CS 3750 Machine Learning
Lecture 7

Monte Carlo methods

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Monte Carlo inference

- Let us assume we have a probability distribution *P*(X) represented e.g. using BBN or MRF, and want calculate *P*(X=x)   (*P*(x) in short)
- We can use exact probabilistic inference, but it may be hard to calculate
- **Monte Carlo approximation**:
  - **Idea:** The probability *P*(x) is approximated using sample frequencies
- **Idea (first method):**
  - Generate a random sample *D* of size *M* from *P*(X)
  - Estimate P(x) as:

$$\hat{P}_D(X = x) = \frac{M_{X=x}}{M}$$

Absolute Error Bound

- **Hoeffding's bound** lets us bound the probability with which the estimate $\hat{P}_D(x)$ differs from $P(x)$ by more than ε

$$P(\hat{P}_D(x) \notin [P(x)-\varepsilon, P(x)+\varepsilon]) \leq 2e^{-2M\varepsilon^2} \leq \delta$$

The bound can be used to decide on how many samples are required to achieve a desired accuracy:

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

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Relative Error Bound

- **Chernoff's bound** lets us bound the probability of the estimate $\hat{P}_D(x)$ exceeding a relative error ε of the true value $P(x)$.

$$P(\hat{P}_D(x) \notin P(x)(1+\in)) \leq 2e^{-MP(x)\varepsilon^2/3}$$

- This leads to the following sample complexity bound:

$$M \geq 3\frac{\ln(2/\delta)}{P(x)\varepsilon^2}$$

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Monte Carlo inference challenges

Two challenges:

•How to generate N (unbiased) examples from the target distribution P(X) ?

– Generating (unbiased) examples from P(X) may be hard, or very inefficient

•How to estimate the expected value of f(x) for p(x):

$$E_P[f] = \sum_x P(x) f(x) \qquad E_P[f] = \int_x p(x) f(x) dx$$

• We can estimate this expectation by generating samples x[1], …, x[M] from P, and then estimating it as:

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

Monte Carlo inference challenges

The estimate:

•Based on M samples samples x[1], …, x[M] generated from P,

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

• Using the central limit theorem, the estimate $\hat{\Phi}$ follows the normal distribution with variance:

$$\frac{\sigma^2}{M}$$

– where $\sigma^2 = \int_x p(x)[f(x) - E_P(f(x))]^2 dx$

is the variance of f(x)

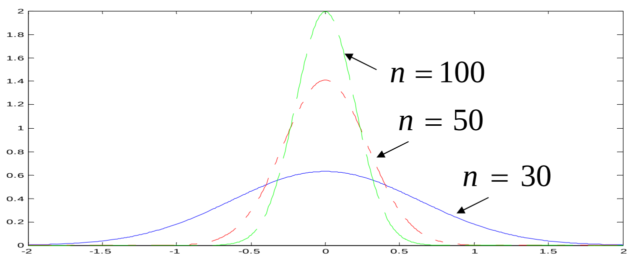
Central limit theorem

- **Central limit theorem:**

  Let random variables $X_1, X_2, \cdots X_n$ form a random sample from a distribution with mean μ and variance σ^2, then if the sample n is large, the distribution

$$\sum_{i=1}^{n} X_i \approx N(n\mu, n\sigma^2) \quad \text{or} \quad \frac{1}{n}\sum_{i=1}^{n} X_i \approx N(\mu, \sigma^2 / n)$$

Effect of increasing the sample size *n* on the sample mean:

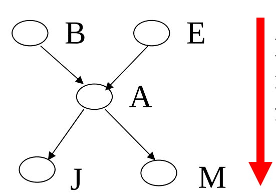


$\mu = 0$

$\sigma^2 = 4$

Example: Monte Carlo for BBNs

- **Sample generation: BBN sampling of the joint is easy**
  - One sample gives one assignment of values to all variables
  - **Example:**



Examples can be generated in a top down manner, following the links

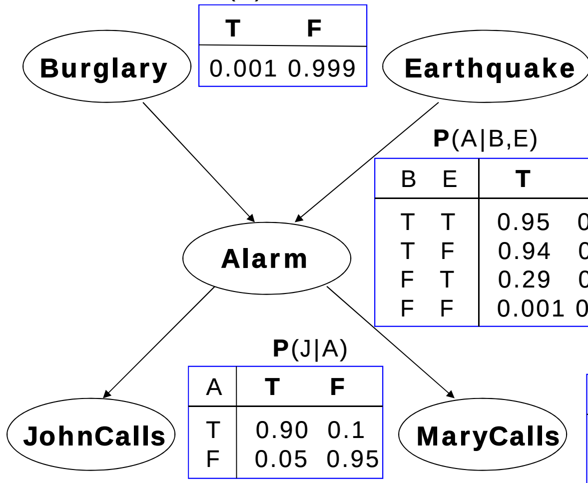
- **MC approximation for BBN joint estimates**:
  - The probability is approximated using sample frequencies

$$\tilde{P}(B = T, J = T) = \frac{N_{B=T, J=T}}{N}$$

$N_{B=T,J=T}$: $\#\, samples \;\; with \;\; B = T, J = T$

N: $total \;\; \#\, samples$

BBN sampling example



P(B)

T	F
0.001	0.999

P(E)

T	F
0.002	0.998

P(A|B,E)

B	E	T	F
T	T	0.95	0.05
T	F	0.94	0.06
F	T	0.29	0.71
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P(J|A)

A	T	F
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F	0.05	0.95

P(M|A)

A	T	F
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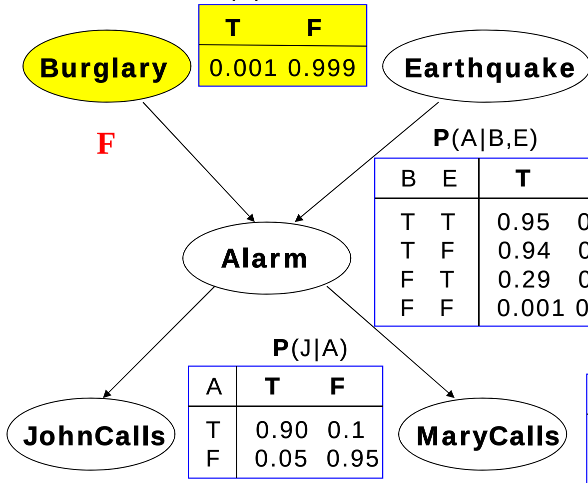
BBN sampling example



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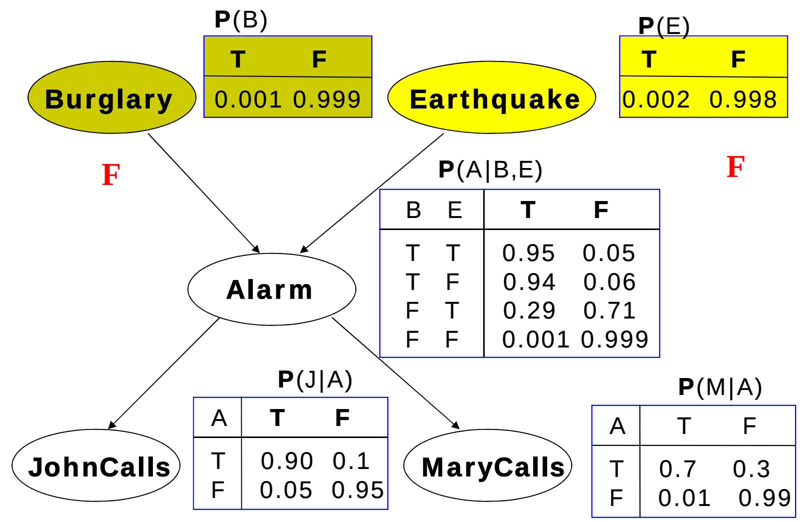

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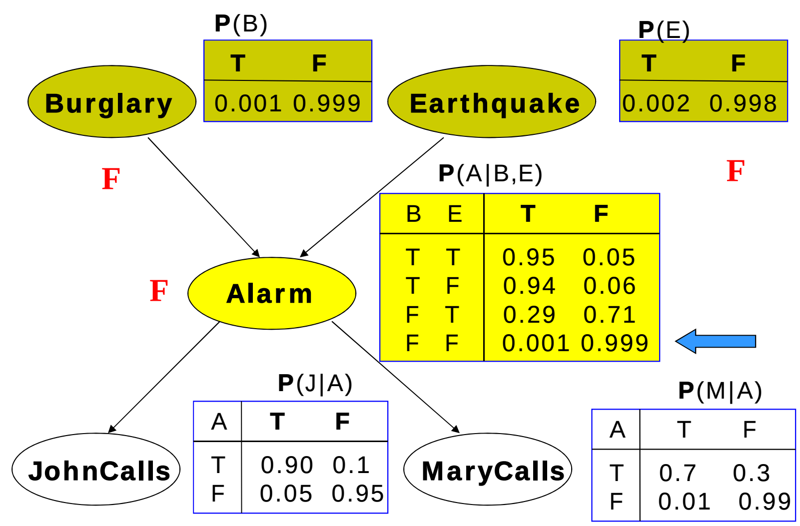

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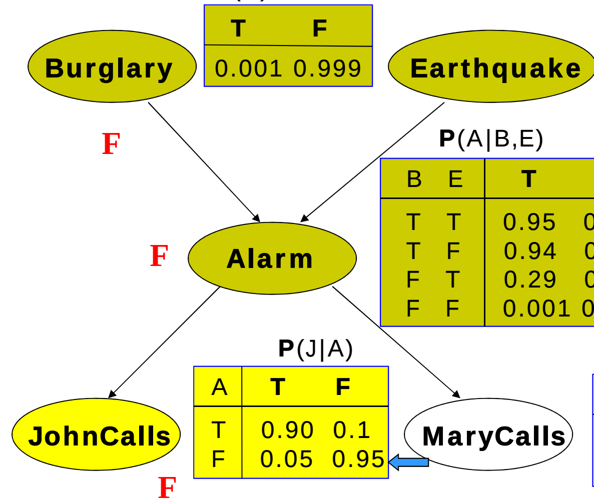

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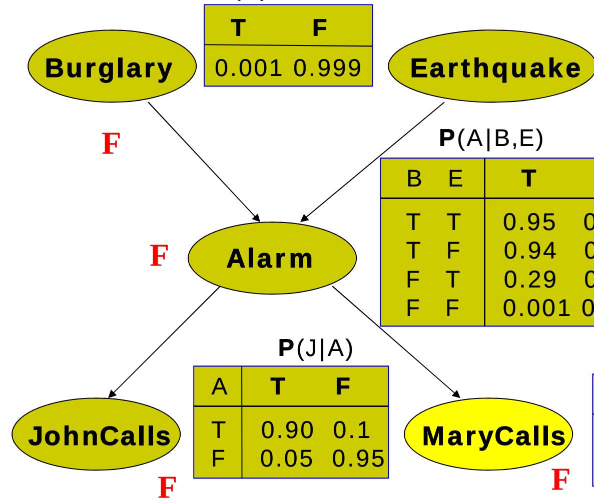
BBN sampling example



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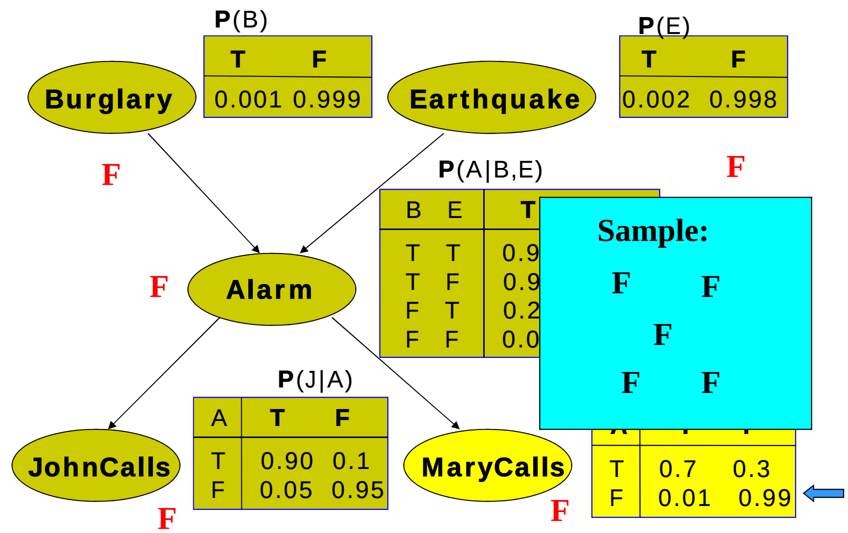


Monte Carlo approaches

- **MC approximation of conditional probabilities**:
  - The probability is approximated using sample frequencies
  - **Example:**

$$\tilde{P}(B=T \mid J=T) = \frac{N_{B=T,J=T}}{N_{J=T}}$$

$\# samples \;\; with \;\; B=T, J=T$

$\# samples \;\; with \;\; J=T$

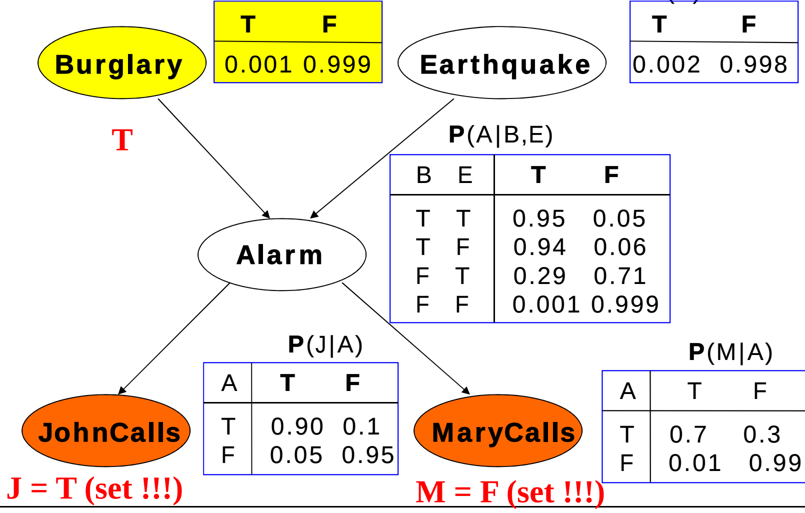
- **Rejection sampling:**
  - Generate samples from the full joint by sampling BBN
  - Use only samples that agree with the condition, the remaining samples are rejected
- **Problem:** many samples can be rejected

Likelihood weighting

- **Avoids inefficiencies of rejection sampling**
  - **Idea:** generate only samples consistent with an evidence (or conditioning event)
  - **If the value is set no sampling**
- **Problem:** using simple counts is not enough since these may occur with different probabilities
- Likelihood weighting:
  - **With every sample keep a weight with which it should count towards the estimate**

$$\tilde{P}(B=T \mid J=T) = \frac{\sum_{samples\ \ with\ \ B=T\ \ and\ \ J=T} w_{B=T}}{\sum_{samples\ \ with\ \ any\ \ value\ \ of\ \ B\ \ and\ \ J=T} w_{B=x}}$$

BBN likelihood weighting example



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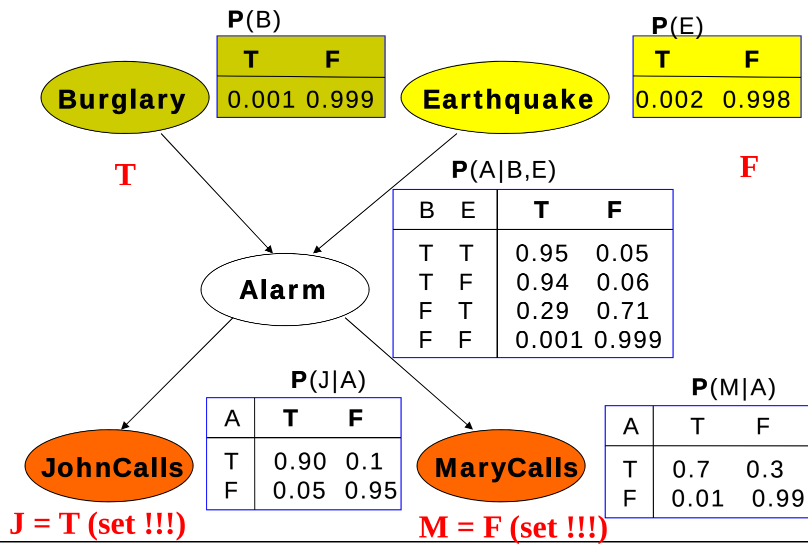

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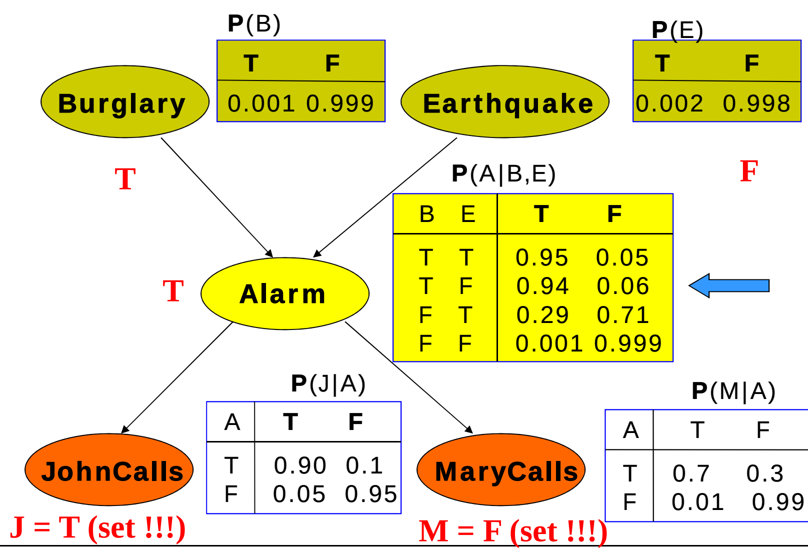
BBN likelihood weighting example



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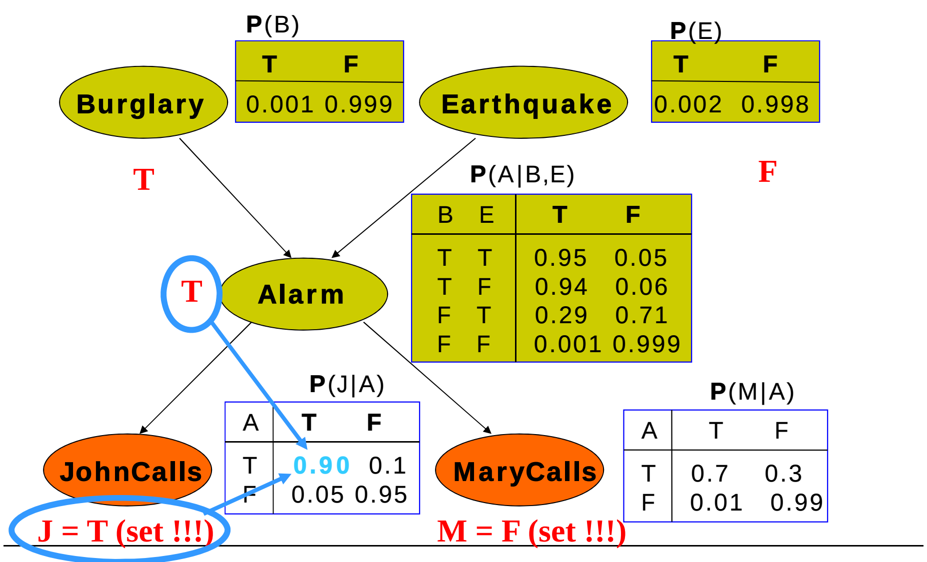

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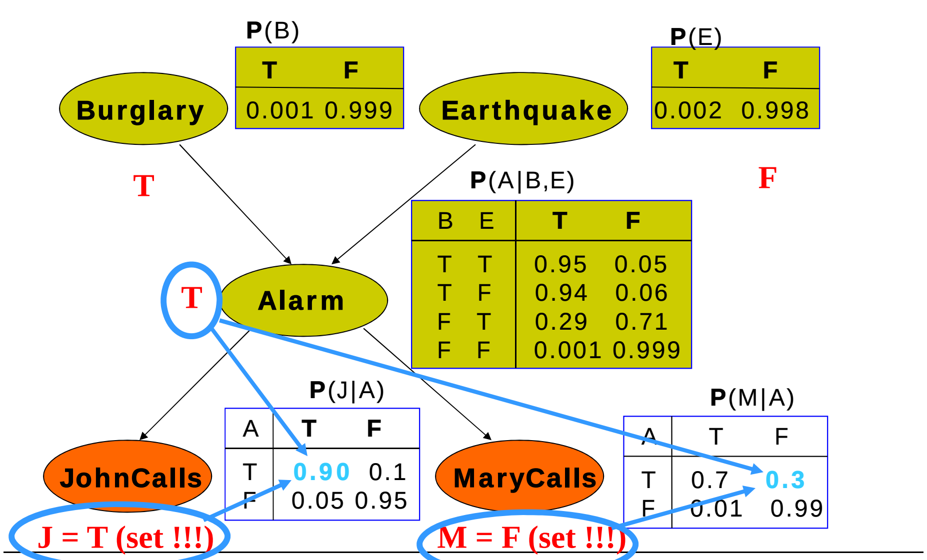
BBN likelihood weighting example



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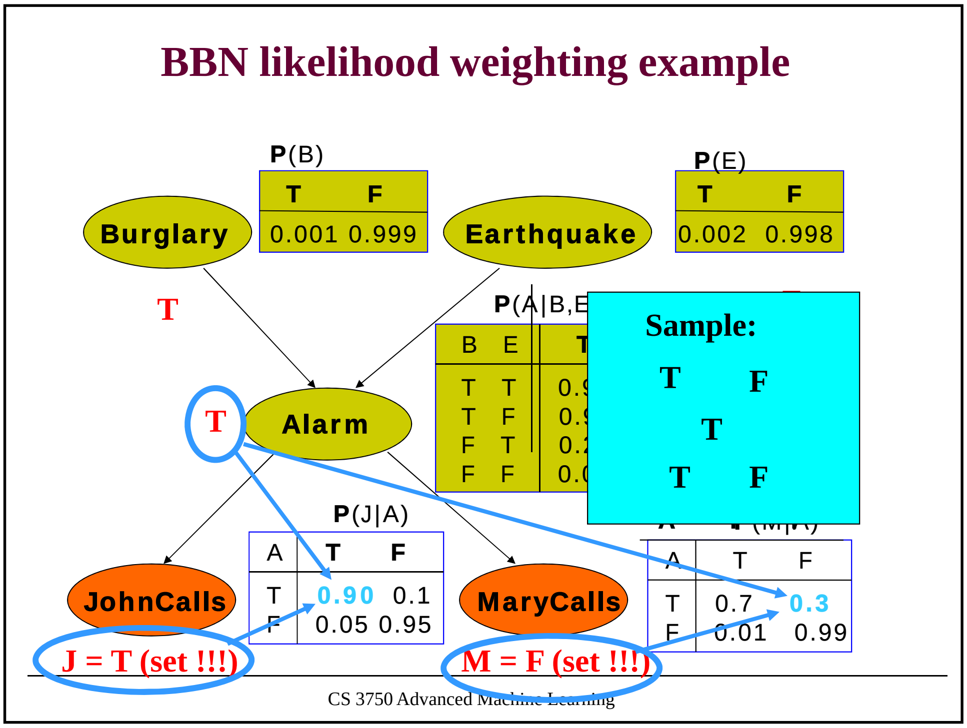
BBN likelihood weighting example
P(B)
T F
0.001 0.999
Burglary
Earthquake
P(E)
T F
0.002 0.998
T
Sample:
T F
T
T F
T
Alarm
P(J|A)
A T F
T 0.90 0.1
F 0.05 0.95
JohnCalls
MaryCalls
A T F
T 0.7 0.3
F 0.01 0.99
J = T (set !!!)
M = F (set !!!)
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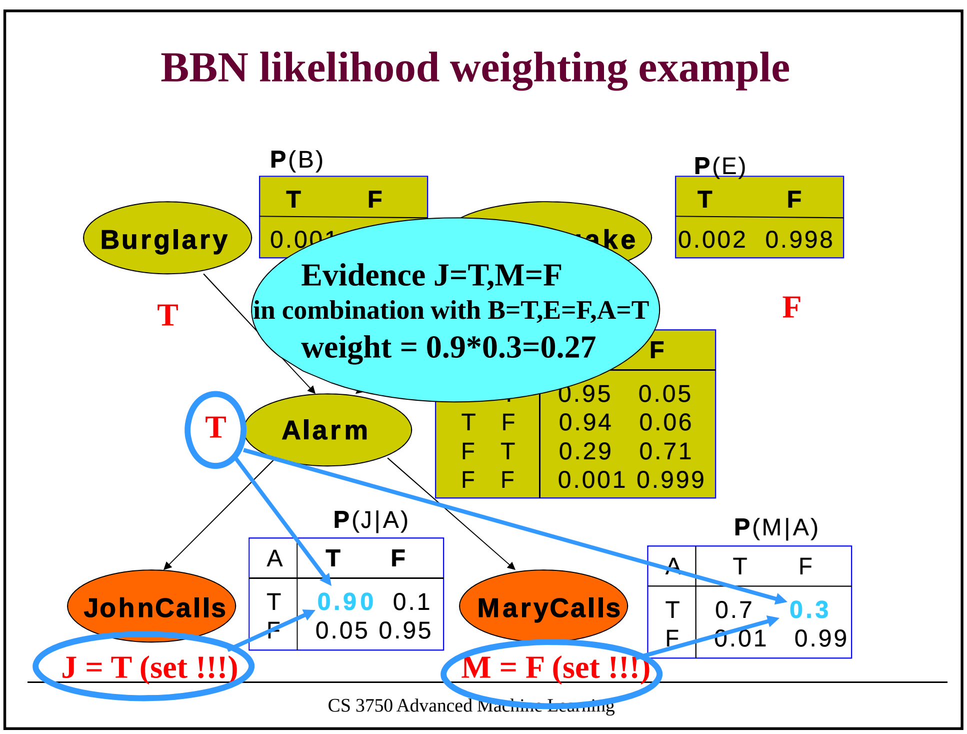
BBN likelihood weighting example
P(B)
T F
Burglary
P(E)
T F
0.002 0.998
T
F
Evidence J=T,M=F
in combination with B=T,E=F,A=T
weight = 0.9*0.3=0.27
F
0.95 0.05
T F 0.94 0.06
F T 0.29 0.71
F F 0.001 0.999
T
Alarm
P(J|A)
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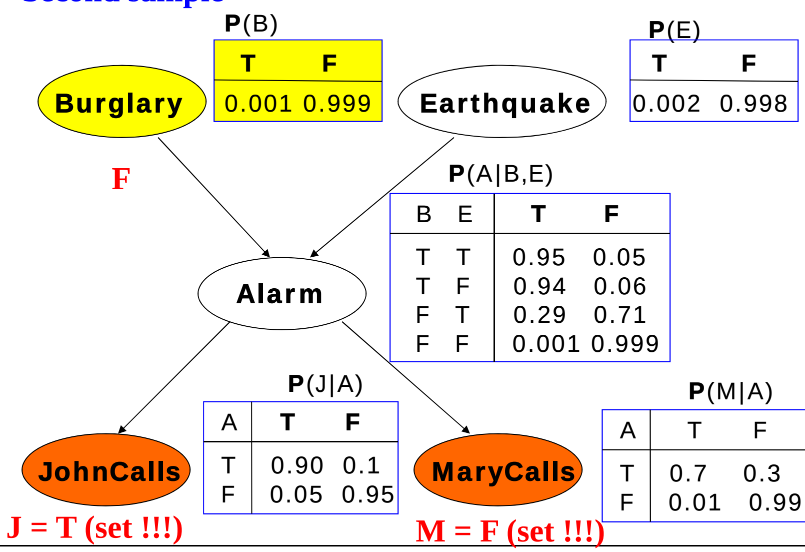
BBN likelihood weighting example

Second sample



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BBN likelihood weighting example

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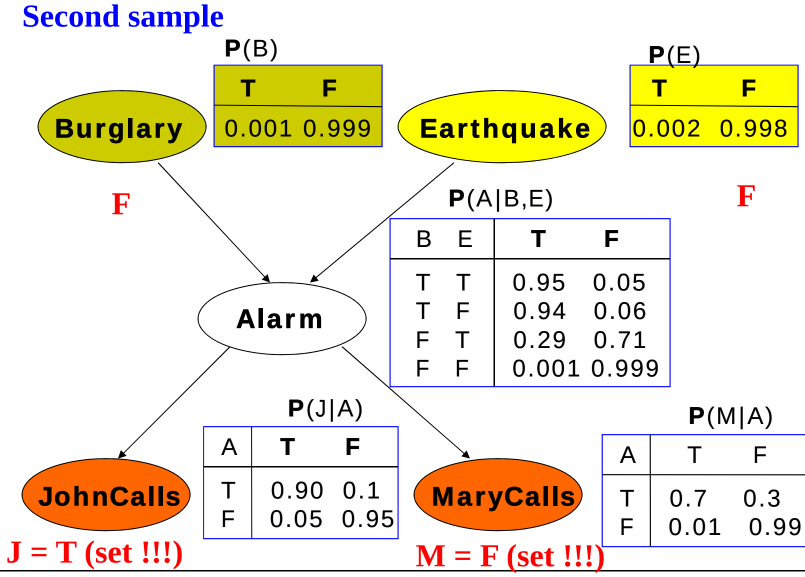

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BBN likelihood weighting example

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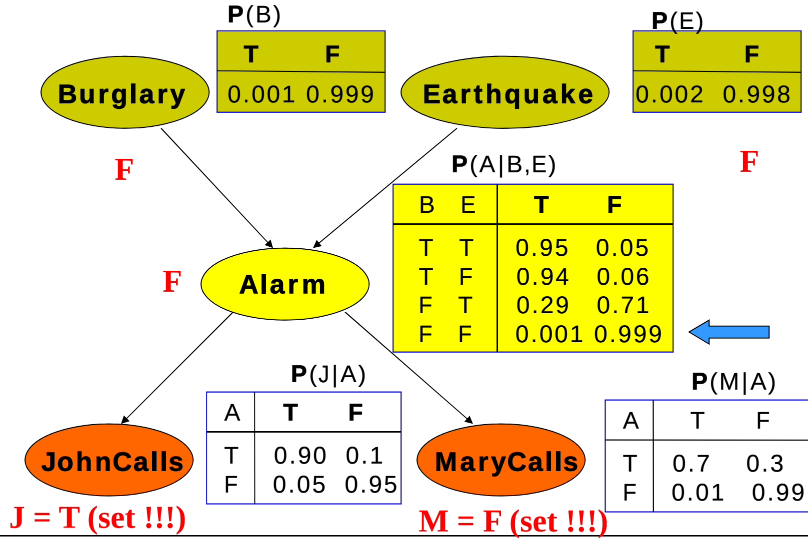

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BBN likelihood weighting example

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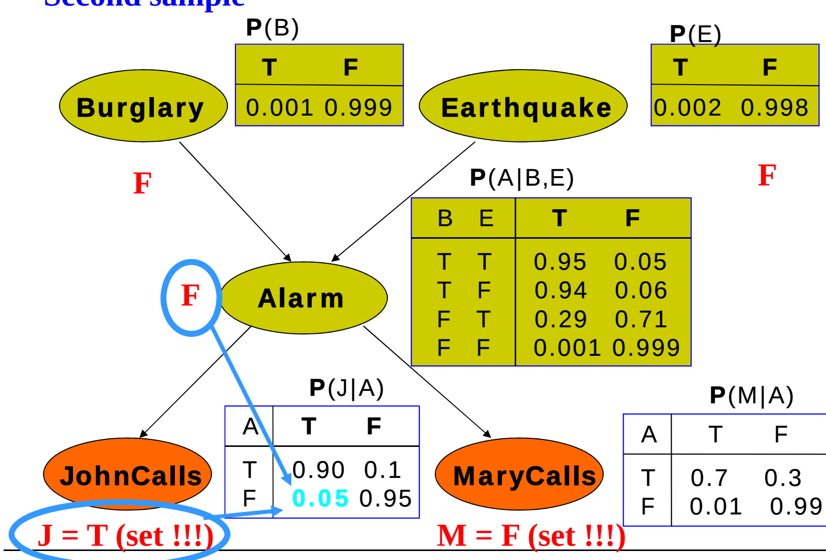

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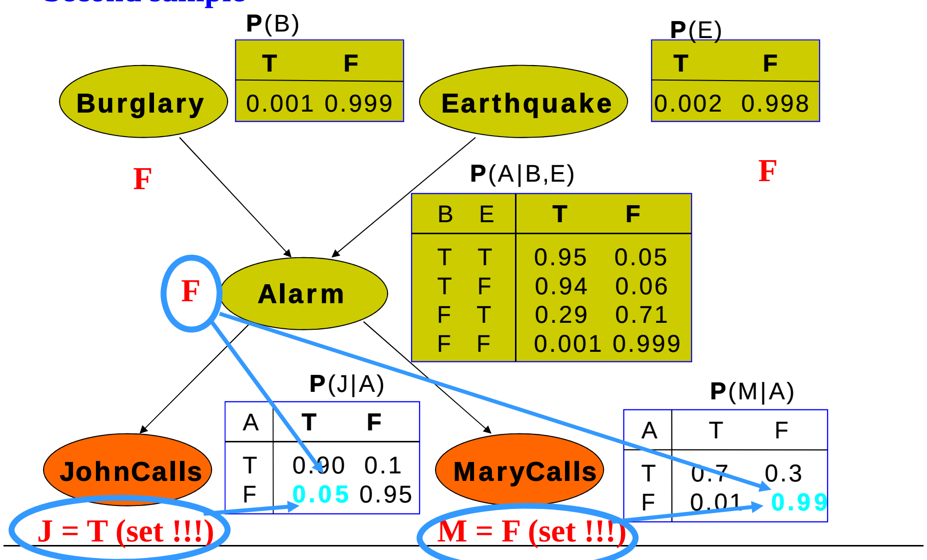

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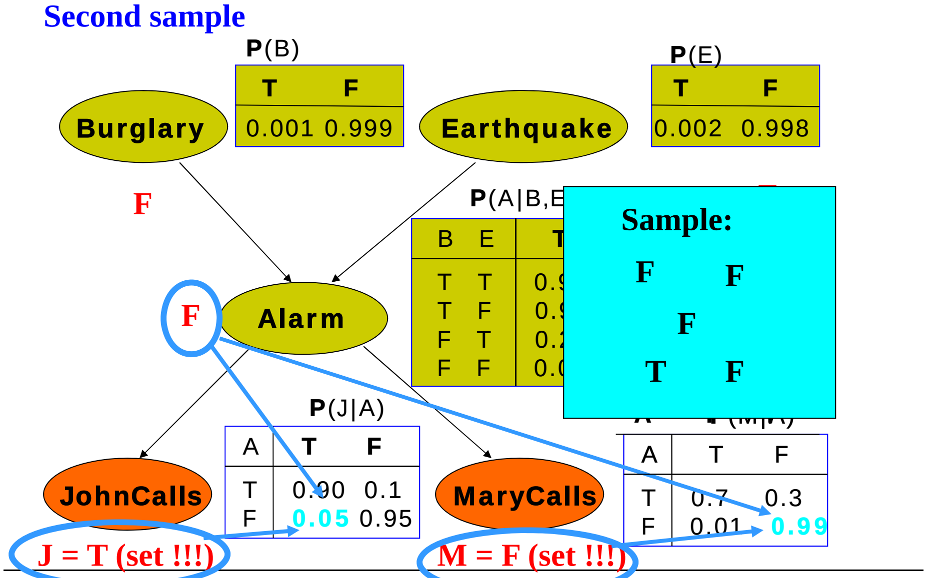

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P(A|B,E

B	E	T
T	T	0.9
T	F	0.9
F	T	0.2
F	F	0.0

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BBN likelihood weighting example

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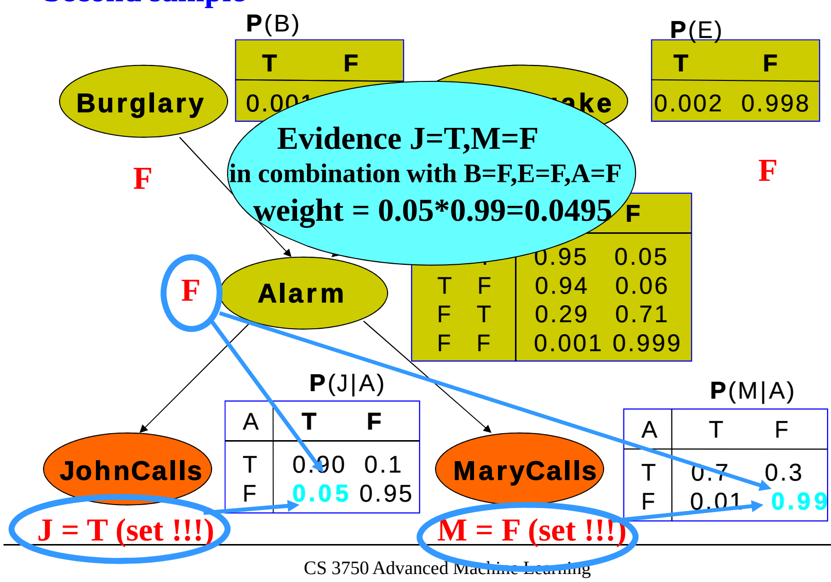
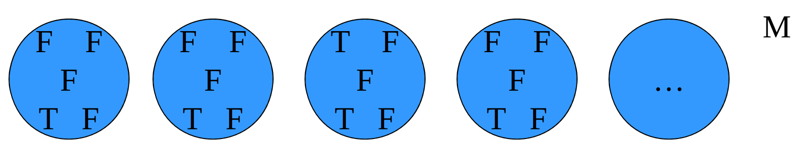


Likelihood weighting

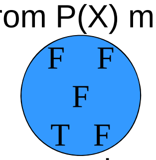
- Assume we have generated the following M samples:



- If we calculate the estimate:

$$P(B=T \mid J=T, M=F) = \frac{\#sample\_with(B=T)}{\#total\_sample}$$

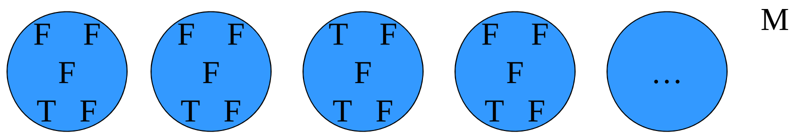
a less likely sample from P(X) may be generated more often.

- For example, sample  is generated more often than in P(X)

- So the samples are not consistent with P(X).

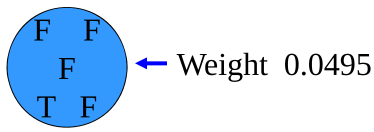
Likelihood weighting

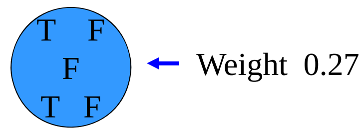
- Assume we have generated the following M samples:



How to make the samples consistent?

Weight each sample by probability with which it agrees with the conditioning evidence P(e).





Likelihood weighting

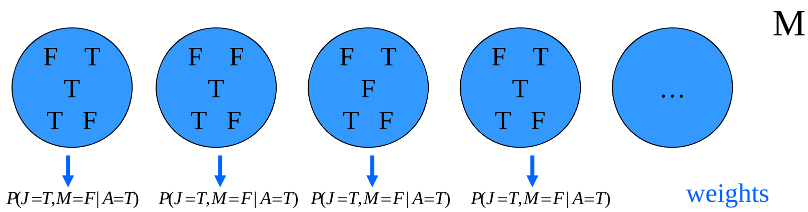
- How to compute weights for the sample?
- Assume the query $P(B=T \mid J=T, M=F)$
- Likelihood weighting:
  - **With every sample keep a weight with which it should count towards the estimate**

$$\tilde{P}(B=T \mid J=T, M=F) = \frac{\sum_{i=1}^{M} 1\{B^{(i)}=T\} w^{(i)}}{\sum_{i=1}^{M} w^{(i)}}$$

$$\tilde{P}(B=T \mid J=T, M=F) = \frac{\sum_{\text{samples with } B=T \text{ and } J=T, M=F} w_{B=T}}{\sum_{\text{samples with any value of } B \text{ and } J=T, M=F} w_{B=x}}$$

Likelihood weighting

- Assume M samples where evidence is enforced:



- We can use P(e) to weight each sample and correct the bias.
- The correct estimate is then:

$$\tilde{P}(A=T \mid J=T, M=F) = \frac{\sum_{i=1}^{M} 1\{A^{(i)}=T\} w^{(i)}}{\sum_{i=1}^{M} w^{(i)}}$$

Importance Sampling

- An approach for estimating the expectation of a function f(x) relative to some distribution P(X) (**target distribution**)
- generally, we can estimate this expectation by generating samples x[1], …, x[M] from P, and then estimating

$$E_P[f] = \frac{1}{M}\sum_{m=1}^{M} f(x[m])$$

- However, we might prefer to generate samples from a different distribution Q (**proposal or sampling distribution**) instead, since it might be impossible or computationally very expensive to generate samples directly from P.

- Q can be arbitrary, but it should dominate P, i.e. Q(x)>0 whenever P(x)>0

Unnormalized Importance Sampling

- Since we generate samples from Q instead of P,
- we need to adjust our estimator to compensate for the incorrect sampling distribution.

$$E_{p(X)}[f(X)] = E_{Q(x)}[f(x)\frac{P(x)}{Q(x)}]$$

- So we can use standard estimator for expectations relative to Q.
- **Method:** We generate a set of M samples D={x[1],…,x[M]} from Q, and estimate:

$$\hat{E}_D(f) = \frac{1}{M}\sum_{m=1}^{M} f(x[m])\frac{P(x[m])}{Q(x[m])}$$

Importance sampling

- This is an unbiased estimator: its mean for any data set is precisely the desired value

$w(x) = P(x)/Q(x)$ - a weighting function, or a correction weight

- We can estimate the distribution of the estimator around its mean: as M $\rightarrow \infty$

$$E_{Q(X)}[f(X)w(X)] - E_{P(X)}[f(X)] \propto N(0;\sigma_Q{}^2/M)$$

where $\sigma_Q{}^2 = [E_{Q(X)}[(f(X)w(X))^2]] - (E_{Q(X)}[f(X)w(X)])^2$

$$\sigma_Q{}^2 = [E_{Q(X)}[(f(X)w(X))^2]] - (E_{P(X)}[f(X)])^2$$

Importance sampling

- When f(X)=1, the variance is simply the variance of the weighting function P(X)/Q(X). Thus, the more different Q is from P, the higher is the variance of the estimator.
- In general, the lowest variance is achieved when

$$Q(X) \propto |f(X)| P(X)$$

- We should avoid cases where our sampling probability Q(X)<<P(X)f(X) in any part of the space, as these cases can lead to very large or even infinite variance.

- Problem with unnormalized IS: P is assumed to be known

Normalized Importance Sampling

- When P is only known up to a normalizing constant α
- We have access to a function P'(X), such that P' is not a normalized distribution, but P'(X)= αP(X)

- In this context, we cannot define the weights relative to P, so we define:

$$w(X) = \frac{P'(X)}{Q(X)}$$

$$E_{P(X)}[f(X)] = \sum_x P(x) f(x) = \sum_x Q(x) f(x) \frac{P(X)}{Q(x)} = \frac{1}{\alpha} \sum_x Q(x) f(x) \frac{P'(x)}{Q(x)}$$

$$= \frac{1}{\alpha} E_{Q(x)}[f(X) w(X)] = \frac{E_{Q(X)}[f(X) w(X)]}{E_{Q(X)}[w(X)]}$$

Why? $E_{Q(X)}[w(X)] = \sum_x Q(x) \frac{P'(x)}{Q(x)} = \sum_x P'(x) = \alpha$

Importance sampling

- Using an empirical estimator for both the numerator and denominator, we can estimate:

$$\hat{E}_D(f) = \frac{\sum_{m=1}^{M} f(x[m])w(x[m])}{\sum_{m=1}^{M} w(x[m])}$$

- Although the normalized estimator is biased, its variance is typically lower than that of the unnormalized estimator. This reduction in variance often outweighs the bias term.
- So normalized estimator is often used in place of the unnormalized estimator, even in cases where P is known and we can sample from it effectively.

Proposal Distribution for estimating conditional probabilities in BBNs

Assume a Bayesian Network

- We want to calculate P(x|e)
- This is hard if we need to go opposite the links and account for the effect of evidence on nondescendants

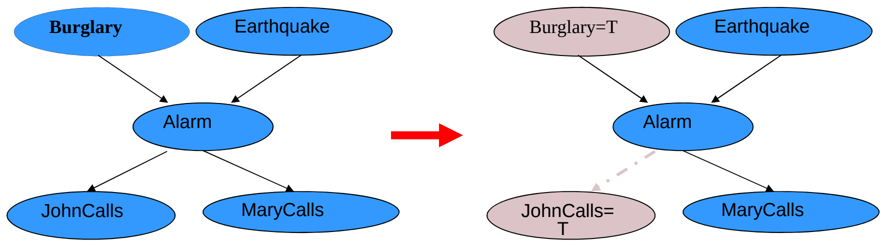
Objective: generate examples efficiently using a simpler proposal distribution Q(x)

Solution: **a mutilated belief network** (Koller, Friedman 2009)

- Idea:
  - Avoid propagation of evidence effects to non-descendants;
  - Disconnect all variables in the evidence from their parents

Mutilated Belief network

- Assume we want to calculate P(x|B=T,J=T) in the Alarm network
- Use B=T and J=T to build a mutilated network



Original network

Mutilated network

Mutilated Belief network

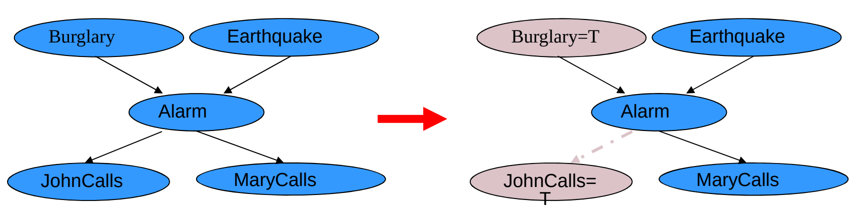
- Assume the evidence is J=j* and B=b*
- **Original network (target distribution):**

$$P(E=e, A=a, M=m, J=j^*, B=b^*) = P(b^*)P(e)P(a\,|\,b^*,e)P(j^*\,|\,a)P(m\,|\,a)$$

- **Mutilated network (proposal distribution):**

$$Q(E=e, A=a, M=m, J=j^*, B=b^*) = P(e)P(a\,|\,b^*,e)P(m\,|\,a)$$

- Note that $w(x) = \dfrac{P(x)}{Q(x)} = P(b^*)P(j^*\,|\,a)$



Original network

Mutilated network

Mutilated Belief network

- Assume the evidence is J=j* and B=b*
- **Original network:**

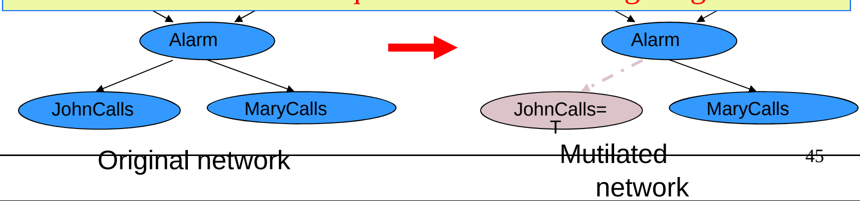
$$P(E=e, A=a, M=m, J=j^*, B=b^*) = P(b^*)P(e)P(a \mid b^*, e)P(j^* \mid a)P(m \mid a)$$

- **Mutilated network:**

$$Q(E=e, A=a, M=m, J=j^*, B=b^*) = P(e)P(a \mid b^*, e)P(m \mid a)$$

- Note that $w(x) = \frac{P(x)}{Q(x)} = P(b^*)P(j^* \mid a)$

So importance sampling with a proposal distribution based on mutilated network is equal to likelihood weighting



Data-Dependent Likelihood Weighting

- **Question:** When to stop? How many samples do we need to see?
- **Intuition:** not every samples contribute equally to the quality of the estimate. A sample with high weight is more compatible with the evidence e, and may provide us with more information.
- **Solution:** We stop sampling when the total weight of the generated particles reaches a pre-defined value.
- **Benefits:** It allows early stopping in cases where we were lucky in our random choice of samples.