Access Code: 280562

#### 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

- Basic idea:
  - Draw N samples from a sampling distribution S
  - Compute an approximate posterior probability  $\widehat{P}$
  - $\hat{P}$  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.

- 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.

- Overall process:
  - The 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.

- 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.

#### Probabilistic Sampling: Example

• Consider random variable C with domain values {red, green, blue} and probability distribution: P(C = red) = 0.6, P(C = green) = 0.1, P(C = blue) = 0.3

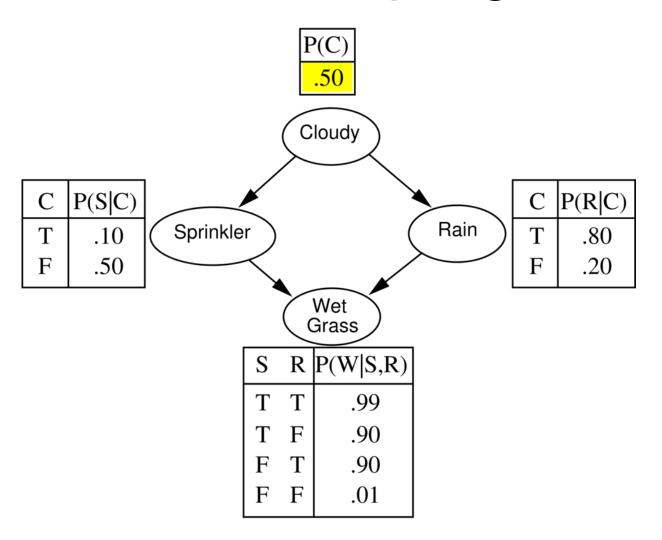
Generating 8 random numbers looks like:

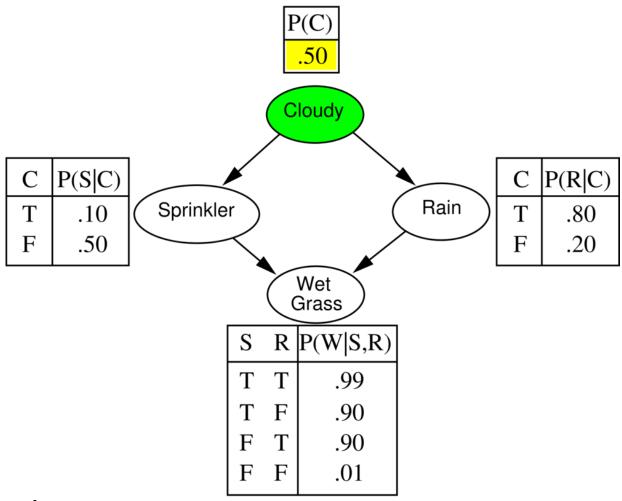


• That gives the following:  $P(C) = <\frac{5}{8}, \frac{1}{8}, \frac{2}{8} >$ 

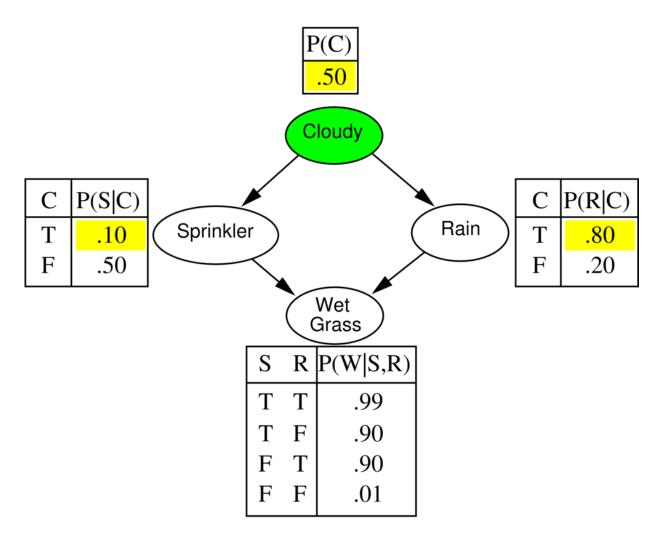
#### Today

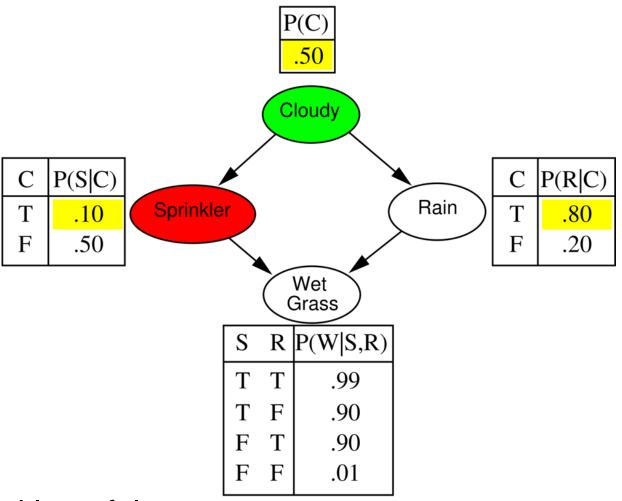
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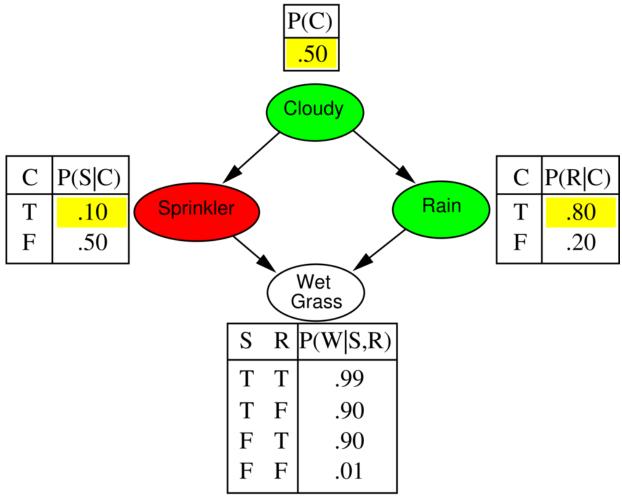


Cloudy = true

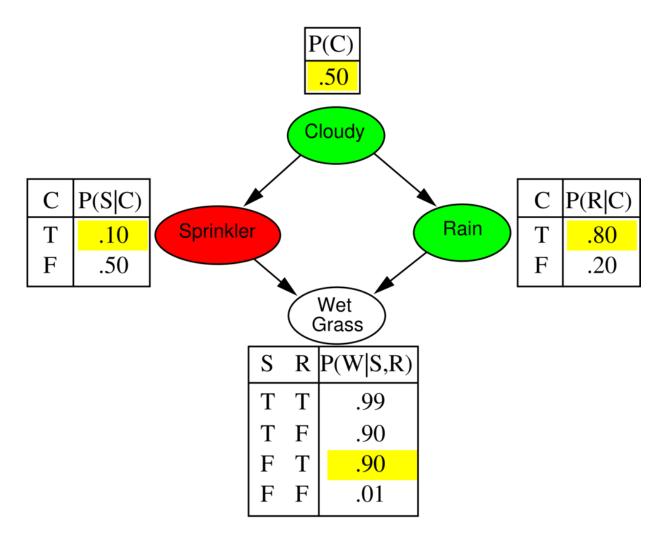


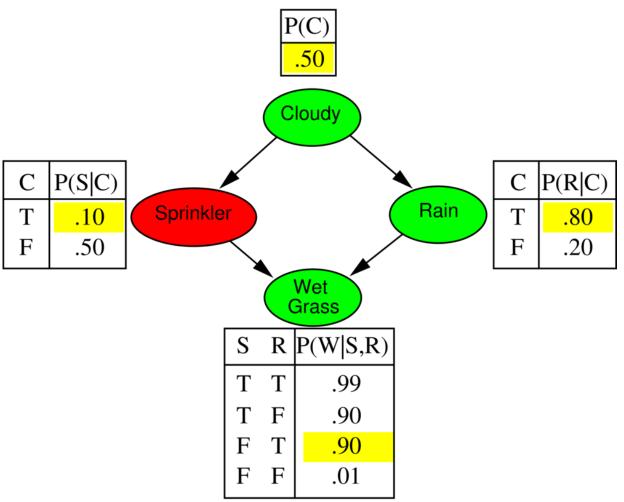


Sprinkler = false



Rain = true





WetGrass = true

- 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, 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 x
   return x
```

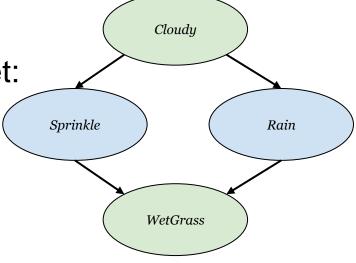
#### Rejection Sampling: Algorithm

```
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 \mathsf{Prior}\text{-Sample}(bn)
if \mathbf{x} is consistent with \mathbf{e} then
\mathbf{N}[x] \leftarrow \mathbf{N}[x]\text{+1} \text{ where } x \text{ is the value of } X \text{ in } \mathbf{x}
return \mathsf{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 | Sprinkler = true) from N=100

- 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

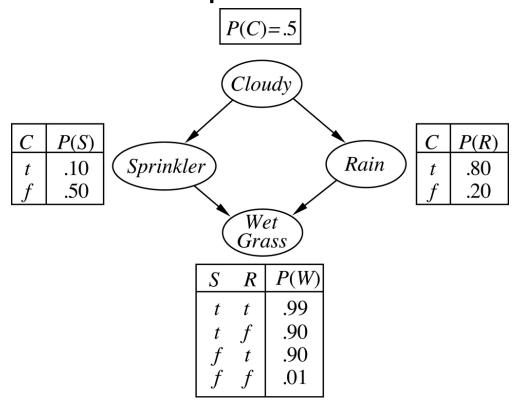
- Rejection sampling uses (conditional) probabilities to sample events, reject those that do not match the evidence, and calculate posterior probabilities.
- For unlikely events, may have to wait a long time to get enough matching samples.
- That can be inefficient.

If that's the case, use alternative algorithms.

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  - Rejection Sampling
  - Likelihood Weighting
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Consider we have the Sprinkler network:



Say we want to establish

P(Rain|Cloudy = true, WetGrass = true)

- 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 =?]

- 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 =?]

- 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 =?]

- 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 up with event [true, false, true, true] and weight w = 0.45.

#### 10 sampled events:

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.

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

- w ← 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, thus  $w = w \times P(wg \mid \neg s, r) = 0.5 \times 0.9 = 0.45$
- Return event [true, false, true, true] with weight w = 0.45

#### Repeating that 10 times:

= 0.0267

$$P(r|c,g) = \frac{\sum_{r} w}{\sum w}$$

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

## 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 \mathsf{Weighted}\text{-Sample}(bn)
\mathbf{W}[x] \leftarrow \mathbf{W}[x] + w where x is the value of X in \mathbf{x} return \mathsf{Normalize}(\mathbf{W}[X])
```

Adds in a new weight for a value of *X*.

## Likelihood Weighting: Algorithm

**function** Weighted-Sample(bn, 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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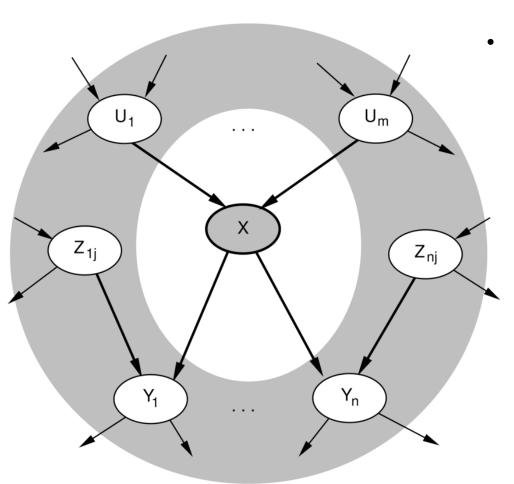
## Gibbs Sampling

- 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 . . . <u>flipping one variable</u> 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  $(Z_i)$ .

- 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.

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

Cloudy

Rain

Sprinkler

- 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]

Next we sample Rain given its Markov blanket.

Cloudy

WetGrass

Rain

Sprinkler

 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.

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

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

- 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:

$$P(C|mb(C)) = \alpha P(C|parents(C)) \qquad P(Y|parents(Y))$$

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

$$= \alpha < P(c), P(\neg c) > \langle P(s|c), P(s|\neg c) > \langle P(\neg r|c), P(\neg r|\neg c) > \rangle$$

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

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

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

$$= \langle 0.048, 0.952 >$$

And then we sample as normal.

### Ideas for your Assignment (optional)

- Implement the Likelihood Weighting algorithm (by extending BayesNetInference.py)
- Implement the Gibbs Sampling algorithm in the code of today's workshop (by extending BayesNetInference.py and related files)

...

But give priority to solving the assignment task first using the code provided during the workshops. Once you have done that, think about implementing your own algs.

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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
- Split continuous data into uniform intervals (e.g., 1, 2, 3,... intervals between min & max).
- Data discretisation using bnlearn\*.

<sup>\*</sup> 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', '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 = ["age", "height", "weight", "ap_hi",
  "ap_lo"]
  df_discrete = bn.discretize(data, edges, continuous_columns,
  max_iterations=1, verbose=3)
```

### Data Discretisation: Example Output

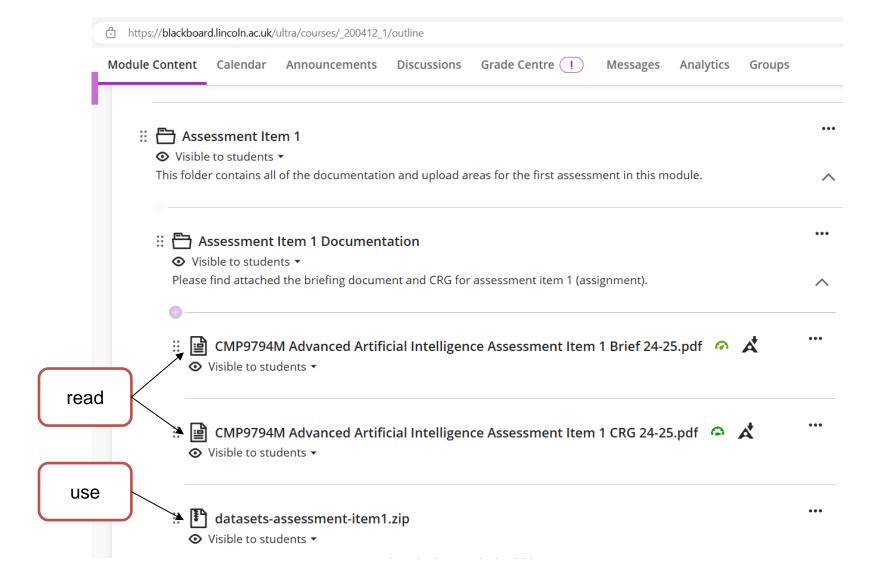
```
(env bnlearn) C:\Lincoln\slides\CMP9794M-2024-25\aai-workshop-w4>python bnlearn DataDiscretisation.py
DATA:
                    height weight ap hi ap lo cholesterol gluc smoke alco active target
             gender
     17623
                                82
                                      150
                       169
                 2
                                             100
                                                            1
                                                                  1
                                                                                       1
     17474
                 1
                       156
                                 56
                                      100
                                              60
                                                                  1
                                                                                       0
                                                                                               0
     14791
                       165
                                      120
                                                                  1
                                                                                               0
     17482
                       154
                                68
                                      100
                                              70
                                                                                       0
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                                                                  1
     21413
                 1
                       157
                                      130
                                              80
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495
                                                                  2
     21111
                 1
                       160
                                71
                                      140
                                              90
                                                                                       1
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496
                                                                  1
                                                                                       1
     19655
                       168
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497
     19594
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498
     19711
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[500 rows x 12 columns]
[bnlearn] >Discretizer for continuous values. Iteration [0].
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    (14213.54, 19994.0]
                              1 (140.45, 190.0] (41.74, 79.5]
                                                                 (2.0499999999999, 138.5]
                                                                                             (-11.0, 88.5]
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                              1 (140.45, 190.0] (79.5, 151.5]
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497
    (14213.54, 19994.0]
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                                                                                             (-11.0, 88.5]
     (19994.0, 23653.0]
                              2 (140.45, 190.0] (41.74, 79.5]
                                                                 (2.04999999999999, 138.5]
                                                                                             (88.5, 575.0]
```

Those outputs can be used by CPT\_Generator.py,
BayesNetInference.py, and ModelEvaluator.py

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# 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.

## Workshop Materials in Github

#### https://github.com/LCAS/CMP9794M

#### **Usage**:

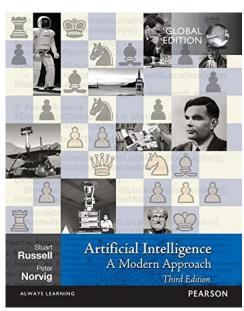
- 1. Open a terminal and change directory to the path where you want to download the repository.
- 2. Terminal prompt> git clone https://github.com/LCAS/CMP9794M
- 3. Open VS Code and you should see the workshop folders, one per week.
- 4. Run the code as done in the workshop sessions.

### 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?