pa}(X_i), i = 1, \dots, n$$

- **Then samples are generated with probability**

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

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

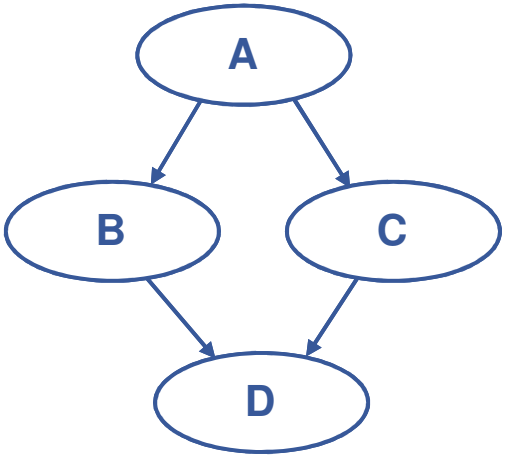
$$\frac{\#\{(x_1, \dots, x_n)\}}{N} \to P(x_1, \dots, x_n) \text{ as } N \to \infty$$



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 $p(x)$

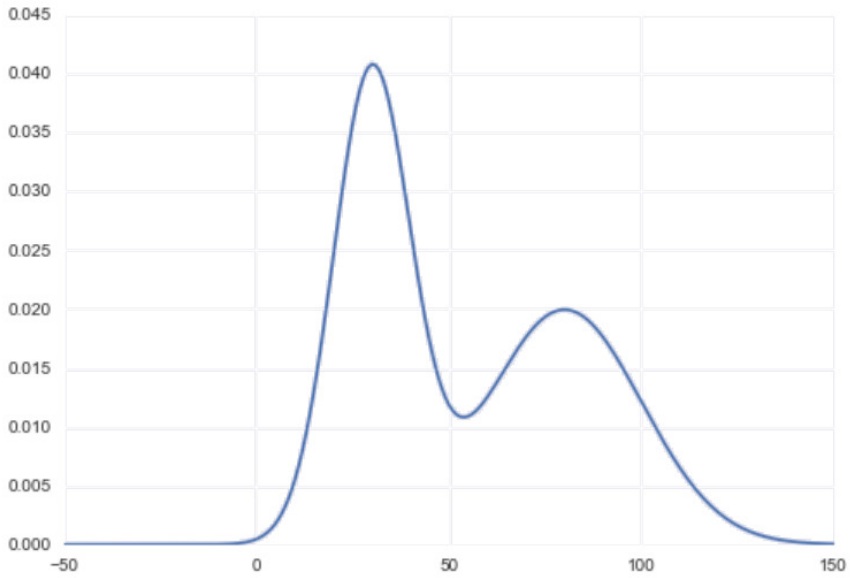
$$p(x) = \tilde{p}(x)/Z_p \Leftrightarrow \tilde{p}(x) = p(x)Z_p$$

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

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



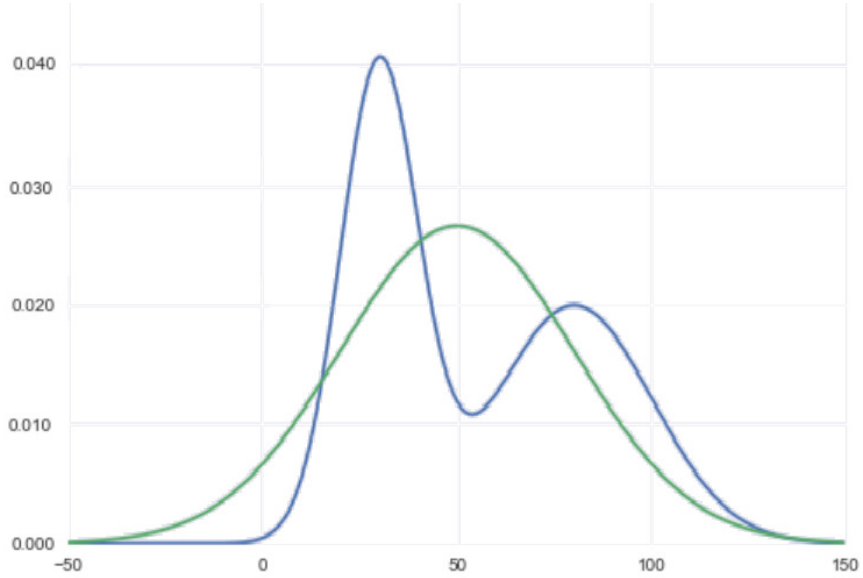
Example: rejection sampling

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

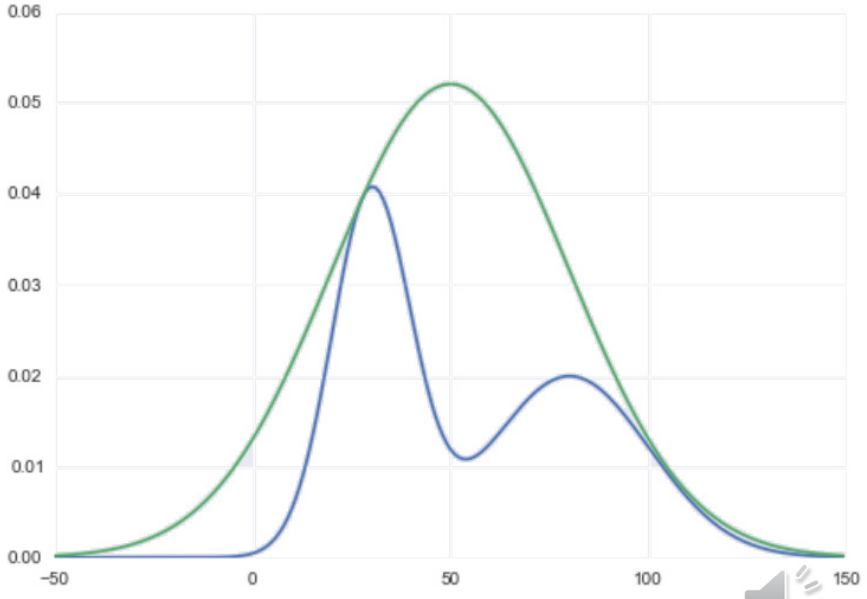
$$X + Y \sim N(30,10) + N(80,20)$$

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**

$$Z \sim q(x)$$

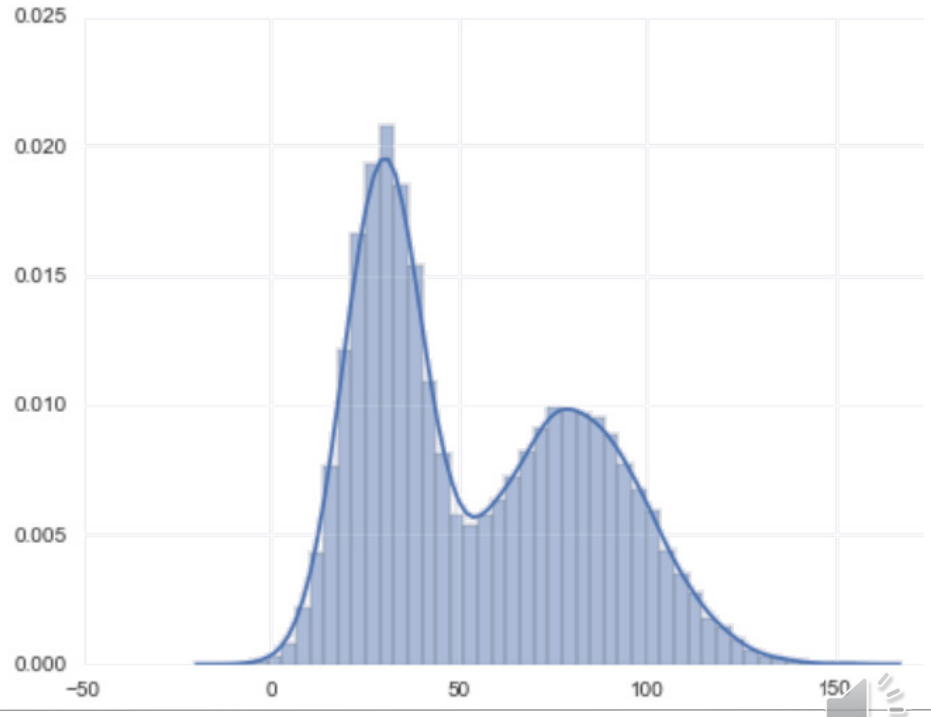
- **Uniformly pick the height**

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

Now (z, u) **is uniform under**

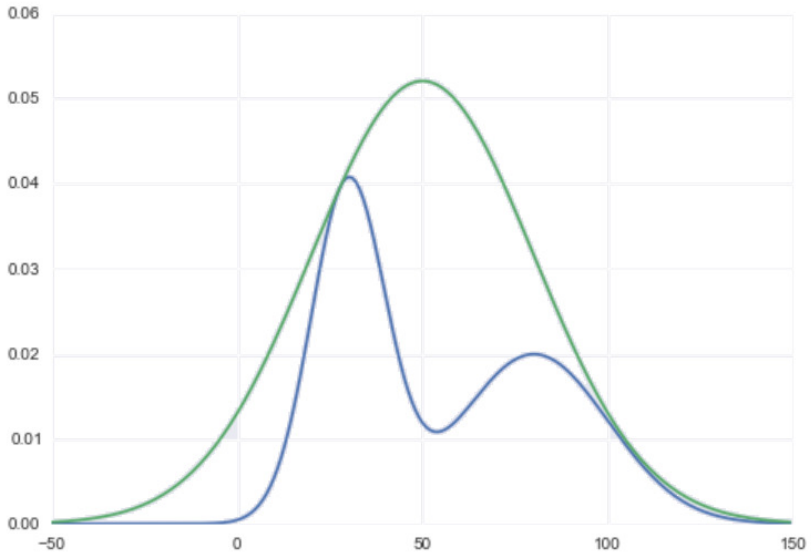
$$kq(x)$$

- **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.**



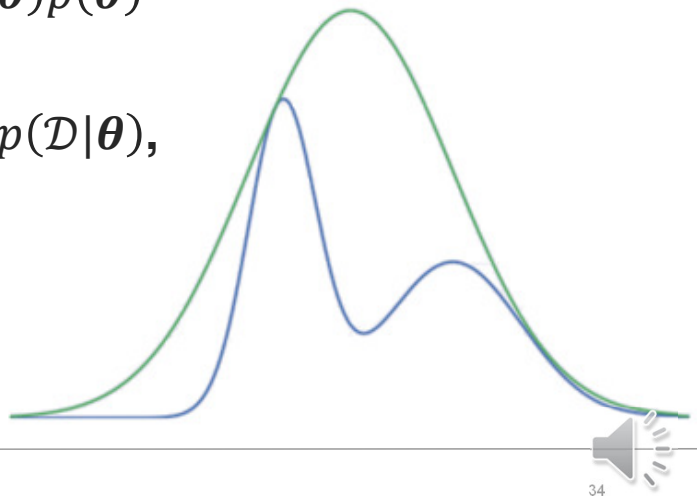
Rejection sampling in Bayesian statistics

- **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**

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



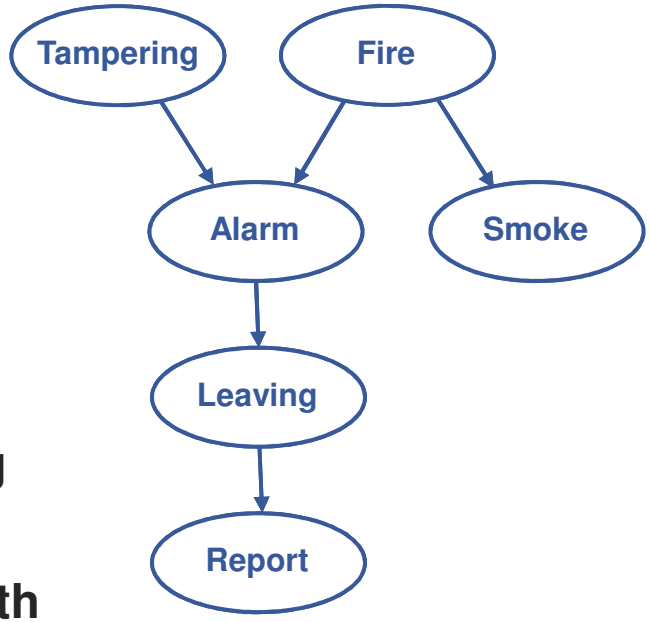
Sampling in Bayesian networks: example

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**

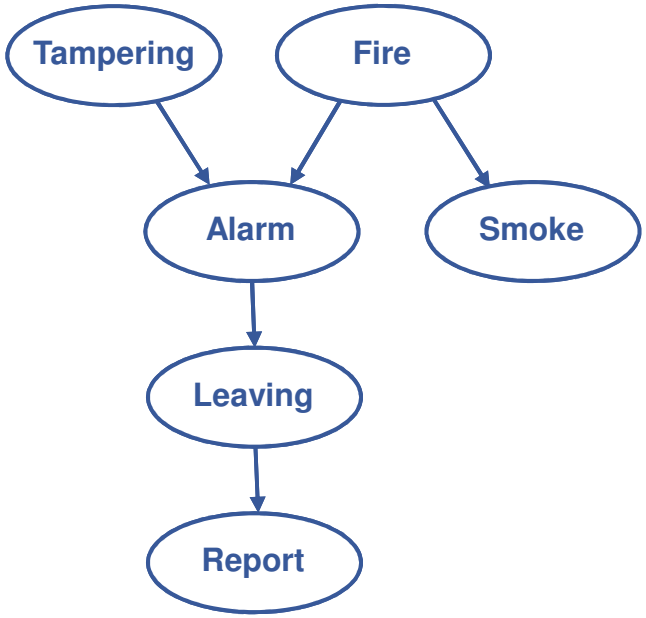
Conditional dependencies are given by the DAG.



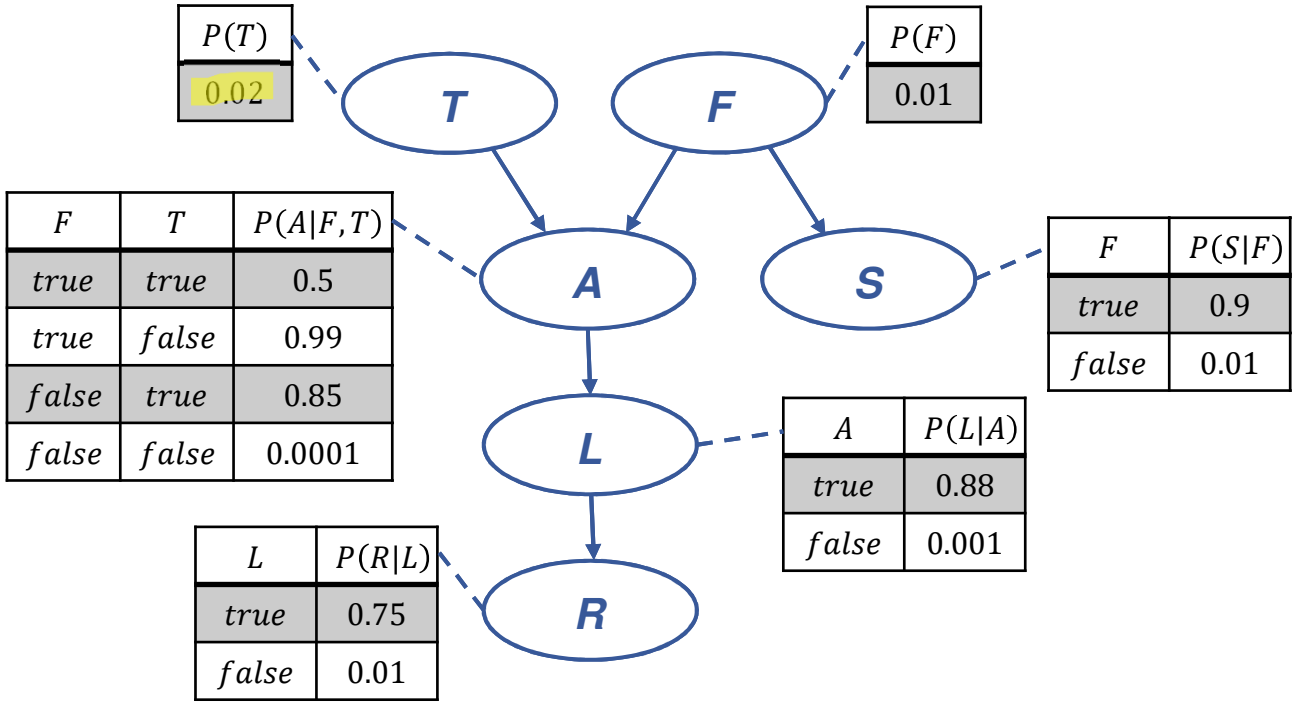
Sampling in Bayesian networks: example

Factorization

$$P(\text{tampering}, \text{fire}, \text{alarm}, \text{smoke}, \text{leaving}, \text{report}) =$$
$$= P(\text{tampering})$$
$$\cdot P(\text{fire})$$
$$\cdot P(\text{alarm} \mid \text{tampering}, \text{fire})$$
$$\cdot P(\text{smoke} \mid \text{fire})$$
$$\cdot P(\text{leaving} \mid \text{alarm}) \cdot$$
$$\cdot P(\text{report} \mid \text{leaving})$$



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

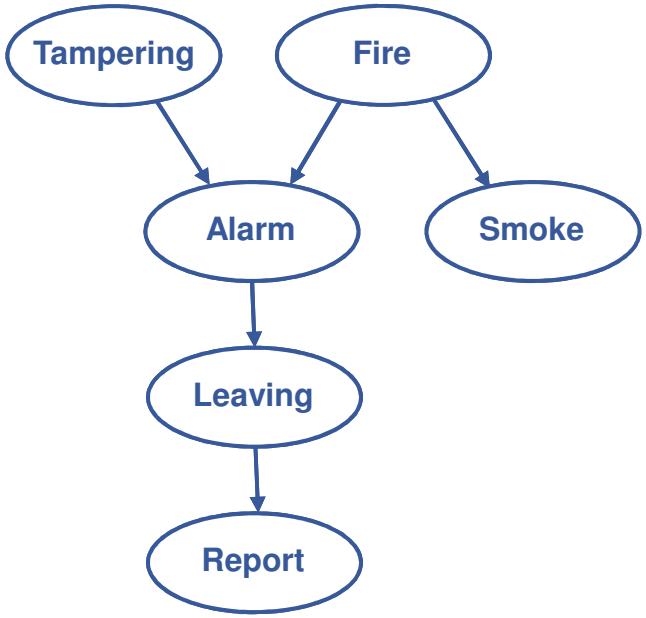
F	$P(S\|F)$
$true$	0.9
$false$	0.01

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 $X_1, X_2, \ldots, X_n$ 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

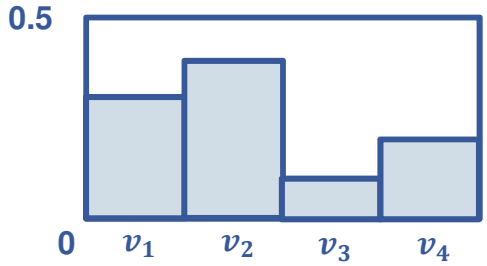
Assume variable X takes values $\{v_1, v_2, v_3, v_4\}$.
Assume

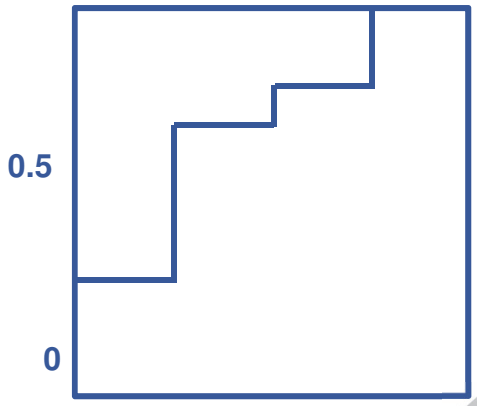
$$P(X = v_1) = 0.3$$
$$P(X = v_2) = 0.4$$
$$P(X = v_3) = 0.1$$
$$P(X = v_4) = 0.2$$

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

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

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

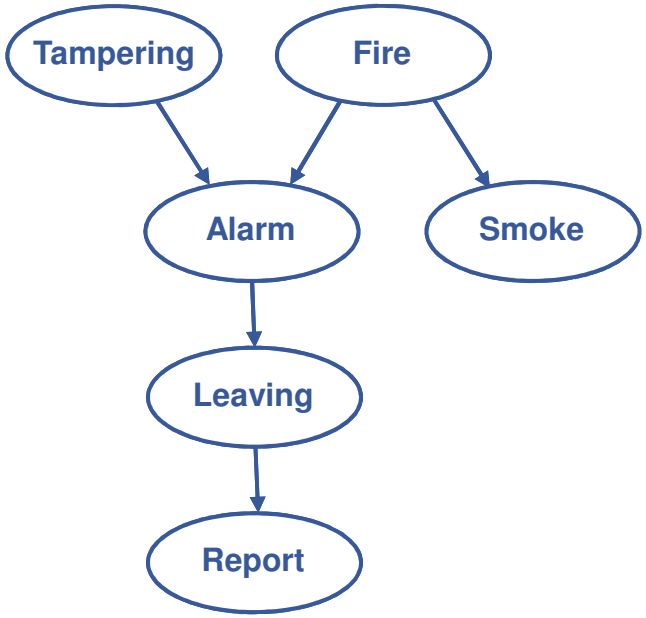
$\Rightarrow A = true$

etc.

Rejection sampling in Bayesian networks

Given some data D rejection sampling estimates the posterior

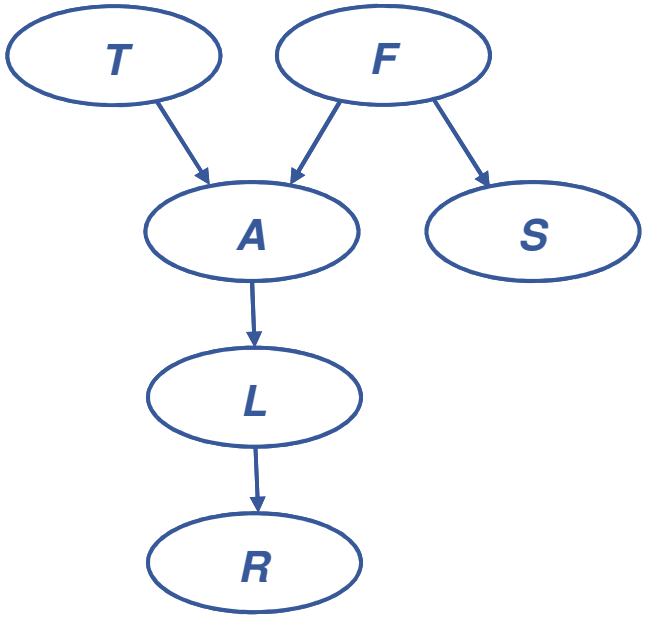
$$P(Y|D) = \frac{P(D|Y)P(Y)}{P(D)}$$



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:

$\approx$ **990** $F = false$

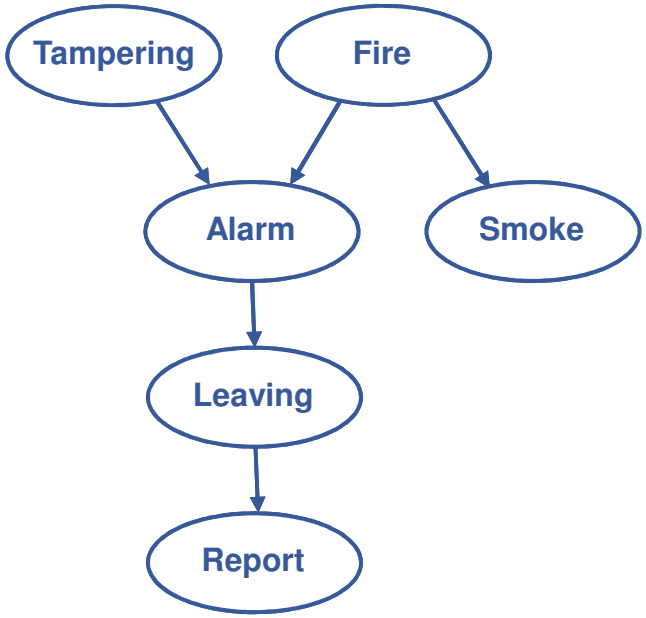
Of these 990

$\approx$ **1% = 10** $S = true$

$\Rightarrow$ **remaining 980 (98%) rejected**

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**

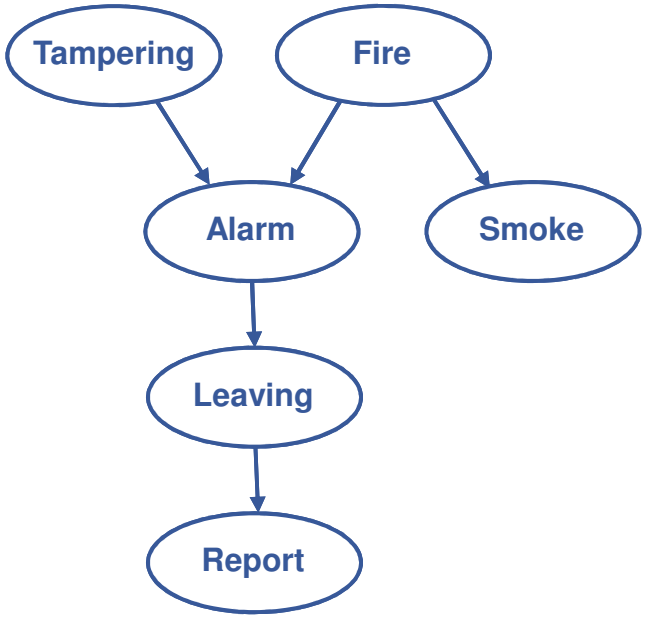
$$S_{LW}(\mathbf{x}, \mathbf{y}) = \prod_{X_i \in \mathbf{X}} P(X_i|\mathrm{pa}(X_i))$$

- **Compute sample weights**

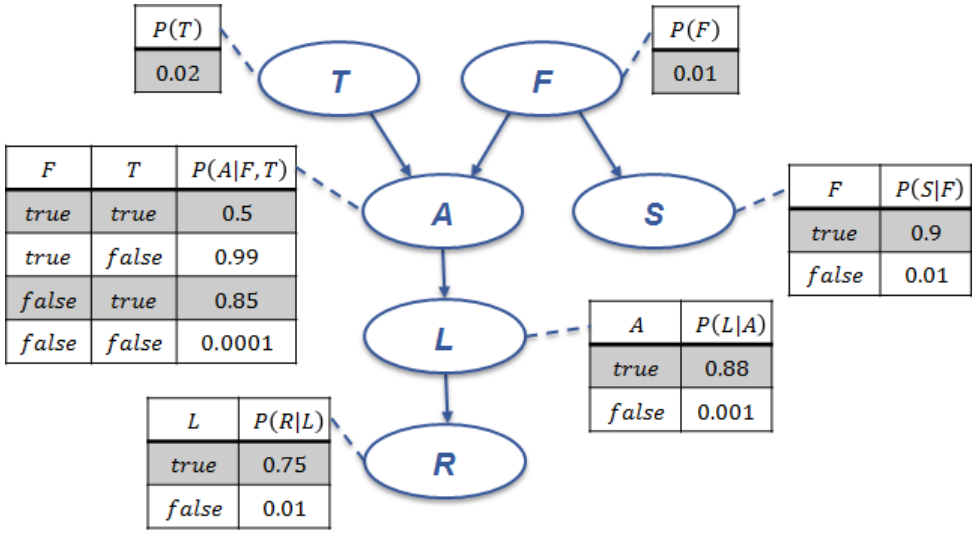
$$w(\mathbf{x}, \mathbf{y}) = \prod_{Y_i \in \mathbf{Y}} P(Y_i|\mathrm{pa}(Y_i))$$

- **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

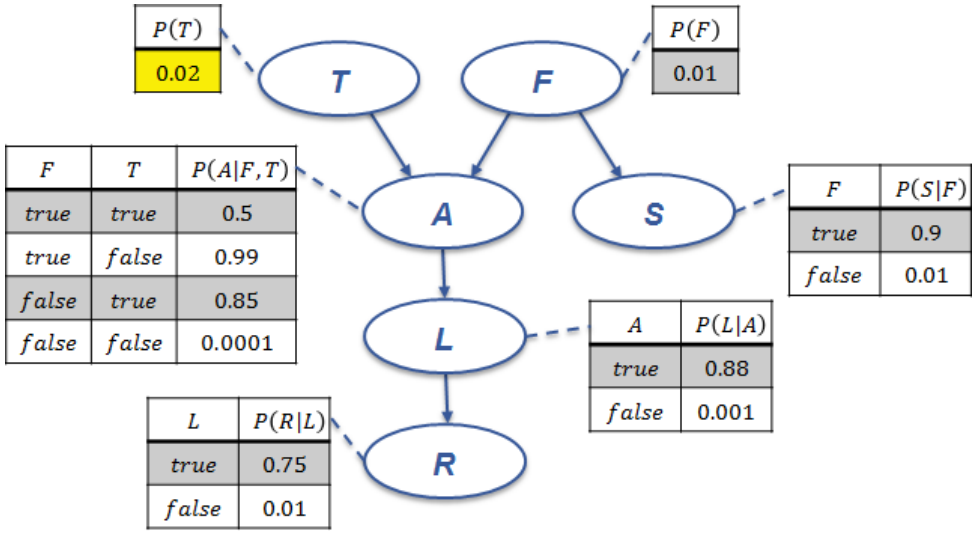


Example: estimate $P(T|S, R^c)$

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

Generate sample:

Likelihood weighting in Bayesian networks



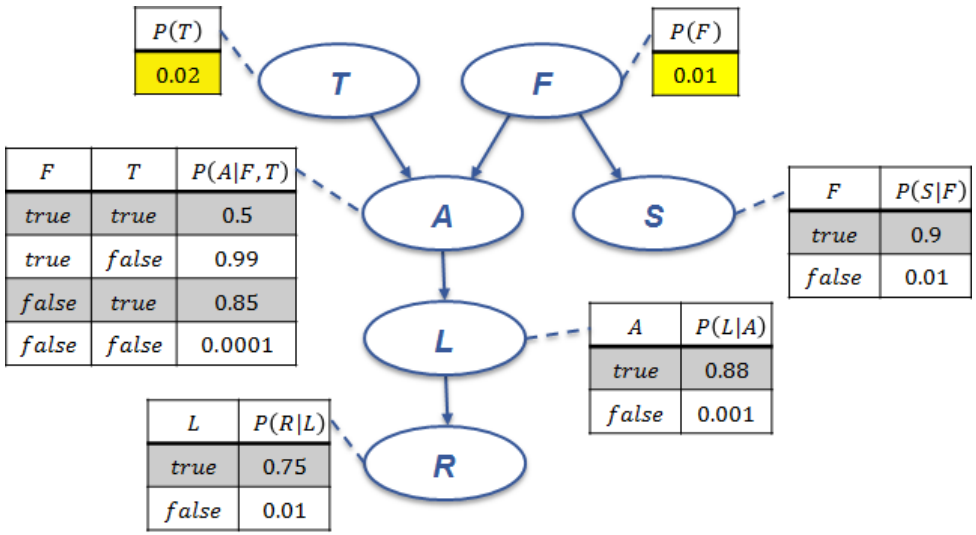
Example: estimate $P(T|S, R^c)$

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

Generate sample:

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

Likelihood weighting in Bayesian networks



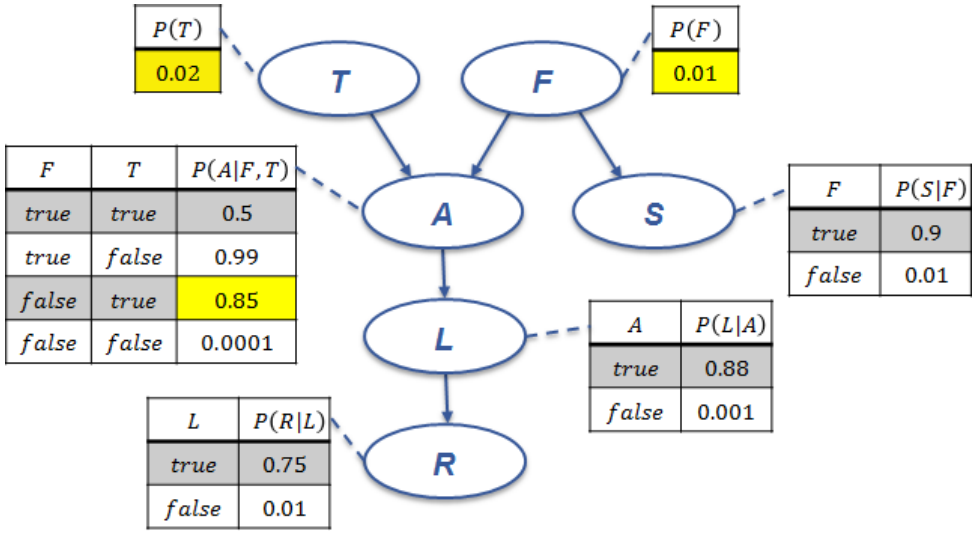
Example: estimate $P(T|S, R^c)$

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



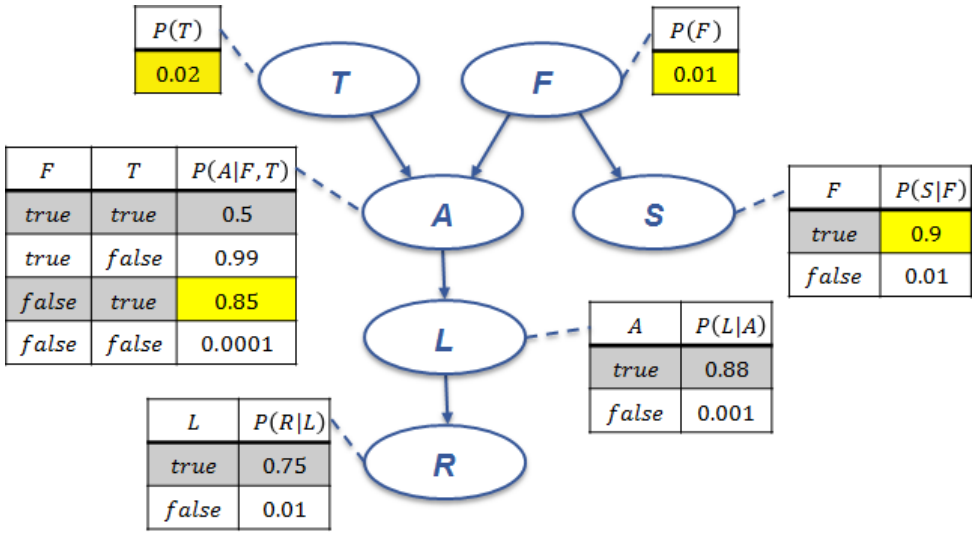
Example: estimate $P(T|S, R^c)$

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



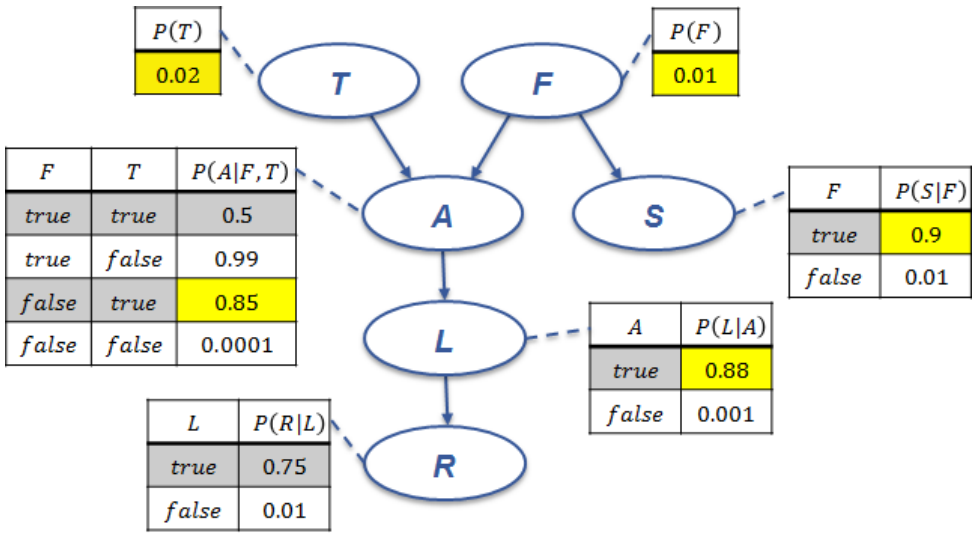
Example: estimate $P(T|S, R^c)$

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



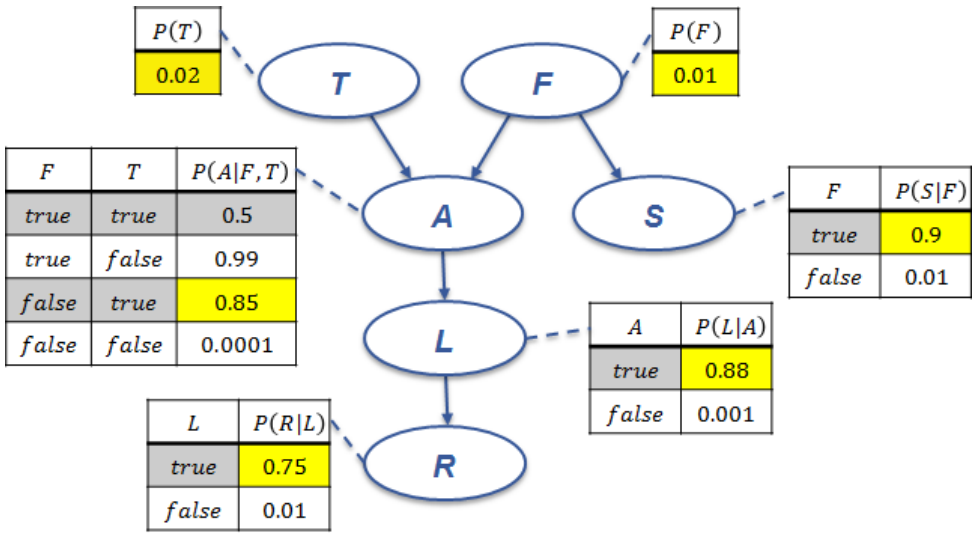
Example: estimate $P(T|S, R^c)$

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



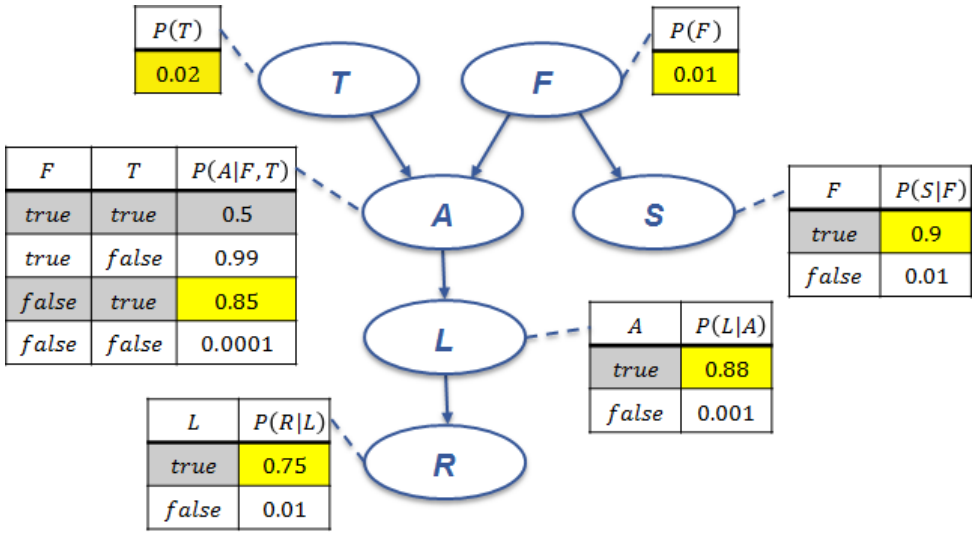
Example: estimate $P(T|S,R^c)$

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



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

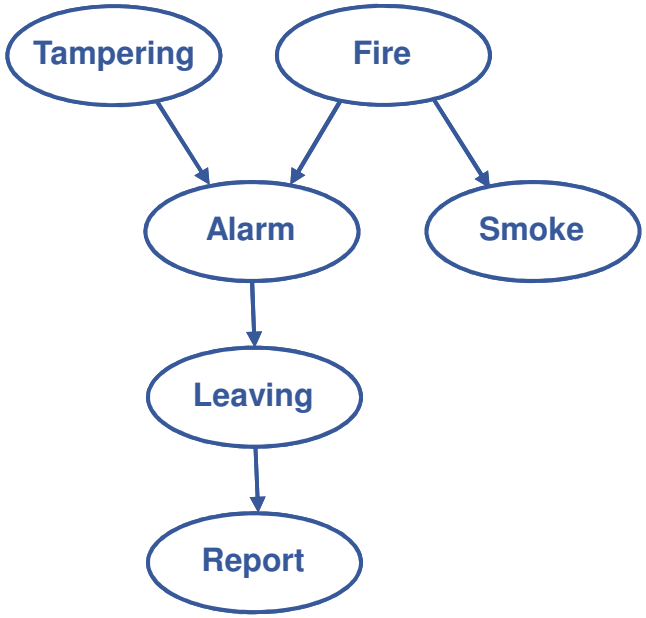
$$P(T|S,R^c) = \frac{\text{sum of weights where } T = true}{\text{sum of all weights}}$$

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

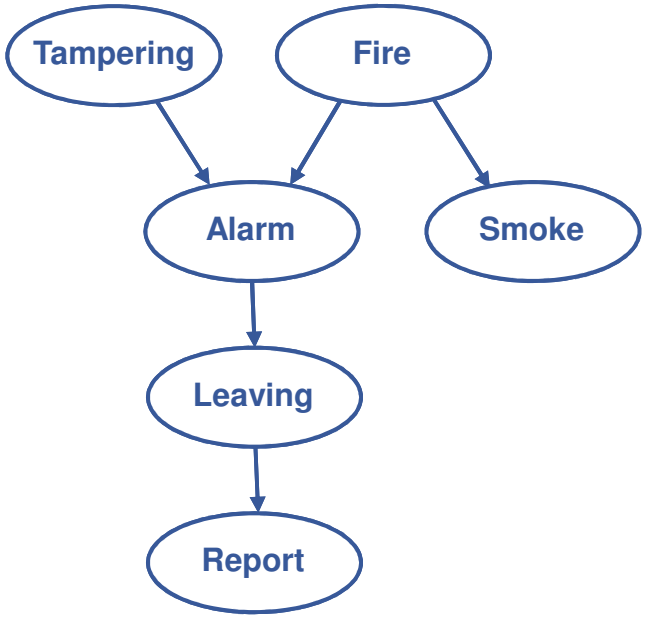
$$\hat{P}(X|Y) = \left(\sum_{x:X|Y} W(x)\right) / \left(\sum_{x} W(x)\right)$$



Likelihood weighting in Bayesian networks

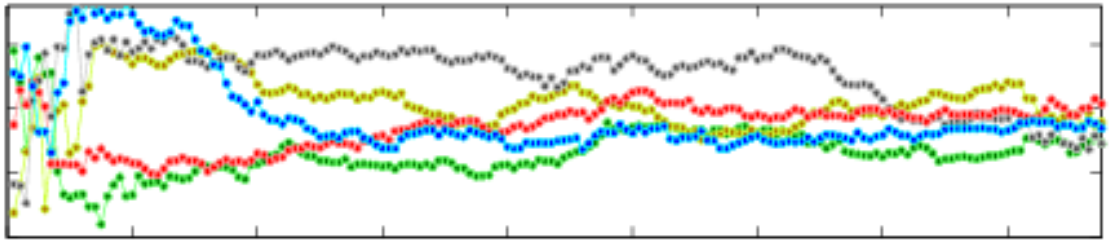
- More efficient than rejection sampling.
- But doesn't solve all our problems:
  - By fixing the evidence nodes, we influence the sampling of the downstream variables, not the upstream ones.

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



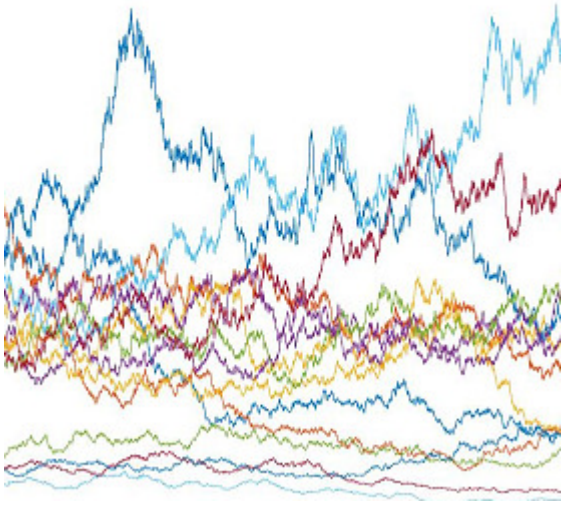
Markov chain Monte Carlo (MCMC)

- 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.



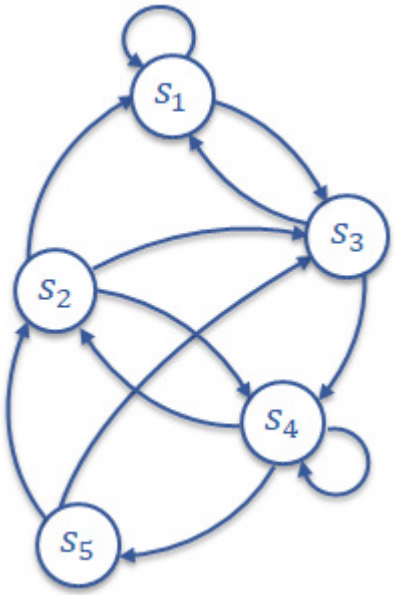
Markov chains

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

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

and where the next jump only depends on the current state

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



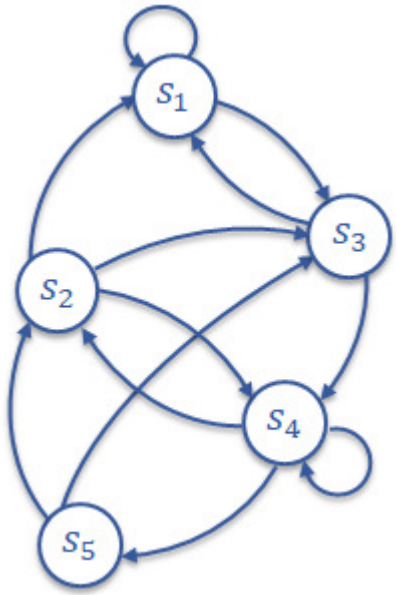
Markov chains

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

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

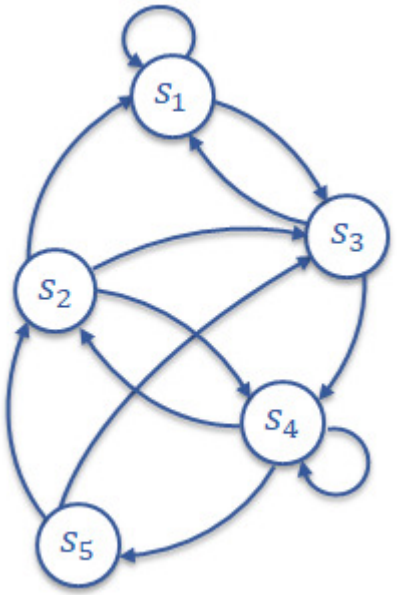
  - **transition probabilities**

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



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.



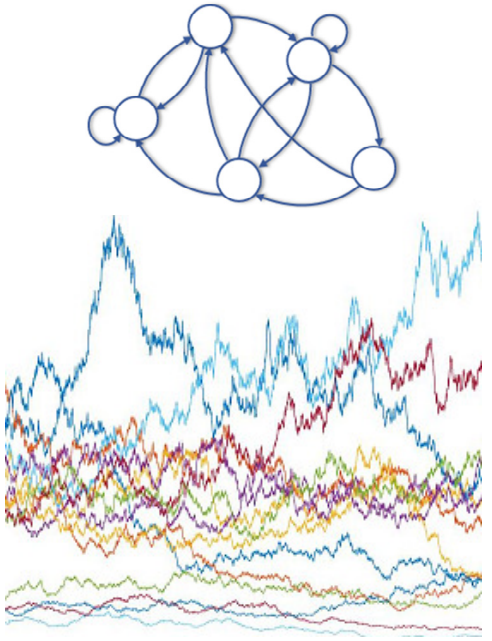
The Metropolis-Hastings algorithm

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.

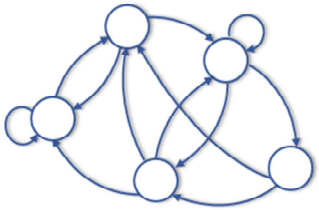


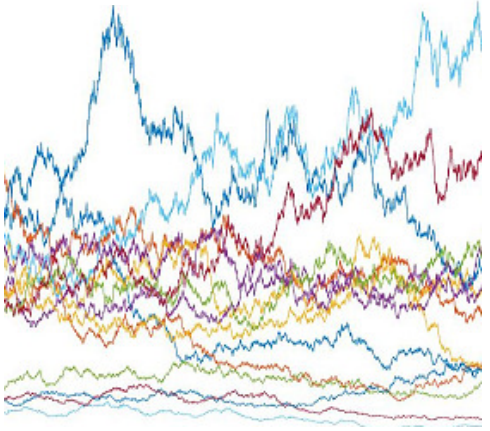
The Metropolis-Hastings algorithm

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 $q(\theta^*|\theta^{(k)})$ (symmetric $q(x|y) = q(y|x)$.)**
3. **Compute the ratio**

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

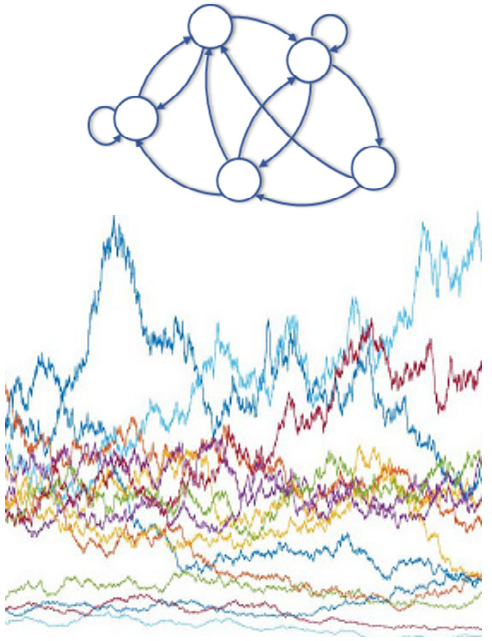
4. **If the jump increases the density ($\alpha > 1$), accept the point: $\theta^{(k+1)} = \theta^*$. If the jump decreases the density ($\alpha < 1$), accept the point with probability α. Else reject it. Return to step 2.**





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 $p(x)$.**



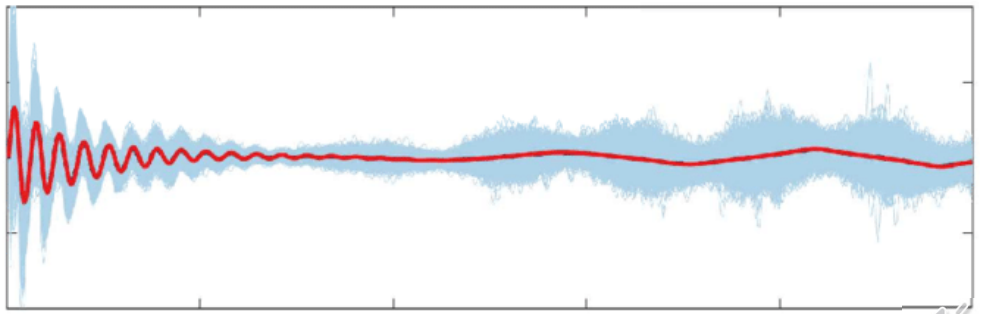
Burn-in period

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.**

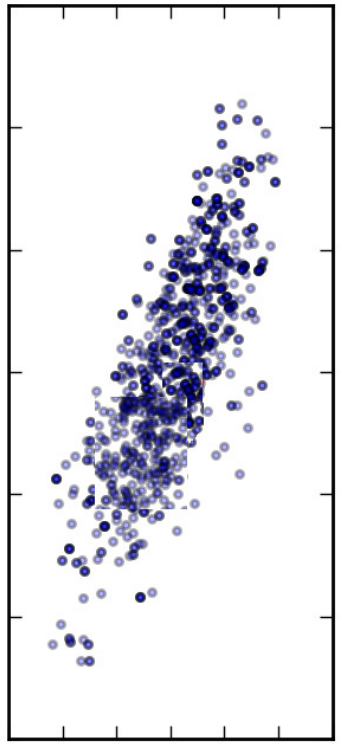
A poor choice of initial values can greatly increase the burn-in period.

- **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.



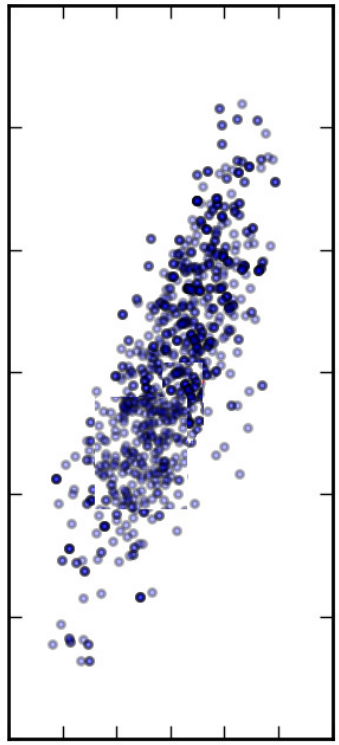
Example: Gibbs sampling

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:

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

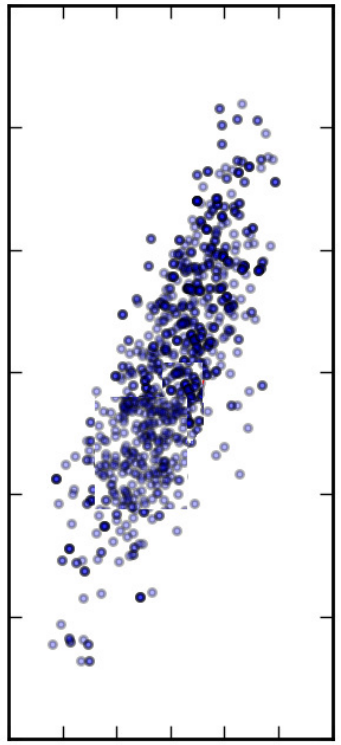


Example: Gibbs sampling

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** $P(X_i|x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_n)$
   c. **Keep all other variables** $x_j' = x_j, \forall j \neq i$
   d. **The new sample is** $x_1', \ldots x_n'$
3. **Alternatively march through the variables in some predefined order.**