CS 3750 Advanced Machine Learning
Lecture 12

Learning Bayesian belief networks

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Administration

Midterm projects:

- Will be given out on Wednesday, October 8, 2003
- **Due on November 3, 2003**
- **Group project:** 2 groups of 2, 1 group of 3 people

Learning probability distribution

Basic settings:

- A set of random variables $\mathbf{X} = \{X_1, X_2, \ldots, X_n\}$
- **A model of the distribution** over variables in $\boldsymbol{X}$ with parameters Θ
- **Data** $D = \{D_1, D_2, .., D_N\}$

Objective: find parameters $\hat{\Theta}$ that describe the observed data the best

Learning Bayesian belief networks:

– parameterizations as defined by the structure of network

Learning of BBN

Learning.

- **Learning of parameters of conditional probabilities**
- **Learning of the network structure**

Variables:

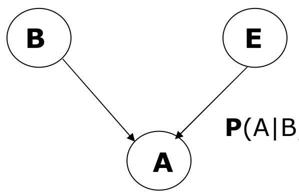
- **Observable** – values present in every data sample
- **Hidden** – they values are never observed in data
- **Missing values** – values sometimes present, sometimes not

Next: All variables are observable

1. Learning of parameters of BBN
2. Learning of the model (BBN structure)

Learning of parameters of BBN

- **Idea:** decompose the estimation problem for the full joint over a large number of variables to a set of smaller estimation problems corresponding to parent-variable conditionals.
- **Example:** Assume A,E,B are binary with *True, False* values



P(A|B,E)

4 estimation problems

- **P**(A|B=T,E=T)
- **P**(A|B=T,E=F)
- **P**(A|B=F,E=T)
- **P**(A|B=F,E=F)

- **Assumption that enables the decomposition:** parameters of conditional distributions are independent

Estimates of parameters of BBN

- Two assumptions that permit the decomposition:
  - **Sample independence**

$$P(D \mid \mathbf{\Theta}, \xi) = \prod_{u=1}^{N} P(D_u \mid \mathbf{\Theta}, \xi)$$

  - **Parameter independence**

$$p(\mathbf{\Theta} \mid D, \xi) = \prod_{i=1}^{n} \prod_{j=1}^{q_i} p(\theta_{ij} \mid D, \xi)$$

Parameters of each conditional (one for every assignment of values to parent variables) can be learned independently

Learning of BBN parameters. Example.

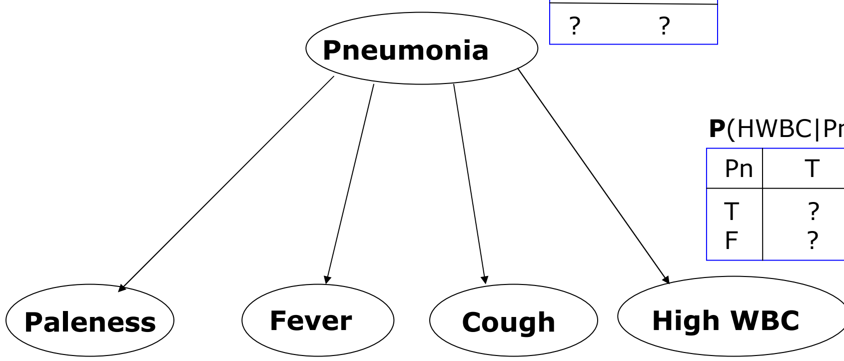
Example:

P(Pneumonia)

T	**F**
?	?

P(HWBC|Pneum)

Pn	T	F
T	?	?
F	?	?

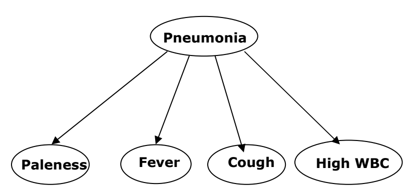


P(Palen|Pneum)	**P**(Fever|Pneum)	**P**(Cough|Pneum)
?	?	?

Learning of BBN parameters. Example.

Data D (different patient cases):

Pal	Fev	Cou	HWB	Pneu
T	T	T	T	F
T	F	F	F	F
F	F	T	T	T
F	F	T	F	T
F	T	T	T	T
T	F	T	F	F
F	F	F	F	F
T	T	F	F	F
T	T	T	T	T
F	T	F	T	T
T	F	F	T	F
F	T	F	F	F



Estimates of parameters of BBN

- Much like multiple **coin toss or roll of a dice** problems.
- A "smaller" learning problem corresponds to the learning of exactly one conditional distribution
- **Example:**

$$\mathbf{P}(Fever \mid Pneumonia = T)$$

- **Problem:** How to pick the data to learn?

Estimates of parameters of BBN

Much like multiple **coin toss or roll of a dice** problems.

- A "smaller" learning problem corresponds to the learning of exactly one conditional distribution

Example:

$$\mathbf{P}(Fever \mid Pneumonia = T)$$

Problem: How to pick the data to learn?

Answer:

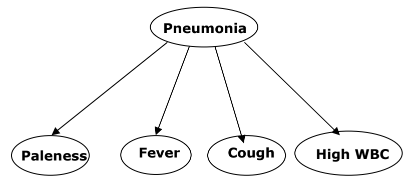
1. Select data points with Pneumonia=T (ignore the rest)
2. Focus on (select) only values of the random variable defining the distribution (Fever)
3. Learn the parameters of the conditional the same way as we learned the parameters of the biased coin or dice

Learning of BBN parameters. Example.

Learn: $\mathbf{P}(Fever \mid Pneumonia = T)$

Step 1: Select data points with Pneumonia=T

Pal	Fev	Cou	HWB	Pneu
T	T	T	T	F
T	F	F	F	F
F	F	T	T	T
F	F	T	F	T
F	T	T	T	T
T	F	T	F	F
F	F	F	F	F
T	T	F	F	F
T	T	T	T	T
F	T	F	T	T
T	F	F	T	F
F	T	F	F	F

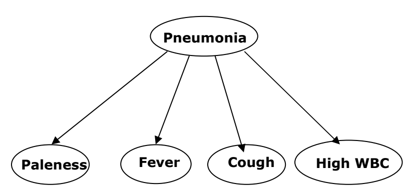


Learning of BBN parameters. Example.

Learn: $\mathbf{P}(Fever \mid Pneumonia = T)$

Step 1: Ignore the rest

Pal	Fev	Cou	HWB	Pneu
F	F	T	T	T
F	F	T	F	T
F	T	T	T	T
T	T	T	T	T
F	T	F	T	T

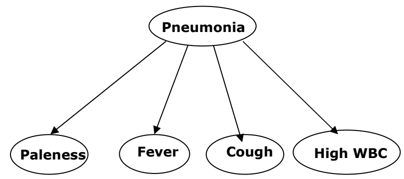


Learning of BBN parameters. Example.

Learn: $\mathbf{P}(Fever \mid Pneumonia = T)$

Step 2: Select values of the random variable defining the distribution of Fever

Pal	Fev	Cou	HWB	Pneu
F	F	T	T	T
F	F	T	F	T
F	T	T	T	T
T	T	T	T	T
F	T	F	T	T

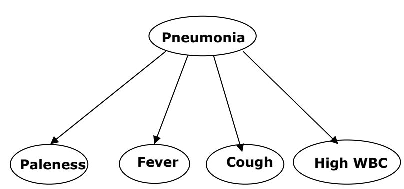


Learning of BBN parameters. Example.

Learn: $\mathbf{P}(Fever \mid Pneumonia = T)$

Step 2: Ignore the rest

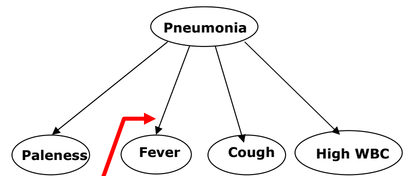
Fev
F
F
T
T
T



Learning of BBN parameters. Example.

Learn: $\mathbf{P}(Fever \mid Pneumonia = T)$

Step 3a: Learning the ML estimate



Fev
F
F
T
T
T

$\mathbf{P}(Fever \mid Pneumonia = T)$

T	F
0.6	0.4

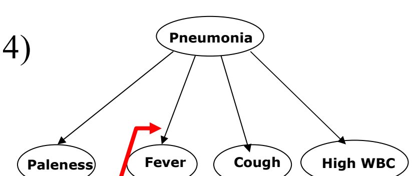
Learning of BBN parameters. Bayesian learning.

Learn: $\mathbf{P}(Fever \mid Pneumonia = T)$

Step 3b: Learning the Bayesian estimate

Assume the prior

$$\theta_{Fever|Pneumonia=T} \sim Beta(3,4)$$

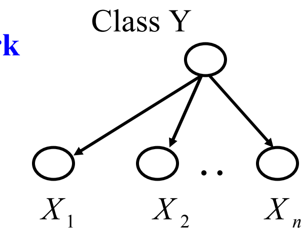


Fev
F
F
T
T
T

Posterior:

$$\theta_{Fever|Pneumonia=T} \sim Beta(6,6)$$

Naïve Bayes model



A **special (simple) Bayesian belief network**

- **used as a generative classifier model**
  - Class variable Y
  - Attributes are independent given Y

$$p(\mathbf{x} \mid Y = i, \mathbf{\Theta}) = \prod_{j=1}^{n} p(x_j \mid Y = i, \Theta_{ij})$$

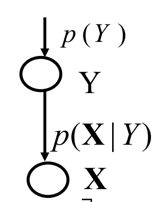
Learning: ML, Bayesian estimates of parameters

Classification: given x we need to determine the class

- Choose the class with the maximum posterior

$$p(Y = i \mid \mathbf{x}, \mathbf{\Theta}) = \frac{p(Y = i \mid \mathbf{\Theta}) p(\mathbf{x} \mid Y = i, \mathbf{\Theta})}{\sum_{j=1}^{k} p(Y = j \mid \mathbf{\Theta}) p(\mathbf{x} \mid Y = j, \mathbf{\Theta})}$$

Naïve Bayes with Gaussians distributions



Generative classification model $p(\mathbf{X}, Y)$

1. Priors on classes

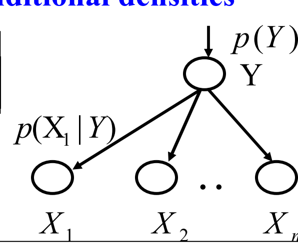
$p(Y = 1), \; p(Y = 2), \; p(Y = 3), \ldots$

Before: Joint class conditional densities (for x)

$$p(\mathbf{x} \mid \boldsymbol{\mu}_j, \mathbf{\Sigma}_j) = \frac{1}{(2\pi)^{d/2} |\mathbf{\Sigma}_j|^{1/2}} \exp\left[-\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu}_j)^T \mathbf{\Sigma}_j^{-1} (\mathbf{x} - \boldsymbol{\mu}_j) \right]$$

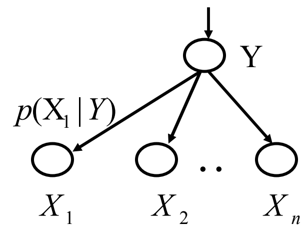
Now: Naïve Bayes - independent class conditional densities

$$p(x_i \mid \mu_{ji}, \sigma_{ji}) = \frac{1}{\sqrt{(2\pi)}\sigma_{ji}} \exp\left[-\frac{1}{2\sigma_{ji}^2} (x_i - \mu_{ji})^2 \right]$$



Naïve Bayes with Gaussians distributions

How to learn the generative model $p(\mathbf{X}, Y)$



1. **Priors on classes**

   $p(Y=1),\ p(Y=2),\ p(Y=3),\ldots$

   ?

2. **Class conditional densities**

$$p(x_i \mid \mu_{ji}, \sigma_{ji}) = \frac{1}{\sqrt{(2\pi)}\sigma_{ji}} \exp\left[-\frac{1}{2\sigma_{ji}^{2}} (x_i - \mu_{ji})^2 \right]$$

Model selection

- **BBN has two components**:
  - **Structure of the network** (models conditional independences)
  - **A set of parameters** (conditional child-parent distributions)

We already know how to learn the parameters for the fixed structure

But how to learn the structure of the BBN?

Assumption:

- All variables are observable in the dataset

Learning the structure

Criteria we can choose to score the structure S

- **Marginal likelihood**

  maximize $P(D \mid S, \xi)$

  ξ - represents the prior knowledge

- **Posterior probability**

  maximize $P(S \mid D, \xi)$

$$P(S \mid D, \xi) = \frac{P(D \mid S, \xi) P(S \mid \xi)}{P(D \mid \xi)}$$

How to compute marginal likelihood $P(D \mid S, \xi)$?

Learning of BBNs

- **Notation**:
  - i ranges over all possible variables $i=1,..,n$
  - $j=1,..,q$ ranges over all possible parent combinations
  - $k=1,..,r$ ranges over all possible variable values
  - $\boldsymbol{\Theta}$ - parameters of the BBN

  θ_{ij} is a vector of θ_{ijk} representing parameters of the conditional probability distribution; such that $\sum_{k=1}^{r} \theta_{ijk} = 1$

  N_{ijk} - a number of instances in the dataset where parents of variable X_i take on values j and X_i has value k

  $N_{ij} = \sum_{k=1}^{r} N_{ijk}$

  α_{ijk} - prior counts (parameters of Beta or Dirichlet priors)

  $\alpha_{ij} = \sum_{k=1}^{r} \alpha_{ijk}$

Marginal likelihood

- Integrate over all possible parameter settings

$$P(D \mid S,\xi) = \int_{\Theta} P(D \mid S,\Theta,\xi)\, p(\Theta \mid S,\xi)\, d\Theta$$

- Using the assumption of parameter and sample independence

$$P(D \mid S,\xi) = \prod_{i=1}^{n} \prod_{j=1}^{q_i} \frac{\Gamma(\alpha_{ij})}{\Gamma(\alpha_{ij} + N_{ij})} \prod_{k=1}^{r_i} \frac{\Gamma(\alpha_{ijk} + N_{ijk})}{\Gamma(\alpha_{ijk})}$$

- We can use **log-likelihood score** instead

$$\log P(D \mid S,\xi) = \sum_{i=1}^{n} \left\{ \sum_{j=1}^{q_i} \log \frac{\Gamma(\alpha_{ij})}{\Gamma(\alpha_{ij} + N_{ij})} + \sum_{k=1}^{r_i} \log \frac{\Gamma(\alpha_{ijk} + N_{ijk})}{\Gamma(\alpha_{ijk})} \right\}$$

Score is decomposable along variables !!!

Trick to compute the marginal likelihood

- Integrate over all possible parameter settings

$$P(D \mid S,\xi) = \int_{\Theta} P(D \mid S,\Theta,\xi)\, p(\Theta \mid S,\xi)\, d\Theta$$

- Posterior of parameters, given data and the structure

$$p(\mathbf{\Theta} \mid D,S,\xi) = \frac{P(D \mid \mathbf{\Theta},S,\xi)\, p(\mathbf{\Theta} \mid S,\xi)}{P(D \mid S,\xi)}$$

Trick

$$P(D \mid S,\xi) = \frac{P(D \mid \mathbf{\Theta},S,\xi)\, p(\mathbf{\Theta} \mid S,\xi)}{p(\mathbf{\Theta} \mid D,S,\xi)}$$

- Gives the solution

$$P(D \mid S,\xi) = \prod_{i=1}^{n} \prod_{j=1}^{q_i} \frac{\Gamma(\alpha_{ij})}{\Gamma(\alpha_{ij} + N_{ij})} \prod_{k=1}^{r_i} \frac{\Gamma(\alpha_{ijk} + N_{ijk})}{\Gamma(\alpha_{ijk})}$$

Learning the structure

Likelihood of data for the BBN (structure and parameters)

$$P(D \mid S, \Theta, \xi)$$

- **measures the goodness of fit of the BBN to data**

Marginal likelihood (for the structure only !!!!)

$$P(D \mid S, \xi)$$

- **Measures more than the goodness of fit.** The score is:
  - different for structures of different complexity
  - Incorporates preferences towards simpler structures, **implements Occam's razor** !!!!

Occam's Razor

- Why there is a preference towards simpler structures ?

Rewrite marginal likelihood as

$$P(D \mid S, \xi) = \frac{\int_{\Theta} P(D \mid S, \Theta, \xi)\, p(\Theta \mid S, \xi)\, d\Theta}{\int_{\Theta} p(\Theta \mid S, \xi)\, d\Theta}$$

We know that $\int_{\Theta} p(\Theta \mid S, \xi)\, d\Theta = 1$

Interpretation: in more complex structures there are more ways how parameters can be set badly
- **The numerator:** count of good assignments
- **The denominator:** count of all assignments

Approximations of probabilistic scores

Approximations of the marginal likelihood and posterior scores

- **Information based measures**
  – Akaike criterion
  – Bayesian information criterion (BIC)
  – Minimum description length (MDL)
- Reflect the tradeoff between the fit to data and preference towards simpler structures

Example: **Akaike criterion.**

Maximize: $score(S) = \log P(D \mid S, \Theta_{ML}, \xi) - \text{compl(S)}$

Bayesian information criterion (BIC)

Maximize:

$$score(S) = \log P(D \mid S, \Theta_{ML}, \xi) - \frac{1}{2}\text{compl(S) logN}$$

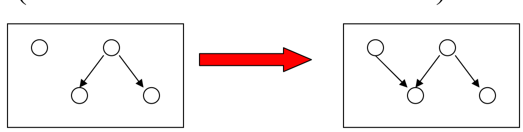
Optimizing the structure

Finding the best structure is an instance of a **combinatorial optimization** problem

- A good feature: the score **is decomposable along variables**:

$$\log P(D \mid S, \xi) = \sum_{i=1}^{n} \left\{ \sum_{j=1}^{q_i} \log \frac{\Gamma(\alpha_{ij})}{\Gamma(\alpha_{ij} + N_{ij})} + \sum_{k=1}^{r_i} \log \frac{\Gamma(\alpha_{ijk} + N_{ijk})}{\Gamma(\alpha_{ijk})} \right\}$$

Algorithm idea: Search the space of structures using local changes (additions and deletions of a link)

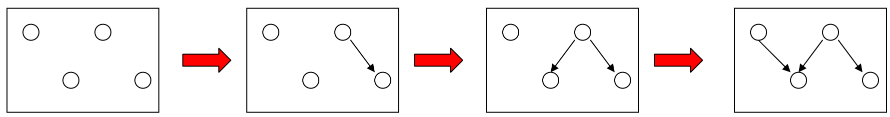


Advantage:

– we do not have to compute the whole score from scratch
– Recompute the partial score for the affected variable

Optimizing the structure. Algorithms

- **Greedy search**
  - Start from the structure with no links
  - Add a link that yields the best score improvement



- **Metropolis algorithm (with simulated annealing)**
  - Local additions and deletions
  - Avoids being trapped in a “local” optima