Bayesian belief networks

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Density estimation

Data: \( D = \{D_1, D_2, \ldots, D_n\} \)
\( D_i = x_i \) a vector of attribute values

Attributes:
- modeled by random variables \( X = \{X_1, X_2, \ldots, X_d\} \) with:
  - Continuous values
  - Discrete values
    E.g. \textit{temperature} with numerical values
    or \textit{chest pain} with discrete values
      [no-pain, mild, moderate, strong]

Underlying true probability distribution:
\( p(X) \)
Density estimation

**Data:** \( D = \{D_1, D_2, ..., D_n\} \)
\( D_i = x_i \) a vector of attribute values

**Objective:** try to estimate the underlying true probability distribution over variables \( X \), \( p(X) \), using examples in \( D \)

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**Standard (iid) assumptions:** Samples
- are independent of each other
- come from the same (identical) distribution (fixed \( p(X) \))

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Learning via parameter estimation

In this lecture we consider **parametric density estimation**

**Basic settings:**
- A set of random variables \( X = \{X_1, X_2, ..., X_d\} \)
- A model of the distribution over variables in \( X \) with parameters \( \Theta \) : \( \hat{p}(X | \Theta) \)
- Data \( D = \{D_1, D_2, ..., D_n\} \)

**Objective:** Find the parameters \( \Theta \) that explain the observed data the best
Parameter estimation

- **Maximum likelihood (ML)**
  - maximize $p(D \mid \Theta, \xi)$
  - yields: one set of parameters $\hat{\Theta}_{ML}$
  - the target distribution is approximated as:
    $$\hat{p}(X) = p(X \mid \hat{\Theta}_{ML})$$

- **Bayesian parameter estimation**
  - uses the posterior distribution over possible parameters
    $$p(\Theta \mid D, \xi) = \frac{p(D \mid \Theta, \xi) p(\Theta \mid \xi)}{p(D \mid \xi)}$$
  - Yields: all possible settings of $\Theta$ (and their “weights”)
  - The target distribution is approximated as:
    $$\hat{p}(X) = p(X \mid D) = \int p(X \mid \Theta) p(\Theta \mid D, \xi) d\Theta$$

Other possible criteria:

- **Maximum a posteriori probability (MAP)**
  - maximize $p(\Theta \mid D, \xi)$ (mode of the posterior)
  - Yields: one set of parameters $\hat{\Theta}_{MAP}$
  - Approximation:
    $$\hat{p}(X) = p(X \mid \hat{\Theta}_{MAP})$$

- **Expected value of the parameter**
  - $\hat{\Theta} = E(\Theta)$ (mean of the posterior)
  - Expectation taken with regard to posterior $p(\Theta \mid D, \xi)$
  - Yields: one set of parameters
  - Approximation:
    $$\hat{p}(X) = p(X \mid \hat{\Theta})$$
Distribution models

• So far we have covered density estimation for “simple” distribution models:
  – Bernoulli
  – Binomial
  – Multinomial
  – Gaussian
  – Poisson

But what if:
• The dimension of $X = \{X_1, X_2, \ldots, X_d\}$ is large
  – Example: patient data
• Compact parametric distributions do not seem to fit the data
  – E.g.: multivariate Gaussian may not fit
• We have only a “small” number of examples to do accurate parameter estimates

Modeling complex distributions

Question: How to model and learn complex multivariate distributions $\hat{p}(X)$ with a large number of variables?

Solution:
• Decompose the distribution using conditional independence relations
• Decompose the parameter estimation problem to a set of smaller parameter estimation tasks

Decomposition of distributions under conditional independence assumption is the main idea behind Bayesian belief networks.
Example

**Problem description:**

- **Disease:** pneumonia
- **Patient symptoms (findings, lab tests):**
  - Fever, Cough, Paleness, WBC (white blood cells) count, Chest pain, etc.

**Representation of a patient case:**

- Symptoms and disease are represented as random variables

**Our objectives:**

- Describe a multivariate distribution representing the relations between symptoms and disease
- Design of inference and learning procedures for the multivariate model

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Modeling uncertainty with probabilities

**Full joint distribution:**

- Assume $X = \{X_1, X_2, \ldots, X_d\}$ are all random variables that define the domain
- Full joint: $P(X)$ or $P(X_1, X_2, \ldots, X_d)$

**Full joint is sufficient** to do any type of probabilistic inference:

- Computation of joint probabilities for sets of variables
  - $P(X_1, X_2, X_3)$
  - $P(X_1, X_{10})$
- Computation of conditional probabilities
  - $P(X_1 \mid X_2 = \text{True}, X_3 = \text{False})$
  - Why? Conditional probability is defined in terms of joint probabilities
  - $P(A \mid B) = \frac{P(A, B)}{P(B)}$
### Marginalization

**Joint probability distribution (for a set variables)**
- Defines probabilities for all possible assignments to values of variables in the set

\[
P(pneumonia, WBCcount)\]

2x3 table

<table>
<thead>
<tr>
<th>Pneumonia</th>
<th>high</th>
<th>normal</th>
<th>low</th>
</tr>
</thead>
<tbody>
<tr>
<td>True</td>
<td>0.0008</td>
<td>0.0001</td>
<td>0.0001</td>
</tr>
<tr>
<td>False</td>
<td>0.0042</td>
<td>0.9929</td>
<td>0.0019</td>
</tr>
</tbody>
</table>

\[
P(WBCcount)\]

**Marginalization** (summing of rows, or columns)
- summing out variables

### Variable independence

- The joint distribution over a subset of variables can be always computed from the joint distribution through marginalization
- **How about the opposite?** Can we recover the joint from the joint over subsets?

\[
P(pneumonia, WBCcount)\]

\[
P(WBCcount)\]

\[
P(Pneumonia)\]
Variable independence

- The joint distribution over a subset of variables can be always computed from the joint distribution through marginalization.
- Can we recover the joint from the joint over subsets? **NO**!
  - Only exception: when variables are independent

\[ P(A, B) = P(A)P(B) \]

<table>
<thead>
<tr>
<th>WBCcount</th>
<th>Pneumonia</th>
<th>Pneumonia</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>True</td>
<td>False</td>
</tr>
<tr>
<td>high</td>
<td>?</td>
<td>?</td>
</tr>
<tr>
<td>normal</td>
<td>?</td>
<td>?</td>
</tr>
<tr>
<td>low</td>
<td>?</td>
<td>?</td>
</tr>
</tbody>
</table>

\[ P(WBCcount) = 0.005 \quad 0.993 \quad 0.002 \]

P(neumonia, WBCcount)  WBCcount  P(Pneumonia)

Conditional probability

**Conditional probability:**
- Probability of A given B

\[ P(A|B) = \frac{P(A,B)}{P(B)} \]

- Conditional probability is defined in terms of joint probabilities
- Joint probabilities can be expressed in terms of conditional probabilities

\[ P(A,B) = P(A|B)P(B) \quad (\text{product rule}) \]

\[ P(X_1, X_2, \ldots X_n) = \prod_{i=1}^{n} P(X_i \mid X_1, \ldots X_{i-1}) \quad (\text{chain rule}) \]

- Conditional probability – is useful for **various probabilistic inferences**

\[ P(\text{Pneumonia} = \text{True} \mid \text{Fever} = \text{True}, \text{WBCcount} = \text{high}, \text{Cough} = \text{True}) \]
Inference

Any query can be computed from the full joint distribution!!!
• **Joint over a subset of variables** is obtained through marginalization:
  \[ P(A = a, C = c) = \sum_i \sum_j P(A = a, B = b_i, C = c, D = d_j) \]

• **Conditional probability over a set of variables**, given other variables’ values is obtained through marginalization and definition of conditionals:
  \[
  P(D = d \mid A = a, C = c) = \frac{P(A = a, C = c, D = d)}{P(A = a, C = c)} = \frac{\sum_i P(A = a, B = b_i, C = c, D = d)}{\sum_i \sum_j P(A = a, B = b_j, C = c, D = d_j)}
  \]

Inference

• Any joint probability can be expressed as a product of conditionals via the **chain rule**.
  \[
  P(X_1, X_2, \ldots X_n) = P(X_n \mid X_1, \ldots X_{n-1})P(X_1 \ldots X_{n-1})
  = P(X_n \mid X_1, \ldots X_{n-1})P(X_{n-1} \mid X_1, \ldots X_{n-2})P(X_1 \ldots X_{n-2})
  = \prod_{i=1}^n P(X_i \mid X_1, \ldots X_{i-1})
  \]

• It is often easier to define the distribution in terms of conditional probabilities:
  - E.g. \( P(\text{Fever} \mid \text{Pneumonia} = T) \)
  - \( P(\text{Fever} \mid \text{Pneumonia} = F) \)
Modeling uncertainty with probabilities

- **Full joint distribution**: joint distribution over all random variables defining the domain
  - it is sufficient to represent the complete domain and to do any type of probabilistic inferences

Problems:
- **Space complexity**. To store full joint distribution requires to remember $O(d^n)$ numbers.
  $n$ – number of random variables, $d$ – number of values
- **Inference complexity**. To compute some queries requires $O(d^n)$ steps.
- **Acquisition problem**. Who is going to define all of the probability entries?

Pneumonia example. Complexities.

- **Space complexity**.
  - Pneumonia (2 values: T,F), Fever (2: T,F), Cough (2: T,F), WBCcount (3: high, normal, low), paleness (2: T,F)
  - Number of assignments: $2 \times 2 \times 2 \times 3 \times 2 = 48$
  - We need to define at least 47 probabilities.

- **Time complexity**.
  - Assume we need to compute the probability of Pneumonia=T from the full joint

$$P(\text{Pneumonia} = T) = \sum_{i \in T,F} \sum_{j \in T,F} \sum_{k = h,n,l} \sum_{u \in T,F} P(\text{Fever} = i, \text{Cough} = j, \text{WBCcount} = k, \text{Pale} = u)$$
  - Sum over $2 \times 2 \times 3 \times 2 = 24$ combinations
Bayesian belief networks (BBNs)

Bayesian belief networks
- Represent the full joint distribution over the variables more compactly with a smaller number of parameters.
- Take advantage of conditional and marginal independences among random variables.

- A and B are independent
  \[ P(A, B) = P(A)P(B) \]
- A and B are conditionally independent given C
  \[ P(A, B | C) = P(A | C)P(B | C) \]
  \[ P(A | C, B) = P(A | C) \]

Alarm system example
- Assume your house has an alarm system against burglary. You live in the seismically active area and the alarm system can get occasionally set off by an earthquake. You have two neighbors, Mary and John, who do not know each other. If they hear the alarm they call you, but this is not guaranteed.
- We want to represent the probability distribution of events:
  - Burglary, Earthquake, Alarm, Mary calls and John calls

Causal relations

[Diagram of causal relationships: Burglary, Earthquake, Alarm, JohnCalls, Mary Calls]
Bayesian belief network

1. Directed acyclic graph
   - **Nodes** = random variables
     Burglary, Earthquake, Alarm, Mary calls and John calls
   - **Links** = direct (causal) dependencies between variables.
     The chance of Alarm being is influenced by Earthquake,
     The chance of John calling is affected by the Alarm

2. Local conditional distributions
   - relating variables and their parents
**Full joint distribution in BBNs**

**Full joint distribution** is defined in terms of local conditional distributions (obtained via the chain rule):

\[
P(X_1, X_2, \ldots, X_n) = \prod_{i=1}^{n} P(X_i \mid pa(X_i))
\]

**Example:**
Assume the following assignment of values to random variables
\[B = T, E = T, A = T, J = T, M = F\]

Then its probability is:
\[
P(B = T, E = T, A = T, J = T, M = F) =
\]
\[
P(B = T)P(E = T)P(A = T \mid B = T, E = T)P(J = T \mid A = T)P(M = F \mid A = T)
\]
Bayesian belief networks (BBNs)

Bayesian belief networks
• Represent the full joint distribution over the variables more compactly using the product of local conditionals.
• But how did we get to local parameterizations?
Answer:
• Graphical structure encodes conditional and marginal independences among random variables
• A and B are independent \( P(A, B) = P(A)P(B) \)
• A and B are conditionally independent given C
  \[
  P(A \mid C, B) = P(A \mid C) \\
  P(A, B \mid C) = P(A \mid C)P(B \mid C)
  \]
• The graph structure implies the decomposition !!!

Independences in BBNs

3 basic independence structures:
1. Burglary
   - Alarm
     - JohnCalls
2. Burglary
   - Earthquake
   - Alarm
3. Alarm
   - JohnCalls
   - MaryCalls
1. JohnCalls is independent of Burglary given Alarm

\[ P(J \mid A, B) = P(J \mid A) \]
\[ P(J, B \mid A) = P(J \mid A)P(B \mid A) \]

2. Burglary is independent of Earthquake (not knowing Alarm)
Burglary and Earthquake become dependent given Alarm !!

\[ P(B, E) = P(B)P(E) \]
Independences in BBNs

1. MaryCalls is independent of JohnCalls given Alarm

$$P(J | A, M) = P(J | A)$$

$$P(J, M | A) = P(J | A)P(M | A)$$

Independence in BBN

- BBN distribution models many conditional independence relations relating distant variables and sets
- These are defined in terms of the graphical criterion called d-separation
- **D-separation in the graph**
  - Let X, Y and Z be three sets of nodes
  - If X and Y are d-separated by Z then X and Y are conditionally independent given Z
- **D-separation**: A is d-separated from B given C if every undirected path between them is blocked with C
- **Path blocking**
  - 3 cases that expand on three basic independence structures
Undirected path blocking

A is d-separated from B given C if every undirected path between them is blocked.
Undirected path blocking

A is d-separated from B given C if every undirected path between them is blocked.

- 1. Path blocking with a linear substructure

- 2. Path blocking with the wedge substructure
**Undirected path blocking**

A is d-separated from B given C if every undirected path between them is **blocked**

- **3. Path blocking with the vee substructure**
  
  ![Diagram](image)

  - X in A
  - Y in B
  - Z or any of its descendants **not** in C

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**Independences in BBNs**

- Earthquake and Burglary are independent given MaryCalls
  - F
- Burglary and MaryCalls are independent (not knowing Alarm)
  - F
- Burglary and RadioReport are independent given Earthquake
  - T
- Burglary and RadioReport are independent given MaryCalls
  - F
Full joint distribution in BBNs

Rewrite the full joint probability using the product rule:

\[ P(B=T, E=T, A=T, J=T, M = F) = \]

Product rule

\[ = P(J= T \mid B= T, E= T, A= T, M = F)P(B= T, E= T, A= T, M = F) \]
Full joint distribution in BBNs

Rewrite the full joint probability using the product rule:

\[ P(B = T, E = T, A = T, J = T, M = F) = \]

\[
\begin{align*}
= & \quad P(J = T \mid B = T, E = T, A = T, M = F) P(B = T, E = T, A = T, M = F) \\
= & \quad P(J = T \mid A = T) P(B = T, E = T, A = T, M = F)
\end{align*}
\]

CS 2750 Machine Learning
Parameter complexity problem

- In the BBN the **full joint distribution** is defined as:
  \[ P(X_1, X_2, \ldots, X_n) = \prod_{i=1}^{n} P(X_i \mid pa(X_i)) \]
- **What did we save?**

Alarm example: 5 binary (True, False) variables

\[
\begin{align*}
\text{# of parameters of the full joint:} & \quad 2^5 = 32 \\
\text{One parameter is for free:} & \quad 2^5 - 1 = 31 \\
\text{# of parameters of the BBN:} & \quad 2^3 + 2(2^2) + 2(2) = 20 \\
\text{One parameter in every conditional is for free:} & \quad 2^2 + 2(2) + 2(1) = 10
\end{align*}
\]