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CMP9794M
Advanced Artificial Intelligence

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Last Week

- Discussion on structure learning

- Algorithms to induce the structure of Bayes nets
  - PC-Stable (step 1 in particular)
  - Hill Climbing
  - Min-Max Hill Climbing

- Multiple metrics to measure the performance of probabilistic models on test data

Today

- **Inference by stochastic simulation**

- Approximate inference in Bayesian nets (BNs)
  - Rejection Sampling
  - Likelihood Weighting
  - Gibbs Sampling

- Data discretisation for learning discrete BNs

- Questions and answers related to assignment

Acknowledgement: Content of slides adapted from Prof. Simon Parsons' slides.

Inference by Stochastic Simulation

- Basic idea:
  - Draw N samples from a sampling distribution S
  - Compute an approximate posterior probability $\hat{P}$
  - $\hat{P}$ converges to the true probability P as the number of samples tends to infinity.
- That can be used when exact inference is intractable (in the case of large Bayes nets or many hidden vars.)
- Let's look at an example of the basic idea.

Inference by Stochastic Simulation

- Imagine we have a stochastic process that generates numbers in the range: 0, 1, . . . 9
- How do we determine the probability of each value being generated?
  - One possibility is to generate lots of numbers (samples) and look at the sample average for each value.
  - If we generate N samples, and m of them are 9, then the sample average is: $\frac{m}{N}$
  - This is an estimate of the probability of 9 being generated.

Inference by Stochastic Simulation

- Overall process:
  - Draw N samples from a sampling distribution S. The "sampling distribution" is generated by the process.
  - Compute an approximate posterior probability $\hat{P}$. It is an estimate (what the hat means) because it is approximate.
  - $\hat{P}$ converges to the true probability P as the number of samples tends to infinity.
- But note that the more samples, the more accurate our estimates will be.

Inference by Stochastic Simulation

- This works for any process where we can just observe the samples:
  - Rain in Lincoln (in October).
  - How many students turn up to Advanced AI.
  - How many apples my apple tree produces.
  - How long it takes me to walk to work.

- However, for our BN we have to generate the samples.

- That is what we will look at next.

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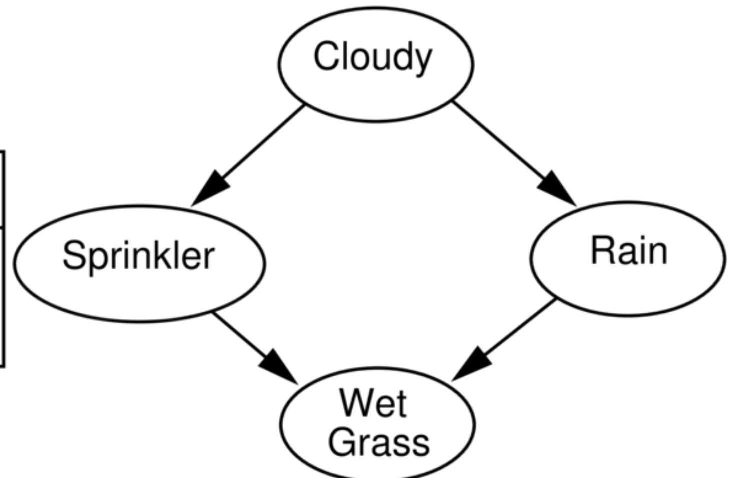
Prior Sampling

P(C)
.50

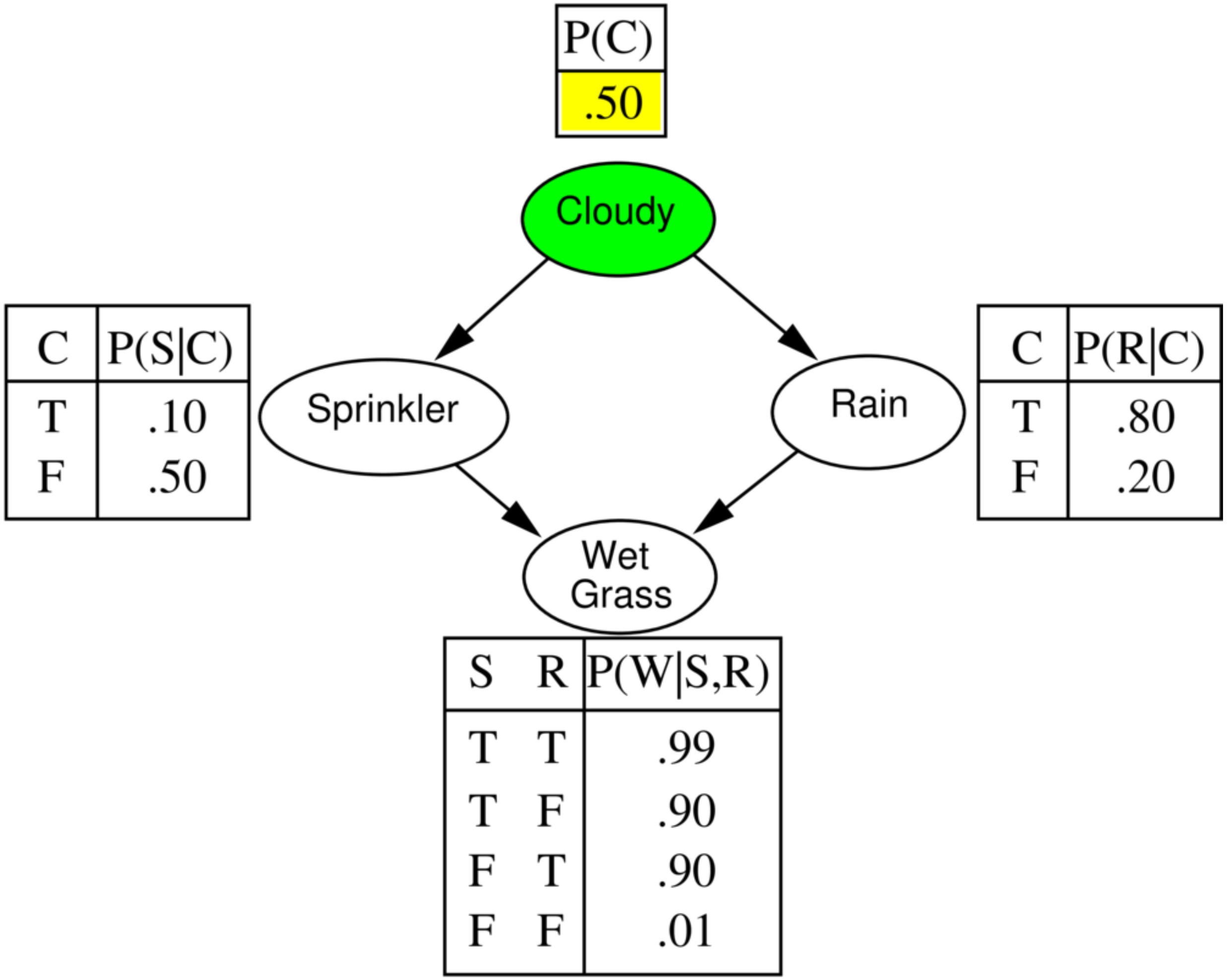
C	P(S|C)
T	.10
F	.50



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

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

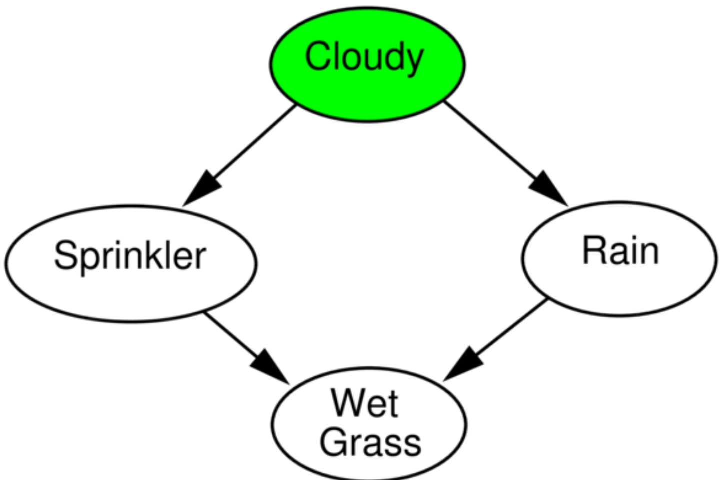
Prior Sampling



Cloudy = true

Prior Sampling

P(C)
.50



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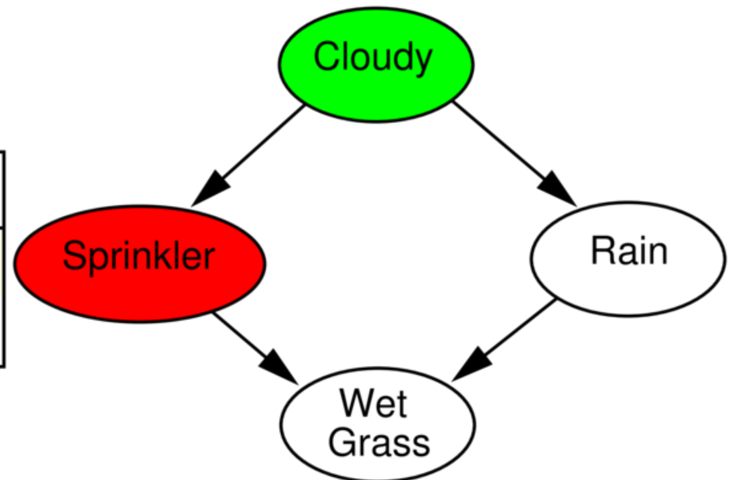

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T	.10
F	.50

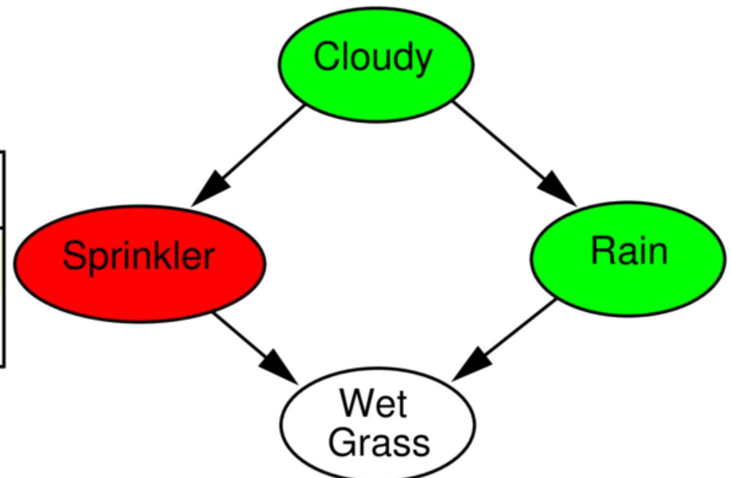
C	P(R|C)
T	.80
F	.20

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

Sprinkler = false

Prior Sampling

P(C)
.50



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

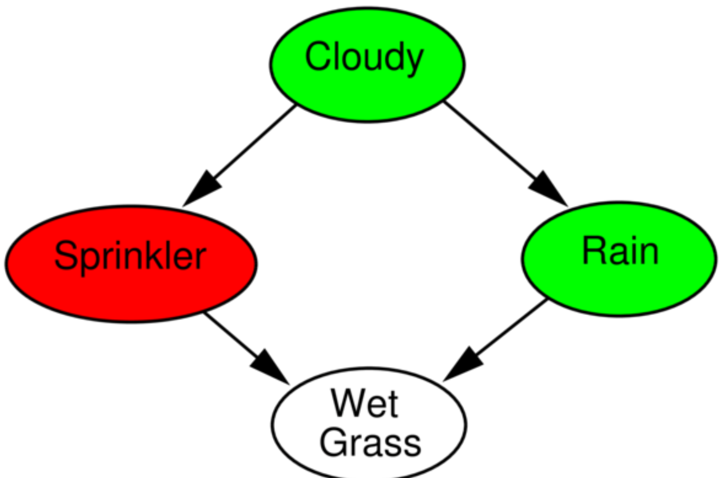
C	P(R|C)
T	.80
F	.20

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

Rain = true

Prior Sampling

P(C)
.50



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

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T	.80
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S	R	P(W|S,R)
T	T	.99
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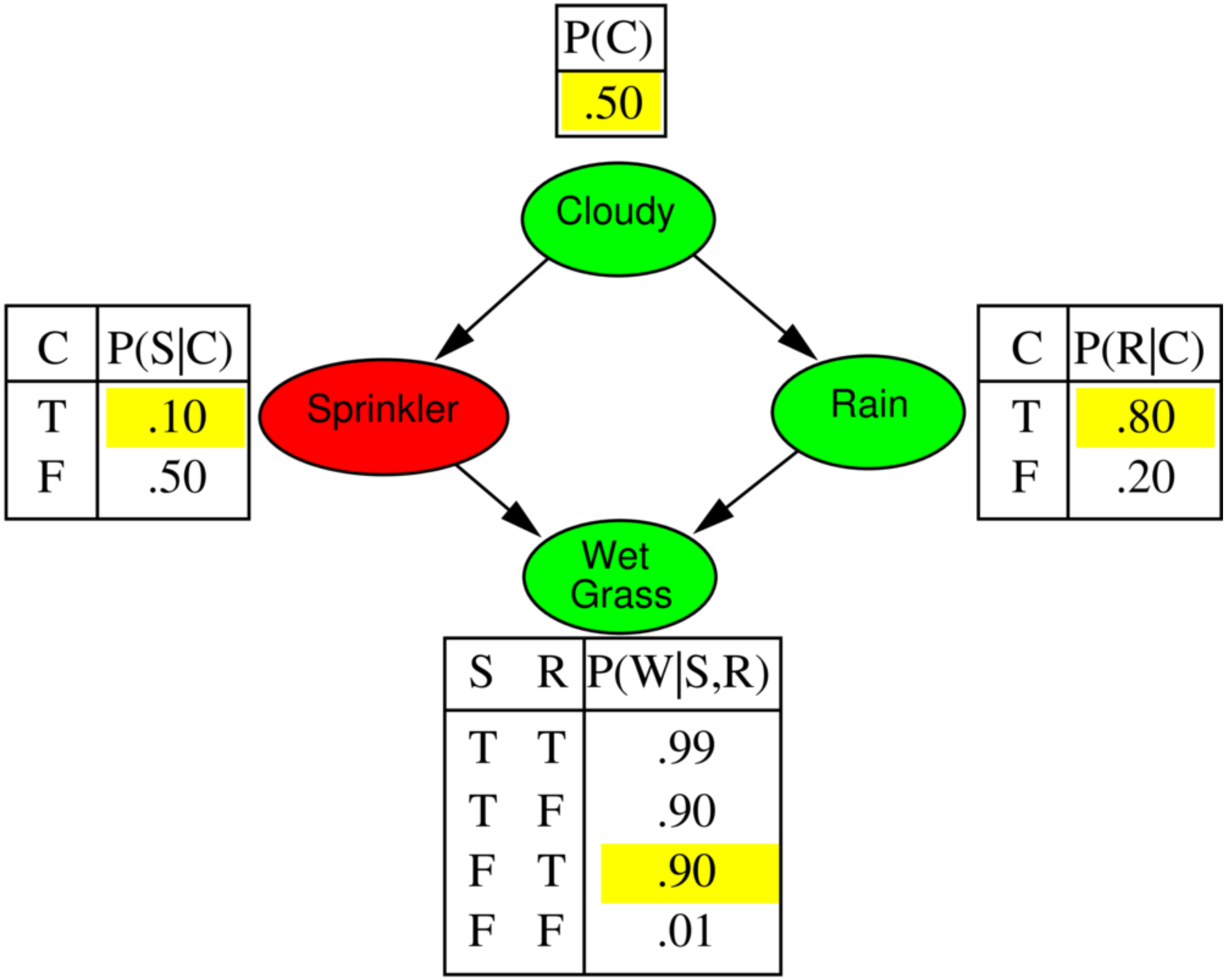
F	T	.90
F	F	.01

Prior Sampling



P(C)
.50

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

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

WetGrass = true

Prior Sampling

- So, we get [$Cloudy = true,\ Sprinkler = false, Rain = true, WetGrass = true$]
- We write this as [$true, false, true, true$], assuming a specific order of random variables (hierarchical).

- If we repeat the process many times (N), we can count the number of times [$true, false, true, true$] is the result (m).
- The proportion $\frac{m}{N}$ gives us $P(c, \neg s, r, w)$
- The more runs, the more accurate the probability.

Prior Sampling: Question for you

- Similarly, the proportion $[false, true, true, true]$ gives us $P(\neg c, s, r, w)$. Thus, given:
  - [true, false, true, true]
  - [false, false, true, true]
  - [true, true, true, true]
  - [true, false, false, true]
  - [true, false, true, true]
  - [true, false, true, false]
- $P(c, \neg s, r, w) \approx ?$
- $P(\neg c, s, r, w) \approx ?$

Prior Sampling: Algorithm

function PRIOR-SAMPLE(bn) **returns** an event sampled from bn

inputs: bn, a belief network specifying joint distribution $\mathbf{P}(X_1, \ldots, X_n)$

$\mathbf{x} \leftarrow$ an event with n elements

for $i = 1$ **to** n **do**

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

given the values of $Parents(X_i)$ in $\mathbf{x}$

return $\mathbf{x}$

Rejection Sampling: Algorithm

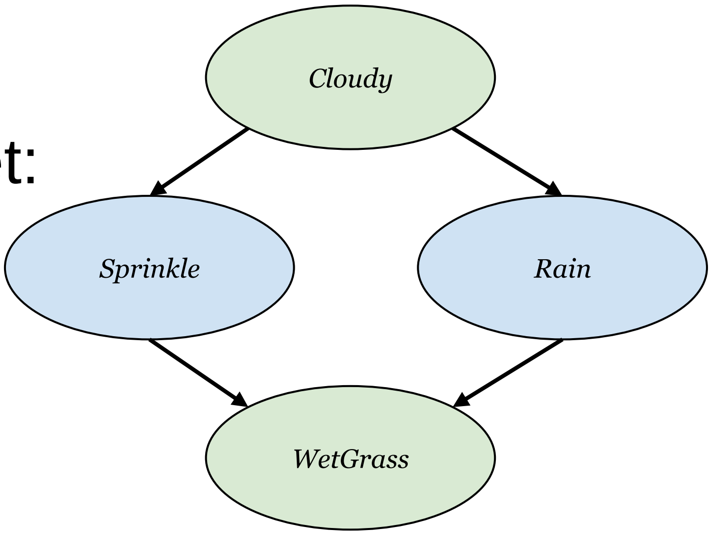
function REJECTION-SAMPLING(X, $\mathbf{e}$, bn, N) **returns** an estimate of $P(X|\mathbf{e})$
local variables: $\mathbf{N}$, a vector of counts over X, initially zero

for $j = 1$ to N **do**
  $\mathbf{x} \leftarrow$ PRIOR-SAMPLE(bn)
  if $\mathbf{x}$ is consistent with $\mathbf{e}$ **then**
    $\mathbf{N}[x] \leftarrow \mathbf{N}[x]+1$ where x is the value of X in $\mathbf{x}$
return NORMALIZE($\mathbf{N}[X]$)

Just calls prior samping, but only counts cases that are consistent with the evidence.

Rejection Sampling: Example

Consider the Sprinkler Bayes net:



Estimate $P(Rain \mid Sprinkler = true)$ from 100 samples

- 73 have $Sprinkler = false$, therefore 73 are rejected
- Out of the remaining samples (27) with $Sprinkler = true$, **8** have $Rain = true$ and **19** have $Rain = false$
- The approximate distribution is $\hat{P}(Rain|Sprinkler = true) = \alpha < 8{,}19 >=< 0.296, 0.704 >$

Rejection Sampling: Summary

- Rejection sampling uses (conditional) probabilities to sample events, reject those that do not match the evidence, and calculate posterior probabilities.
- For unlikely events, may have to wait a long time to get enough matching samples.
- That can be inefficient.
- So, use alternative algorithms.

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- Approximate inference in Bayesian nets (BNs)
  - Rejection Sampling
  - **Likelihood Weighting**
  - Gibbs Sampling
- Data discretisation for learning discrete BNs
- Questions and answers related to assignment

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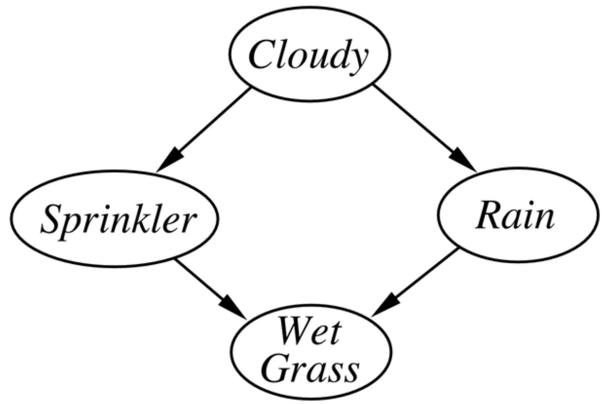
Likelihood Weighting: Example

Consider we have the Sprinkler network:

$P(C) = .5$



C	$P(S)$
t	.10
f	.50

C	$P(R)$
t	.80
f	.20

S	R	$P(W)$
t	t	.99
t	f	.90
f	t	.90
f	f	.01

Say we want to establish

$$P(Rain \mid Cloudy = true, WetGrass = true)$$

Likelihood Weighting: Example

- We pick a variable ordering as before, say: *Cloudy, Sprinkler, Rain, WetGrass*.
- Set the weight $w = 1$ and we start.
- Deal with each variable in order.

- $Cloudy$ is true, so:
  - $w = w * P(Cloudy = true) = 1 * 0.5 = 0.5$
- Event:
  - $[Cloudy = true, Sprinkler = ?, Rain = ?, WetGrass = ?]$

Likelihood Weighting: Example

- $Sprinkler$ is not an evidence variable, so we do not know whether it is true or false.
- Sample a value just as we did for prior sampling:
  - $P(Sprinkler|Cloudy = true) =< 0.1, 0.9 >$
- Let's assume this returns false.
- w remains the same.

Only update weights in the case of evidence variables.

- Event:
  - $[Cloudy = true, Sprinkler = false, Rain = ?, WetGrass = ?]$

Likelihood Weighting: Example

- $Rain$ is not an evidence variable, so we also do not know whether it is true or false.
- Sample a value just as we did for prior sampling:
  - $P(Rain|Cloudy = true) =< 0.8, 0.2 >$
- Let's assume this returns true.
- w remains the same.

- Event:
  - $[Cloudy = true, Sprinkler = false, Rain = true, WetGrass = ?]$

Likelihood Weighting: Example

- $WetGrass$ is an evidence variable, with value true, so we set:
  - $w = w * P(WetGrass = true | Sprinkler = false, Rain = true) = 0.5 * 0.90 = 0.45$

- Event:
  - $[Cloudy = true, Sprinkler = false, Rain = true, WetGrass = true]$

- So we end with the event [*true*, *false*, *true*, *true*] and weight $w = 0.45$.

Likelihood Weighting: Example

10 samples:

$Cloudy$	$Sprinkler$	$Rain$	$GrassWet$	w
$true$	$false$	$true$	$true$	0.45
$true$	$true$	$true$	$true$	0.475
$true$	$false$	$false$	$true$	0.05
$true$	$false$	$true$	$true$	0.45
$true$	$false$	$true$	$true$	0.45
$true$	$false$	$true$	$true$	0.45
$true$	$true$	$true$	$true$	0.475
$true$	$false$	$true$	$true$	0.45
$true$	$false$	$false$	$true$	0.05
$true$	$false$	$true$	$true$	0.45

To find $P(Rain = true | Cloudy = true, WetGrass = true)$ we add up the green-related weights and divide by the sum of all the weights.

Likelihood Weighting: Full Example

Query $P(R \mid c, g)$, assuming order [*Cloudy*, *Sprinkler*, *Rain*, *WetGrass*]

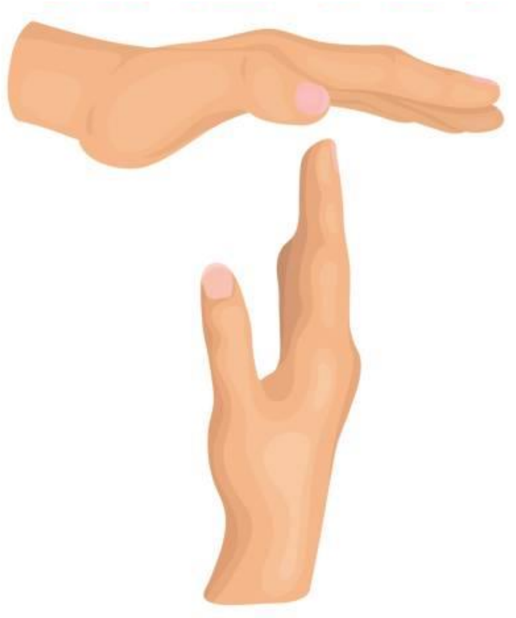
- $w \leftarrow 1$
- *Cloudy* is evidence, therefore $w = w \times P(c) = 1 \times 0.5 = 0.5$
- *Sprinkler* is not evidence, therefore sample from $P(S \mid c)$ − assume *false*
- *Rain* is not evidence, therefore sample from $P(R \mid c)$ − assume *true*
- *WetGrass* is evidence, therefore $w = w \times P(g \mid \neg s, r) = 0.5 \times 0.9 = 0.45$
- Return event $[true, false, true, true]$ with weight $w = 0.45$

Repeating that 10 times:

$$
\begin{aligned}
P(r|c,g) &= \frac{\sum_r w}{\sum w} \\
&= \frac{0.45 + 0.475 + 0.45 + 0.45 + 0.45 + 0.475 + 0.45 + 0.45}{0.45 + 0.475 + 0.05 + 0.45 + 0.45 + 0.45 + 0.475 + 0.45 + 0.05 + 0.45} \\
&= 0.9733
\end{aligned}
$$

$$
\begin{aligned}
P(\neg r|c,g) &= \frac{\sum_{\neg r} w}{\sum w} \\
&= \frac{0.05 + 0.05}{0.45 + 0.475 + 0.05 + 0.45 + 0.45 + 0.45 + 0.475 + 0.45 + 0.05 + 0.45} \\
&= 0.0267
\end{aligned}
$$

Break



Likelihood Weighting: Algorithm

function LIKELIHOOD-WEIGHTING($X, \mathbf{e}, bn, N$) **returns** an estimate of $P(X|\mathbf{e})$

local variables: $\mathbf{W}$, a vector of weighted counts over X, initially zero

for $j = 1$ to N **do**

$\mathbf{x}, w \leftarrow$ WEIGHTED-SAMPLE(bn)

$\mathbf{W}[x] \leftarrow \mathbf{W}[x] + w$ where x is the value of X in $\mathbf{x}$

return NORMALIZE($\mathbf{W}[X]$)

Adds in a new weight for a value of X.

Likelihood Weighting: Algorithm

function WEIGHTED-SAMPLE(bn, $\mathbf{e}$) **returns** an event and a weight

$\mathbf{x} \leftarrow$ an event with n elements; $w \leftarrow 1$
for i = 1 **to** n **do**
  if X_i has a value x_i in $\mathbf{e}$
    then $w \leftarrow w \times P(X_i = x_i \mid parents(X_i))$
   else $x_i \leftarrow$ a random sample from $\mathbf{P}(X_i \mid parents(X_i))$
return $\mathbf{x}$, w

Generates a new sample.

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  - **Gibbs Sampling**
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Acknowledgement: Content of slides adapted from Prof. Simon Parsons.

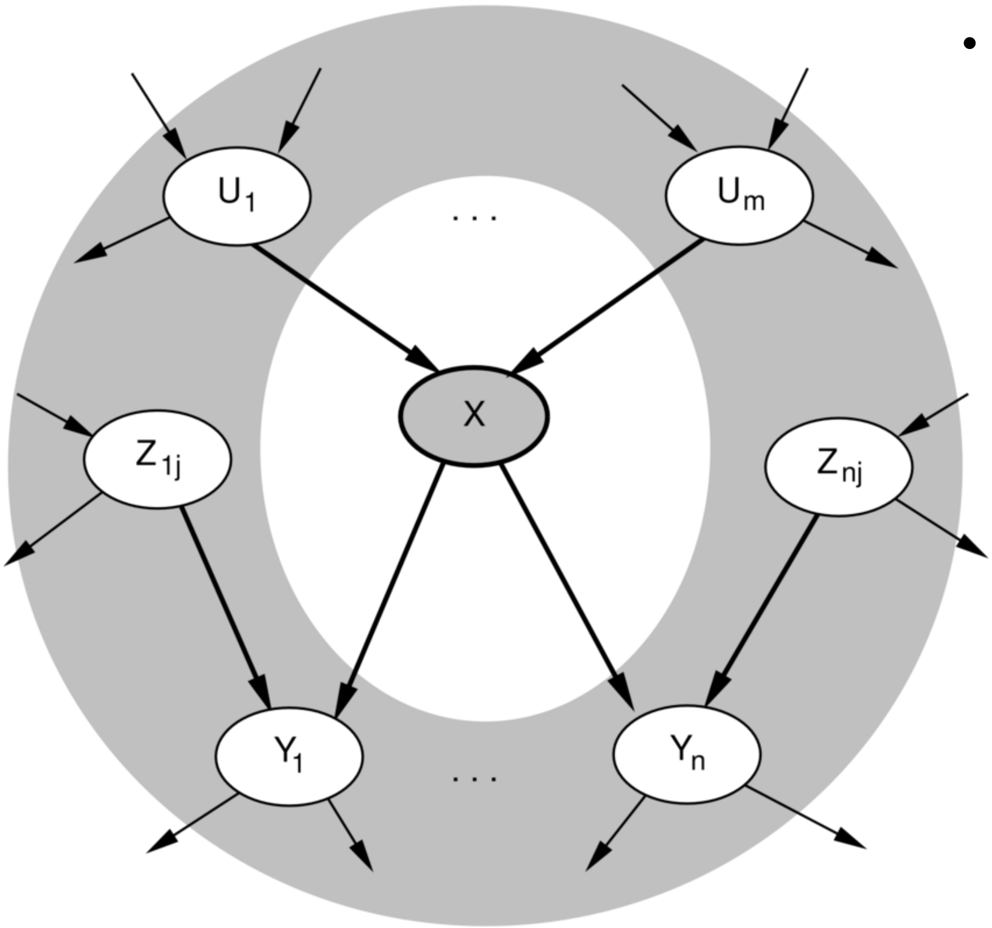
Gibbs Sampling

- A rather different approach to sampling.
- Part of the Markov Chain Monte Carlo (MCMC) family of algorithms.
- Idea: Don’t generate each sample from scratch.
- Generate samples by making a random change to the previous sample.

Gibbs Sampling

- Gibbs sampling starts with an arbitrary state.
- So, pick state with evidence variables fixed at observed values (if *Cloudy*=*true*, we pick that).
- Generate next state by randomly sampling from a non-evidence variable – but conditional on the current values of the Markov blanket.
- “The algorithm therefore wanders randomly around the state space . . . flipping one variable at a time, but keeping evidence variables fixed”.

Markov Blanket



- The Markov blanket of X is:
  - Its parents (U_i);
  - Its children (Y_i); and
  - Its children's (other) parents (Z_i).

Gibbs Sampling: Example

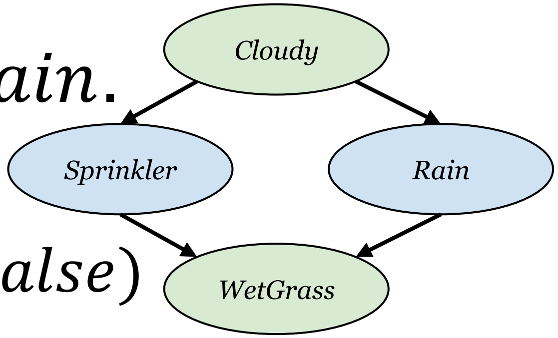
- Start with a query:
  - $P(Rain|Sprinkler = true, WetGrass = true)$
- Our initial state takes values of evidence variables:
  - $[Cloudy =?, Sprinkler = true, Rain =?, WetGrass = true]$

  and the other two are initialised randomly, e.g.:
  - $[Cloudy = true, Sprinkler = true, Rain = false, WetGrass = true]$
- Now we can start the main sampling process.

Gibbs Sampling: Example

- First we sample $Cloudy$ given the current state of its Markov blanket.

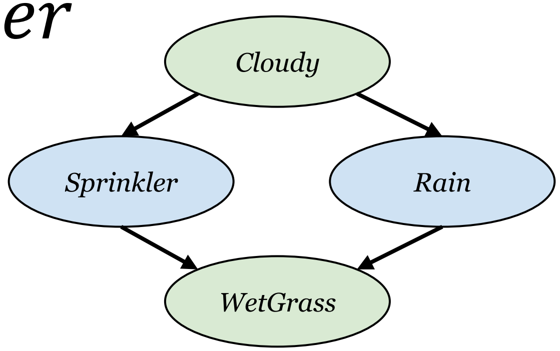
- Markov blanket is $Sprinkler$ and $Rain$.
- So, sample from:
  - $P(Cloudy|Sprinkler = true, Rain = false)$



- Suppose we get $Cloudy = false$, then the new state is:
  - $[Cloudy = false, Sprinkler = true, Rain = false, WetGrass = true]$

Gibbs Sampling: Example

- Next we sample $Rain$ given its Markov blanket.
- Markov blanket is $Cloudy$, $Sprinkler$ and $WetGrass$
- So, sample from:
  - $P(Rain|Cloudy = false, Sprinkler = true, WetGrass = false)$



- Suppose we get $Rain = true$, then new state is:
  - $[Cloudy = false, Sprinkler = true, Rain = true, WetGrass = true]$
- Then repeat the sampling.

Gibbs Sampling: Example

- Each state visited during this process contributes to our estimate for:
  - $P(Cloudy|Sprinkler = true, WetGrass = true)$
- Say the process visits 80 states:
  - In 20, $Cloudy = true$
  - In 60, $Cloudy = false$
- Then
  - $P(Cloudy|Sprinkler = true, WetGrass = true)$
  - $= Normalise(< 20,60 >)$
  - $=< 0.25,0.75 >$

Gibbs Sampling: Algorithm

function GIBBS-ASK(X, **e**, bn, N) **returns** an estimate of $P(X|\mathbf{e})$
local variables: $\mathbf{N}[X]$, a vector of counts over X, initially zero
$\mathbf{Z}$, the nonevidence variables in bn
$\mathbf{x}$, the current state of the network, initially copied from **e**

initialize $\mathbf{x}$ with random values for the variables in $\mathbf{Z}$
for $j = 1$ to N **do**
  for each Z_i in $\mathbf{Z}$ **do**
    sample the value of Z_i in $\mathbf{x}$ from $\mathbf{P}(Z_i|mb(Z_i))$
      given the values of $MB(Z_i)$ in $\mathbf{x}$
    $\mathbf{N}[x] \leftarrow \mathbf{N}[x] + 1$ where x is the value of X in $\mathbf{x}$
return NORMALIZE($\mathbf{N}[X]$)

Gibbs Sampling: Markov Blanket

- All of this begs the question: "***How do we sample a variable given the state of its Markov blanket?***"

- For a value x of a variable X:

$$P(X|mb(X)) = \alpha P(X|parents(X)) \prod_{Y \in Children(X)} P(Y|parents(Y))$$

  where $mb(X)$ is the Markov blanket of X.

- Given $P(X|mb(X))$, we can sample from it just as we have before.

Gibbs Sampling: Markov Blanket

- Given $P(X|mb(X))$, we can sample from it just as we have before.

- For the sprinker example, consider we want to compute:
  - $P(Cloudy|Sprinkler = true, Rain = false)$

- Then we need:

$$P(X|mb(X)) = \alpha P(X|parents(X)) \prod_{Y \in Children(X)} P(Y|parents(Y))$$

$$P(C|mb(C)) = \alpha P(C|parents(C)) \prod_{Y \in Children(C)} P(Y|parents(Y))$$

Gibbs Sampling: Markov Blanket

- Which gives us:

$$P(C|mb(C)) = \alpha P(C|parents(C)) \prod_{Y \in Children(C)} P(Y|parents(Y))$$

$$= \alpha P(C)P(s|C)P(\neg r|C)$$

$$= \alpha < 0.5, 0.5 >< 0.1, 0.5 >< 0.2, 0.8 >$$

$$= \alpha < 0.5 * 0.1 * 0.2, 0.5 * 0.5 * 0.8 >$$

$$= \alpha < 0.01, 0.2 >$$

$$=< 0.048, 0.952 >$$

- And then we sample as normal.

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- **Data discretisation for learning discrete BNs**

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How to train discrete Bayes Nets with Continuous Random Variables?

1. Manual discretisation of continuous data—to be able to use the methods discussed so far.
   – Age (years/days/minutes): young, middle aged, old
   – Temperature: very cold, cold, mild, hot, very hot

2. Split continuous data into uniform intervals (e.g., 1, 2, 3,… intervals between $\min$ & $\max$).

3. Jointly discretising data and performing structure learning (*bnlearn* implements this*).

* Chen, Y., et al. "Learning Discrete Bayesian Networks from Continuous Data", JAIR, 2017

API for Data Discretisation

bnlearn.discretize(data, edges, continuous_columns, max_iterations, verbose**)**

Example code snippet (using cardiovascular_data):

```
data = pd.read_csv(TRAINING_DATA, encoding='latin')
edges = [('target', 'ï»¿age'),('target', 'gender'),('target', 'height'),('target', 'weight'),('target', 'ap_hi'),('target', 'ap_lo'),('target', 'cholesterol'),('target', 'gluc'),('target', 'smoke'),('target', 'alco'),('target', 'active')]
continuous_columns = ["ï»¿age", "height", "weight", "ap_hi", "ap_lo"]
df_discrete = bn.discretize(data, edges, continuous_columns, max_iterations=1, verbose=3)
```

Data Discretisation: Example Output

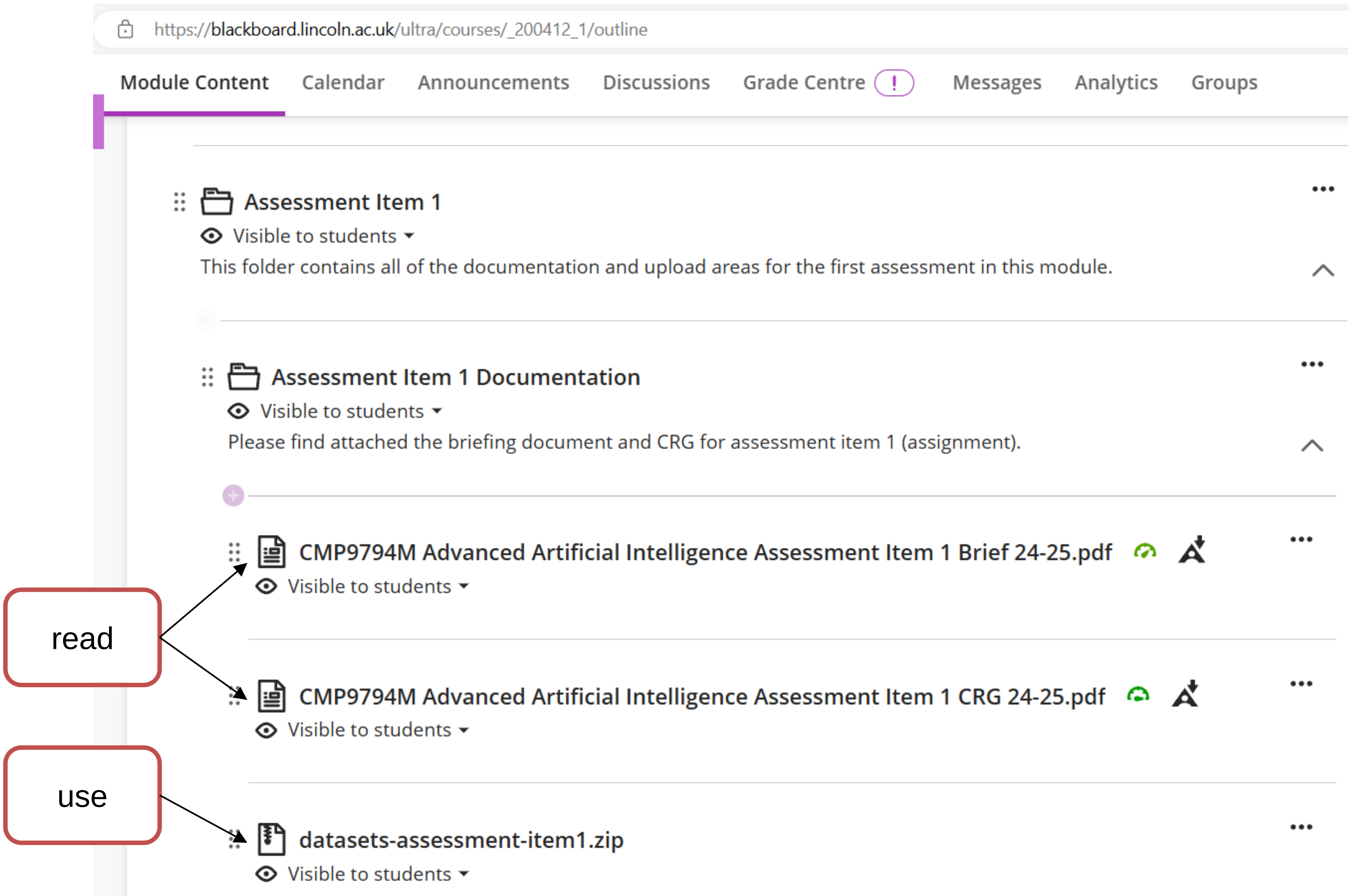
```
(env_bnlearn) C:\Lincoln\slides\CMP9794M-2024-25\aai-workshop-w4>python bnlearn_DataDiscretisation.py
DATA:
      ï»¿age  gender  height  weight  ap_hi  ap_lo  cholesterol  gluc  smoke  alco  active  target
0     17623       2     169      82    150    100            1     1      0     0       1       1
1     17474       1     156      56    100     60            1     1      0     0       0       0
2     14791       2     165      60    120     80            1     1      0     0       0       0
3     17482       1     154      68    100     70            1     1      0     0       0       0
4     21413       1     157      69    130     80            1     1      0     0       1       0
..      ...     ...     ...     ...    ...    ...          ...   ...    ...   ...     ...     ...
495   21111       1     160      71    140     90            1     2      0     0       1       0
496   19655       1     168      82    120     90            1     1      0     0       1       0
497   19594       2     174      54    120     80            2     2      1     0       1       0
498   19711       1     162     100    120     80            3     1      0     0       1       1
499   21242       2     168      79    130     90            1     1      0     0       1       0

[500 rows x 12 columns]
[bnlearn] >Discretizer for continuous values. Iteration [0].
                 ï»¿age  gender           height          weight                            ap_hi           ap_lo  cholest
0    (14213.54, 19994.0]       2  (140.45, 190.0]  (79.5, 151.5]                    (138.5, 563.0]  (88.5, 575.0]
1    (14213.54, 19994.0]       1  (140.45, 190.0]  (41.74, 79.5]  (2.0499999999999, 138.5]  (-11.0, 88.5]
2    (14213.54, 19994.0]       2  (140.45, 190.0]  (41.74, 79.5]  (2.0499999999999, 138.5]  (-11.0, 88.5]
3    (14213.54, 19994.0]       1  (140.45, 190.0]  (41.74, 79.5]  (2.0499999999999, 138.5]  (-11.0, 88.5]
4     (19994.0, 23653.0]       1  (140.45, 190.0]  (41.74, 79.5]  (2.0499999999999, 138.5]  (-11.0, 88.5]
..                   ...     ...              ...            ...                       ...            ...
495   (19994.0, 23653.0]       1  (140.45, 190.0]  (41.74, 79.5]            (138.5, 563.0]  (88.5, 575.0]
496  (14213.54, 19994.0]       1  (140.45, 190.0]  (79.5, 151.5]  (2.0499999999999, 138.5]  (88.5, 575.0]
497  (14213.54, 19994.0]       2  (140.45, 190.0]  (41.74, 79.5]  (2.0499999999999, 138.5]  (-11.0, 88.5]
498  (14213.54, 19994.0]       1  (140.45, 190.0]  (79.5, 151.5]  (2.0499999999999, 138.5]  (-11.0, 88.5]
499   (19994.0, 23653.0]       2  (140.45, 190.0]  (41.74, 79.5]  (2.0499999999999, 138.5]  (88.5, 575.0]
```

Those outputs can be used by `CPT_Generator.py`, `BayesNetInference.py`, and `ModelEvaluator.py`

Today

- Inference by stochastic simulation
- Approximate inference in Bayesian nets (BNs)
  - Rejection Sampling
  - Likelihood Weighting
  - Gibbs Sampling
- Data discretisation for learning discrete BNs
- **Questions and answers related to assignment**

Assessment Item 1: Assignment



First 4 Weeks of this Semester

We have asked and answered the following when training and evaluating Bayesian Networks (BNs):

1. Where do the probabilities come from?

   A: Usually from training data (MLE, not the only one)

2. Where does the structure come from?

   A: Prior knowledge or structure learning (preferred)

3. How to do probabilistic inference?

   A: Inference by enumeration, variable elimination, rejection sampling, likelihood weighting, Gibbs sampling

4. What code to use for training/evaluating BNs?

   A: Module's code and bnlearn code – you've got both.

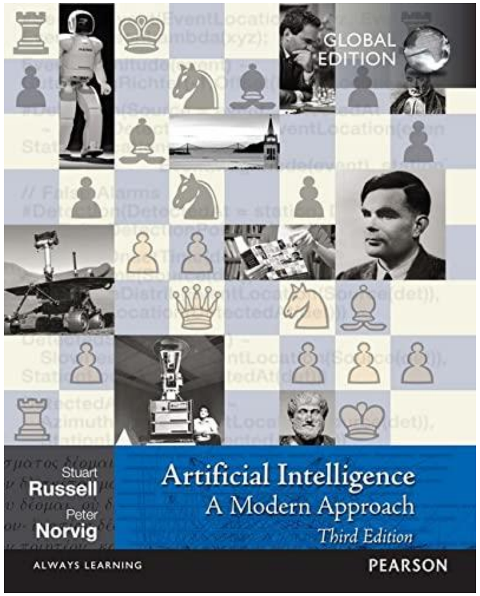
Today

- Approximate inference should be used if exact inference becomes unfeasible/impractical.

- We looked at algorithms for approximate inference in Bayes nets—based on sampling.
  - Rejection sampling
  - Likelihood weighting
  - Gibbs sampling

Readings:

Russell & Norvig 2016. [Chapter 14.5]



This and Next Week

Workshop (today):
Code for approximate probabilistic inference via Rejection Sampling, Gibbs Sampling, etc.

Lecture (next week):
Gaussian Bayesian Networks
Reading 1: Koller & Friedman 2009. Section 7.2
Reading 2: Bishop. C. 2006. Section 8.1.4

Any other questions?