### Inference in belief networks

Chapter 15.3-4 + new

#### Outline

- Exact inference by enumeration
- $\diamondsuit$  Exact inference by variable elimination
- Approximate inference by stochastic simulation
- Approximate inference by Markov chain Monte Carlo

#### Inference tasks

Simple queries: compute posterior marginal  $P(X_i|\mathbf{E}=\mathbf{e})$ e.g., P(NoGas|Gauge = empty, Lights = on, Starts = false)

Conjunctive queries:  $P(X_i, X_j | \mathbf{E} = \mathbf{e}) = P(X_i | \mathbf{E} = \mathbf{e})P(X_j | X_i, \mathbf{E} = \mathbf{e})$ 

Optimal decisions: decision networks include utility information; probabilistic inference required for P(outcome|action, evidence)

Value of information: which evidence to seek next?

Sensitivity analysis: which probability values are most critical?

Explanation: why do I need a new starter motor?

### Inference by enumeration

tually constructing its explicit representation Slightly intelligent way to sum out variables from the joint without ac-

Simple query on the burglary network:

$$\mathbf{P}(B|J=true, M=true)$$

$$= \mathbf{P}(B, J=true, M=true)/P(J=true, M=true)$$

$$= \alpha \mathbf{P}(B, J=true, M=true)$$

$$= \alpha \sum_{e} \sum_{a} \mathbf{P}(B, e, a, J=true, M=true)$$

Rewrite full joint entries using product of CPT entries:

$$P(B = true|J = true, M = true)$$

$$= \alpha \sum_{e} \sum_{a} P(B = true) P(e) P(a|B = true, e) P(J = true|a) P(M = true|a)$$

$$= \alpha P(B = true) \sum_{e} P(e) \sum_{a} P(a|B = true, e) P(J = true|a) P(M = true|a)$$

### Enumeration algorithm

# Exhaustive depth-first enumeration: O(n) space, $O(d^n)$ time

```
inputs: X, the query variable
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           EnumerationAsk(X, \mathbf{e}, bn) returns a distribution over X
                                                                                                                                                                                     EnumerateAll(vars, \mathbf{e}) returns a real number
                                                                                                                                                                                                                                                                         return Normalize(\mathbf{Q}(X))
                                                                                                                                      if EMPTY?(vars) then return 1.0
                                                                                                                                                                                                                                                                                                                                                                                                                   for each value x_i of X do
                                                                                                                                                                                                                                                                                                                                                                                                                                                                        \mathbf{Q}(x) \leftarrow a distribution over X
if Y has value y in e
                                                                                                                                                                                                                                                                                                                                                                  extend e with value x_i for X
                                             Y \leftarrow \text{First}(vars)
                                                                                                                                                                                                                                                                                                                              \mathbf{Q}(x_i) \leftarrow \text{EnumerateAll}(\text{Vars}[bn], \mathbf{e})
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  e, evidence specified as an event
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   bn, a belief network specifying joint distribution \mathbf{P}(X_1,\ldots,X_n)
```

then return  $P(y \mid Pa(Y)) \times \text{ENUMERATEALL(REST}(vars), \mathbf{e})$ else return  $\Sigma_y P(y \mid Pa(Y)) \times \text{ENUMERATEALL}(\text{REST}(vars), \mathbf{e}_y)$ 

where  $\mathbf{e}_y$  is  $\mathbf{e}$  extended with Y = y

### Inference by variable elimination

Enumeration is inefficient: repeated computation e.g., computes P(J=true|a)P(M=true|a) for each value of e

storing intermediate results (factors) to avoid recomputation Variable elimination: carry out summations right-to-left,

$$\begin{split} \mathbf{P}(B|J=true,M=true) \\ &= \alpha \underbrace{\mathbf{P}(B)}_{B} \underbrace{\sum_{e} P(e) \sum_{a} \mathbf{P}(a|B,e)}_{E} \underbrace{P(J=true|a)}_{J} \underbrace{P(M=true|a)}_{M} \\ &= \alpha \mathbf{P}(B) \underbrace{\sum_{e} P(e) \sum_{a} \mathbf{P}(a|B,e) P(J=true|a) f_{M}(a)}_{M} \\ &= \alpha \mathbf{P}(B) \underbrace{\sum_{e} P(e) \sum_{a} \mathbf{P}(a|B,e) f_{J}(a) f_{M}(a)}_{=\alpha \mathbf{P}(B) \underbrace{\sum_{e} P(e) \sum_{a} f_{A}(a,b,e) f_{J}(a) f_{M}(a)}_{=\alpha \mathbf{P}(B) \underbrace{\sum_{e} P(e) f_{\bar{A}JM}(b,e)}_{=\alpha f_{B}(b) \times f_{\bar{E}\bar{A}JM}(b)} \text{ (sum out } E) \\ &= \alpha f_{B}(b) \times f_{\bar{E}\bar{A}JM}(b) \text{ (sum out } E) \end{split}$$

# Variable elimination: Basic operations

Pointwise product of factors  $f_1$  and  $f_2$ :

$$f_1(x_1, \dots, x_j, y_1, \dots, y_k) \times f_2(y_1, \dots, y_k, z_1, \dots, z_l)$$

$$= f(x_1, \dots, x_j, y_1, \dots, y_k, z_1, \dots, z_l)$$
E.g.,  $f_1(a, b) \times f_2(b, c) = f(a, b, c)$ 

factors outside the summation: Summing out a variable from a product of factors: move any constant

$$\sum_x f_1 \times \cdots \times f_k = f_1 \times \cdots \times f_i \sum_x f_{i+1} \times \cdots \times f_k = f_1 \times \cdots \times f_i \times f_{\bar{X}}$$

assuming  $f_1, \ldots, f_i$  do not depend on X

### Variable elimination algorithm

```
function ELIMINATIONASK(X, \mathbf{e}, bn) returns a distribution over X
return Normalize(PointwiseProduct(factors))
                                                                                                                                                                                        for each var in vars do
                                                                                                                                                                                                                                           factors \leftarrow [\ ]; \ vars \leftarrow \texttt{Reverse}(\texttt{Vars}[bn])
                                                                                                                                                                                                                                                                                                          if X \in \mathbf{e} then return observed point distribution for X
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            inputs: X, the query variable
                                                       factors \leftarrow [\text{MakeFactor}(var, \mathbf{e})|factors]
if var is a hidden variable then factors \leftarrow \text{SumOut}(var, factors)
                                                                                                                                                                                                                                                                                                                                                                                                                                                          e, evidence specified as an event
                                                                                                                                                                                                                                                                                                                                                                                                bn, a belief network specifying joint distribution \mathbf{P}(X_1,\ldots,X_n)
```

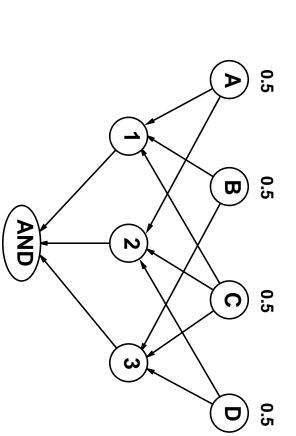
### Complexity of exact inference

### Singly connected networks (or polytrees):

- any two nodes are connected by at most one (undirected) path
- time and space cost of variable elimination are  $O(d^k n)$

#### Multiply connected networks:

- can reduce 3SAT to exact inference
- equivalent to counting 3SAT models  $\Rightarrow$ NP-hard #P-complete



- A V B V C
- < D ∨ ~A
- W v C v ~D

## Inference by stochastic simulation

#### Basic idea:

- 1) Draw N samples from a sampling distribution  $\hat{S}$
- 2) Compute an approximate posterior probability  $\hat{P}$
- 3) Show this converges to the true probability P

#### Outline:

- Sampling from an empty network
- Rejection sampling: reject samples disagreeing with evidence
- Likelihood weighting: use evidence to weight samples
- MCMC: sample from a stochastic process whose stationary distribution is the true posterior

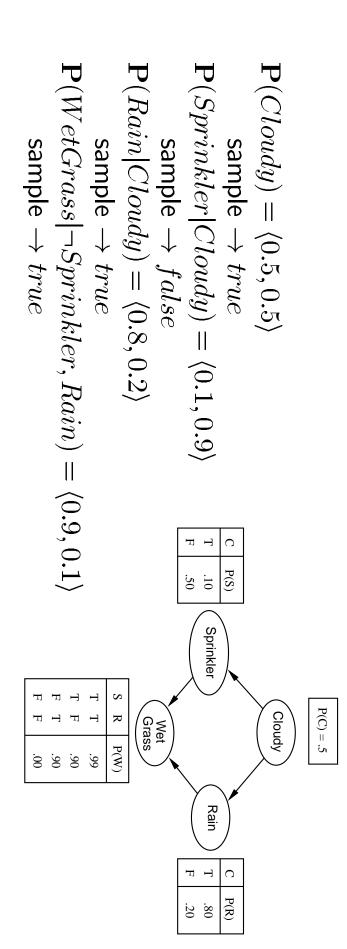
## Sampling from an empty network

function PriorSample(bn) returns an event sampled from  $P(X_1,...,X_n)$  specified by bn  $\mathbf{x} \leftarrow$  an event with n elements

for i = 1 to n do

 $x_i \leftarrow \text{a random sample from } \mathbf{P}(X_i \mid Parents(X_i))$ 

return x



# Sampling from an empty network contd.

Probability that PRIORSAMPLE generates a particular event  $S_{PS}(x_1 \dots x_n) = \prod_{i=1}^n P(x_i | Parents(X_i)) = P(x_1 \dots x_n)$ 

i.e., the true prior probability

for any set of variables Y. Let  $N_{PS}(\mathbf{Y}=\mathbf{y})$  be the number of samples generated for which  $\mathbf{Y}=\mathbf{y}$ ,

Then 
$$\hat{P}(\mathbf{Y}=\mathbf{y}) = N_{PS}(\mathbf{Y}=\mathbf{y})/N$$
 and  $\lim_{N \to \infty} \hat{P}(\mathbf{Y}=\mathbf{y}) = \sum_{\mathbf{h}} S_{PS}(\mathbf{Y}=\mathbf{y}, \mathbf{H}=\mathbf{h})$   $= \sum_{\mathbf{h}} P(\mathbf{Y}=\mathbf{y}, \mathbf{H}=\mathbf{h})$   $= P(\mathbf{Y}=\mathbf{y})$ 

That is, estimates derived from PRIORSAMPLE are consistent

#### Rejection sampling

## $\mathbf{P}(X|\mathbf{e})$ estimated from samples agreeing with $\mathbf{e}$

```
function RejectionSampling(X,\mathbf{e},bn,N) returns an approximation to P(X|\mathbf{e})
return Normalize(N[X])
                                                                                                                                                                                                        for j = 1 to N do
                                                                                                                                                                                                                                                               N[X] \leftarrow a vector of counts over X, initially zero
                                                                                                            if x is consistent with e then
                                                                                                                                                           \mathbf{x} \leftarrow \text{PriorSample}(bn)
                                                           N[x] \leftarrow N[x]+1 where x is the value of X in x
```

E.g., estimate P(Rain|Sprinkler = true) using 100 samples 27 samples have Sprinkler = trueOf these, 8 have Rain = true and 19 have Rain = false.

 $\mathbf{P}(Rain|Sprinkler = true) = \text{Normalize}(\langle 8, 19 \rangle) = \langle 0.296, 0.704 \rangle$ 

Similar to a basic real-world empirical estimation procedure

### Analysis of rejection sampling

$$\hat{\mathbf{P}}(X|\mathbf{e}) = \kappa \mathbf{N}_{PS}(X,\mathbf{e})$$
 (algorithm defn.)  
 $= \mathbf{N}_{PS}(X,\mathbf{e})/N_{PS}(\mathbf{e})$  (normalized by  $N_{PS}(\mathbf{e})$ )  
 $\approx \mathbf{P}(X,\mathbf{e})/P(\mathbf{e})$  (property of  $\mathbf{P}_{RIORSAMPLE}$ )  
 $= \mathbf{P}(X|\mathbf{e})$  (defn. of conditional probability)

Hence rejection sampling returns consistent posterior estimates

Problem: hopelessly expensive if  $P(\mathbf{e})$  is small

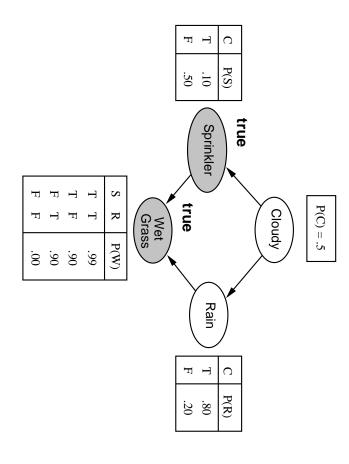
### Likelihood weighting

and weight each sample by the likelihood it accords the evidence Idea: fix evidence variables, sample only nonevidence variables

```
function LikelihoodWeighting(X, \mathbf{e}, bn, N) returns an approximation to P(X|\mathbf{e})
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                function Weighted Sample (bn, \mathbf{e}) returns an event and a weight
return Normalize(\mathbf{W}[X])
                                                                                                                                                                                                                                                                                                                                                                                                      return \mathbf{x}, w
                                                                                                                                                                                      for j = 1 to N do
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         for i = 1 to n do
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   \mathbf{x} \leftarrow \text{an event with } n \text{ elements; } w \leftarrow 1
                                                                                                                                                                                                                                              \mathbf{W}[X] \leftarrow a vector of weighted counts over X, initially zero
                                                                                                                            \mathbf{x}, w \leftarrow \text{WeightedSample}(bn)
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                if X_i has a value x_i in \mathbf{e}
                                                          \mathbf{W}[x] \leftarrow \mathbf{W}[x] + w where x is the value of X in \mathbf{x}
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  then w \leftarrow w \times P(X_i = x_i \mid Parents(X_i))
                                                                                                                                                                                                                                                                                                                                                                                                                                                      else x_i \leftarrow a random sample from P(X_i \mid Parents(X_i))
```

### Likelihood weighting example

Estimate  $\mathbf{P}(Rain|Sprinkler = true, WetGrass = true)$ 



#### LW example contd

Sample generation process:

- 1.  $w \leftarrow 1.0$
- 2. Sample  $\mathbf{P}(Cloudy) = \langle 0.5, 0.5 \rangle$ ; say true
- 3. Sprinkler has value true, so

$$w \leftarrow w \times P(Sprinkler = true|Cloudy = true) = 0.1$$

- Sample  $\mathbf{P}(Rain|Cloudy = true) = \langle 0.8, 0.2 \rangle$ ; say true
- 5. WetGrass has value true, so

$$w \leftarrow w \times P(WetGrass = true|Sprinkler = true, Rain = true) = 0.099$$

### Likelihood weighting analysis

Sampling probability for WEIGHTEDSAMPLE is

$$S_{WS}(\mathbf{y}, \mathbf{e}) = \prod_{i=1}^{l} P(y_i | Parents(Y_i))$$

Note: pays attention to evidence in ancestors only

⇒ somewhere "in between" prior and posterior distribution

Weight for a given sample y, e is  $w(\mathbf{y}, \mathbf{e}) = \prod_{i=1}^{m} P(e_i | Parents(E_i))$ 

Weighted sampling probability is

$$S_{WS}(\mathbf{y}, \mathbf{e})w(\mathbf{y}, \mathbf{e})$$

$$= \prod_{i=1}^{l} P(y_i|Parents(Y_i)) \quad \prod_{i=1}^{m} P(e_i|Parents(E_i))$$

$$= P(\mathbf{y}, \mathbf{e}) \text{ (by standard global semantics of network)}$$

but performance still degrades with many evidence variables Hence likelihood weighting returns consistent estimates

# Approximate inference using MCMC

"State" of network = current assignment to all variables

Sample each variable in turn, keeping evidence fixed Generate next state by sampling one variable given Markov blanket

```
function MCMC-Ask(X, \mathbf{e}, bn, N) returns an approximation to P(X|\mathbf{e})
return Normalize(\mathbb{N}[X])
                                                                                                                                                                                                                                                                                                                    initialize \mathbf{x} with random values for the variables in \mathbf{Y}
                                                                                                                                                                                                                                                         for j = 1 to N do
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    local variables: N[X], a vector of counts over X, initially zero
                                                                                                                               for each Y_i in Y do
                                                                                                                                                                                   N[x] \leftarrow N[x] + 1 where x is the value of X in x
                                                           sample the value of Y_i in x from \mathbf{P}(Y_i|MB(Y_i)) given the values of MB(Y_i) in x
                                                                                                                                                                                                                                                                                                                                                                                                                  \mathbf{x}, the current state of the network, initially copied from \mathbf{e}
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                \mathbf{Y}, the nonevidence variables in bn
```

each state is exactly proportional to its posterior probability Approaches stationary distribution: long-run fraction of time spent in

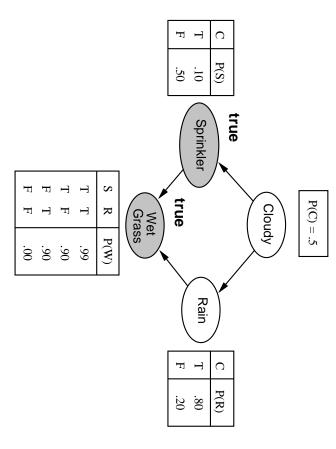
#### MCMC Example

Estimate  $\mathbf{P}(Rain|Sprinkler = true, WetGrass = true)$ 

Sample Cloudy then Rain, repeat.

Count number of times Rain is true and false in the samples.

Markov blanket of Cloudy is Sprinkler and RainMarkov blanket of Rain is Cloudy, Sprinkler, and WetGrass



### MCMC example contd.

Random initial state: Cloudy = true and Rain = false

- 1.  $\mathbf{P}(Cloudy|MB(Cloudy)) = \mathbf{P}(Cloudy|Sprinkler, \neg Rain)$ sample  $\rightarrow false$
- 2.  $\mathbf{P}(Rain|MB(Rain)) = \mathbf{P}(Rain|\neg Cloudy, Sprinkler, WetGrass)$ sample  $\rightarrow true$

Visit 100 states

31 have Rain = true, 69 have Rain = false

 $\hat{\mathbf{P}}(Rain|Sprinkler = true, WetGrass = true)$  $= \text{Normalize}(\langle 31, 69 \rangle) = \langle 0.31, 0.69 \rangle$ 

### MCMC analysis: Outline

Transition probability  $q(\mathbf{y} \to \mathbf{y}')$ 

**D**ccupancy probability  $\pi_t(\mathbf{y})$  at time t

Equilibrium condition on  $\pi_t$  defines stationary distribution  $\pi(\mathbf{y})$ Note: stationary distribution depends on choice of  $q(\mathbf{y} \to \mathbf{y}')$ 

Pairwise detailed balance on states guarantees equilibrium

Gibbs sampling transition probability:

⇒ detailed balance with the true posterior sample each variable given current values of all others

sampling conditioned on each variable's Markov blanket For Bayesian networks, Gibbs sampling reduces to

### Stationary distribution

 $\pi_t(\mathbf{y}) = \mathsf{probability}$  in state  $\mathbf{y}$  at time t $\pi_{t+1}(\mathbf{y}') = \text{probability in state } \mathbf{y}' \text{ at time } t+1$ 

 $\pi_{t+1}$  in terms of  $\pi_t$  and  $q(\mathbf{y} \to \mathbf{y}')$ 

$$\pi_{t+1}(\mathbf{y}') = \sum_{\mathbf{y}} \pi_t(\mathbf{y}) q(\mathbf{y} \to \mathbf{y}')$$

Stationary distribution:  $\pi_t = \pi_{t+1} = \pi$ 

$$\pi(\mathbf{y}') = \sum_{\mathbf{y}} \pi(\mathbf{y}) q(\mathbf{y} \to \mathbf{y}')$$
 for all  $\mathbf{y}'$ 

If  $\pi$  exists, it is unique (specific to  $q(\mathbf{y} \to \mathbf{y}')$ )

In equilibrium, expected "outflow" = expected "inflow"

#### Detailed balance

" $\mathbb{D}$ utflow" = "inflow" for each pair of states:

$$\pi(\mathbf{y})q(\mathbf{y} \to \mathbf{y}') = \pi(\mathbf{y}')q(\mathbf{y}' \to \mathbf{y})$$
 for all  $\mathbf{y}, \mathbf{y}'$ 

Detailed balance 
$$\Rightarrow$$
 stationarity:  

$$\Sigma_{\mathbf{y}}\pi(\mathbf{y})q(\mathbf{y} \to \mathbf{y}') = \Sigma_{\mathbf{y}}\pi(\mathbf{y}')q(\mathbf{y}' \to \mathbf{y})$$

$$= \pi(\mathbf{y}')\Sigma_{\mathbf{y}}q(\mathbf{y}' \to \mathbf{y})$$

$$= \pi(\mathbf{y}')$$

probability q that is in detailed balance with desired  $\pi$ MCMC algorithms typically constructed by designing a transition

#### Gibbs sampling

Sample each variable in turn, given all other variables

Sampling  $Y_i$ , let  $\bar{\mathbf{Y}}_i$  be all other nonevidence variables Current values are  $y_i$  and  $\bar{\mathbf{y}}_i$ ;  $\mathbf{e}$  is fixed Transition probability is given by

$$q(\mathbf{y} \to \mathbf{y}') = q(y_i, \bar{\mathbf{y}}_i \to y_i', \bar{\mathbf{y}}_i) = P(y_i'|\bar{\mathbf{y}}_i, \mathbf{e})$$

This gives detailed balance with true posterior  $P(\mathbf{y}|\mathbf{e})$ :  $\pi(\mathbf{y})q(\mathbf{y}\to\mathbf{y}') = P(\mathbf{y}|\mathbf{e})P(y_i'|\bar{\mathbf{y}}_i,\mathbf{e}) = P(y_i,\bar{\mathbf{y}}_i|\mathbf{e})P(y_i'|\bar{\mathbf{y}}_i,\mathbf{e})$  $= P(y_i|\bar{\mathbf{y}}_i,\mathbf{e})P(\bar{\mathbf{y}}_i|\mathbf{e})P(y_i'|\bar{\mathbf{y}}_i,\mathbf{e}) \quad \text{(chain rule)}$  $q(\mathbf{y}' \to \mathbf{y})\pi(\mathbf{y}') = \pi(\mathbf{y}')q(\mathbf{y}' \to \mathbf{y})$  $P(y_i|\bar{\mathbf{y}}_i,\mathbf{e})P(y_i',\bar{\mathbf{y}}_i|\mathbf{e})$  (chain rule backwards)

### Markov blanket sampling

A variable is independent of all others given its Markov blanket:

$$P(y_i'|\bar{\mathbf{y}}_i,\mathbf{e}) = P(y_i'|MB(Y_i))$$

Probability given the Markov blanket is calculated as follows:

$$P(y_i'|MB(Y_i)) = P(y_i'|Parents(Y_i)) \prod_{Z_j \in Children(Y_i)} P(z_j|Parents(Z_j))$$

c not too large just cd multiplications if  $Y_i$  has c children and d values; can cache it if Hence computing the sampling distribution over  $Y_i$  for each flip requires

Main computational problems:

- 1) Difficult to tell if convergence has been achieved
- 2) Can be wasteful if Markov blanket is large:

 $P(Y_i|MB(Y_i))$  won't change much (law of large numbers)

# Performance of approximation algorithms

Absolute approximation:  $|P(X|\mathbf{e}) - \hat{P}(X|\mathbf{e})| \le \epsilon$ 

Relative approximation:  $\frac{|P(X|\mathbf{e}) - \hat{P}(X|\mathbf{e})|}{P(X|\mathbf{e})} \le \epsilon$ 

Relative  $\Rightarrow$  absolute since  $0 \le P \le 1$  (may be  $O(2^{-n})$ )

Randomized algorithms may fail with probability at most  $\delta$ 

Polytime approximation:  $poly(n, \epsilon^{-1}, \log \delta^{-1})$ 

are NP-hard for any  $\epsilon, \delta < 0.5$ approximation for either deterministic or randomized algorithms Theorem (Dagum and Luby, 1993): both absolute and relative

(Absolute approximation polytime with no evidence—Chernoff bounds)