Density estimation with hidden variables and missing values

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Administration

Midterm: Wednesday, March 17, 2004
• In class
• Closed book
• Material covered by Spring break, excluding learning of the BBN structures
• Last year midterm is on the web

No new homework
Project proposals

Due: Wednesday, March 24, 2004
• 1-2 pages long
Proposal
• Written proposal:
  1. Outline of a learning problem, type of data you have available. Why is the problem important?
  2. Learning methods you plan to try and implement for the problem. References to previous work.
  3. How do you plan to test, compare learning approaches
  4. Schedule of work (approximate timeline of work)
• A PPT (3 slide) summary of points 1-4

Learning the structure of the BBN
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?

Learning the structure

Criteria we can choose to score the structure S

- **Marginal likelihood**
  maximize \( P(D \mid S, \xi) \)

\( \xi \) - represents the prior knowledge

- **Maximum 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
  - $\Theta$ - parameters of the BBN
    - $\Theta_{ij}$ is a vector of $\Theta_{jk}$ representing parameters of the conditional probability distribution; such that $\sum_{k=1}^{r} \Theta_{jk} = 1$
  - $N_{ijk}$ - a number of instances in the dataset where parents of variable $X_i$ take on values $j$ and $X_i$ has value $k$
  - $N_{ij} = \sum_{k=1}^{r} N_{ijk}$
  - $\alpha_{ijk}$ - prior counts (parameters of Beta and 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
  \[
P(D \mid S, \xi) = \prod_{i=1}^{n} \prod_{j=1}^{q} \frac{\Gamma(\alpha_{ij})}{\Gamma(\alpha_{ij} + N_{ij})} \prod_{k=1}^{r} \frac{\Gamma(\alpha_{ijk} + N_{ijk})}{\Gamma(\alpha_{ijk})}
  \]
- We can use **log-likelihood score** instead
  \[
  \log P(D \mid S, \xi) = \sum_{i=1}^{n} \left[ \sum_{j=1}^{q} \log \frac{\Gamma(\alpha_{ij})}{\Gamma(\alpha_{ij} + N_{ij})} + \sum_{k=1}^{r} \log \frac{\Gamma(\alpha_{ijk} + N_{ijk})}{\Gamma(\alpha_{ijk})} \right]
  \]
  **Score is decomposable along variables !!!**
Computing the marginal likelihood

• From the iid assumption:

\[ P(D \mid S, \Theta) = \prod_{i=1}^{N} \prod_{j=1}^{q_i} \prod_{k=1}^{r_i} P(x_i^k \mid \text{parents}_i^j, \Theta) \]

• Let \( r_i \) = number of values that attribute \( x_i \) can take
  \( q_i \) = number of possible parent combinations
  \( N_{ijk} \) = number of cases in \( D \) where \( x_i \) has value \( k \) and parents with values \( j \).

\[
= \prod_{i=1}^{n} \prod_{j=1}^{q_i} \prod_{k=1}^{r_i} P(x_i = k \mid \text{parents}_i = j, \Theta)^{N_{ijk}}
= \prod_{i=1}^{n} \prod_{j=1}^{q_i} \prod_{k=1}^{r_i} \theta_{ijk}^{N_{ijk}}
\]

Computing the marginal likelihood

• From parameter independence

\[ p(\Theta \mid S, \xi) = \prod_{i=1}^{n} \prod_{j=1}^{q_i} p(\Theta_{ij} \mid S, \xi) \]

• Priors for \( p(\Theta_{ij} \mid S, \xi) \)
  – \( \Theta_{ij} = (\Theta_{ij1}, \ldots, \Theta_{ijr_i}) \) is a vector of parameters;
  – we use a Dirichlet distribution with parameters \( \alpha \) to represent it

\[
P(\Theta_{ij} \mid S, \xi) = P(\Theta_{ij1}, \ldots, \Theta_{ijr_i} \mid S, \xi) = \text{Dirichlet}(\Theta_{ij1}, \ldots, \Theta_{ijr_i} \mid \alpha)
= \frac{\Gamma(\sum_{k=1}^{r_i} \alpha_{ijk})}{\prod_{k=1}^{r_i} \Gamma(\alpha_{ijk})} \prod_{k=1}^{r_i} \Theta_{ijk}^{\alpha_{ijk} - 1}
\]

CS 2750 Machine Learning
Computing the marginal likelihood

- **Combine things together:**

\[
P(D \mid S, \Theta) = \int \frac{P(D \mid S, \Theta)P(\Theta \mid S)}{d\Theta}
\]

\[
= \int \prod_{i} \prod_{j} \prod_{k} \Gamma^{N_{ij}} \cdot \frac{\Gamma(\sum_{k=1}^{r} \alpha_{ijk})}{\prod_{k=1}^{r} \Gamma(\alpha_{ijk})} \prod_{k=1}^{r} \Gamma^{a_{ijk}-1} d\Theta
\]

\[
= \prod_{i} \prod_{j} \prod_{k} \frac{\Gamma(\sum_{k=1}^{r} \alpha_{ijk})}{\prod_{k=1}^{r} \Gamma(\alpha_{ijk})} \int \prod_{k=1}^{r} \Gamma^{N_{ij} + a_{ijk} - 1} d\Theta
\]

\[
= \prod_{i} \prod_{j} \prod_{k} \frac{\Gamma(\alpha_{ijk})}{\prod_{k=1}^{r} \Gamma(\alpha_{ijk})} \prod_{k=1}^{r} \Gamma(\alpha_{ijk} + N_{ijk})
\]

Learning the structure

- **Likelihood of data for the BBN** (structure + parameters)

\[P(D \mid S, \Theta, \xi)\]

measures the goodness of fit of the BBN to data

- **Marginal likelihood** (for the structure only)

\[P(D \mid S, \xi)\]

- **Does not measure only a goodness of fit. It 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
  \[
  P(D | S, \xi) = \frac{\int P(D | S, \Theta, \xi) p(\Theta | S, \xi) d\Theta}{\int p(\Theta | S, \xi) d\Theta}
  \]
  We know that \( \int p(\Theta | S, \xi) d\Theta = 1 \)

  **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:**
\[
\text{score}(S) = \log P(D | S, \Theta_{ML}, \xi) - \text{compl}(S)
\]

**Bayesian information criterion (BIC)**

**Maximize:**
\[
\text{score}(S) = \log P(D | S, \Theta_{ML}, \xi) - \frac{1}{2} \text{compl}(S) \log N
\]
Optimizing the structure

Finding the best structure is a **combinatorial optimization** problem

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

\[
\log P(D \mid S, \xi) = \sum_{i=1}^{n} \sum_{j=1}^{q_i} \log \frac{\Gamma(\alpha_{y_j})}{\Gamma(\alpha_{y_j} + N_{y_j})} + \sum_{k=1}^{r} \log \frac{\Gamma(\alpha_{g_{ik}} + N_{g_{ik}})}{\Gamma(\alpha_{g_{ik}})}
\]

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

![Diagram of structure changes](image)

**Advantage**:
- we do not have to compute the whole score from scratch
- Recompute the partial score for the affected variable

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Optimizing the structure. Algorithms

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

![Diagram of greedy search](image)

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

![Diagram of Metropolis algorithm](image)
Density estimation with hidden variables and missing values

Learning probability distribution

Basic learning settings:
• A set of random variables \( X = \{X_1, X_2, \ldots, X_n\} \)
• A model of the distribution over variables in \( X \) with parameters \( \Theta \)
• Data \( D = \{D_1, D_2, \ldots, D_N\} \)
  \( s.t. \quad D_i = (x_1^i, x_2^i, \ldots, x_n^i) \)

Objective: find parameters \( \hat{\Theta} \) that describe the data

Assumptions considered so far:
– Known parameterizations
– No hidden variables
– No-missing values
Hidden variables

Modeling assumption:
Variables \( X = \{X_1, X_2, \ldots, X_n\} \) are related through hidden variables

Why to add hidden variables?
- More flexibility in describing the distribution \( P(X) \)
- Smaller parameterization of \( P(X) \)
  - New independences can be introduced via hidden variables

Example:

- Latent variable models
  - hidden classes (categories)

\[ P(X | C = i) \]

Observed data

Hidden variable model. Example.

- We want to represent the probability model of a population in a two dimensional space \( X = \{X_1, X_2\} \)
Hidden variable model

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Observed data
**Hidden variable model**

- We want to represent the probability model of a population in a two dimensional space \( \mathbf{X} = \{X_1, X_2\} \)

**Observed data**

**Model**: 3 Gaussians with a hidden class variable

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**Mixture of Gaussians**

Probability of the occurrence of a data point \( \mathbf{x} \) is modeled as

\[
p(\mathbf{x}) = \sum_{i=1}^{k} p(C = i) p(\mathbf{x} \mid C = i)
\]

where

\[p(C = i)\]

= probability of a data point coming from class \( C=i \)

\[p(\mathbf{x} \mid C = i) \approx N(\mu_i, \Sigma_i)\]

= class-conditional density (modeled as Gaussian) for class \( i \)
Mixture of Gaussians

- Density function for the Mixture of Gaussians model

Naïve Bayes with a hidden class variable

Introduction of a hidden variable can reduce the number of parameters defining $P(X)$

Example:
- Naïve Bayes model with a hidden class variable
  
  **Hidden class variable**
  
  \[ \begin{align*}
  &C \\
  &X_1 \\& \quad \cdots \\ &X_n
  \end{align*} \]

  Attributes are independent given the class

- Useful in customer profiles
  - Class value = type of customers
Missing values

A set of random variables \( X = \{X_1, X_2, \ldots, X_n\} \)

- **Data** \( D = \{D_1, D_2, \ldots, D_N\} \)
- **But some values are missing**
  \[
  D_i = (x^i_1, x^i_2, \ldots, x^i_n) \\
  \text{Missing value of } x^i_2 \\
  D_{i+1} = (x^i_2, \ldots, x^i_n) \\
  \text{Missing values of } x^i_1, x^i_2 \\
  \text{Etc.}
  \]

- **Example:** medical records
- **We still want to estimate parameters of** \( P(X) \)

Density estimation

**Goal:** Find the set of parameters \( \hat{\Theta} \)

**Estimation criteria:**
- **ML** \( \max_{\Theta} p(D \mid \Theta, \xi) \)
- **Bayesian** \( p(\Theta \mid D, \xi) \)

**Possible optimization methods for the ML:** gradient-ascent, conjugate gradient, Newton-Rhapson, etc.

- **Problem:** No or very small advantage from the structure of the corresponding belief network

**Expectation-maximization (EM) method**
- An alternative optimization method
- Suitable when there are missing or hidden values
- **Takes advantage of the structure of the belief network**