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 $D$

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

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

**Example: modeling of disease – symptoms relations**

- **Disease:** pneumonia
- **Patient symptoms (findings, lab tests):**
  - Fever, Cough, Paleness, WBC (white blood cells) count, Chest pain, etc.
- **Model of the full joint distribution:**
  \[ P(\text{Pneumonia, Fever, Cough, Paleness, WBC, Chest pain}) \]

One probability per assignment of values to variables:
\[ P(\text{Pneumonia} = T, \text{Fever} = T, \text{Cough} = T, \text{WBC} = \text{High}, \text{Chest pain} = T) \]

Bayesian belief networks (BBNs)

**Bayesian belief networks** (late 80s, beginning of 90s)

**Key features:**
- 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
- **X and Y are independent** \( P(X, Y) = P(X)P(Y) \)
- **X and Y are conditionally independent given Z**

\[
P(X, Y \mid Z) = P(X \mid Z)P(Y \mid Z) \\
P(X \mid Y, Z) = P(X \mid Z)
\]
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:
• Chain rule +
• 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
\[
P(A \mid C, B) = P(A \mid C) \quad P(A, B \mid C) = P(A \mid C)P(B \mid C)
\]
• The graph structure implies the decomposition !!!

Independences in BBNs

3 basic independence structures:

1. 
\[
\text{Burglary} \rightarrow \text{Alarm} \rightarrow \text{JohnCalls}
\]

2. 
\[
\text{Burglary} \rightarrow \text{Alarm} \rightarrow \text{Earthquake}
\]

3. 
\[
\text{Alarm} \rightarrow \text{JohnCalls} \rightarrow \text{MaryCalls}
\]
Independences in BBNs

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

2. JohnCalls

3. MaryCalls is independent of JohnCalls given Alarm

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

Independences in BBN

• BBN distribution models many conditional independence relations among distant variables and sets of variables
• These are defined in terms of the graphical criterion called d-separation
• D-separation and independence
  – 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
**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

```
    X ------ Z ------ Y  
     |           |     
   X in A     Z in C     Y in B
```

- 2. Path blocking with the wedge substructure

```
    X ------ Z ------ Y  
     |     
   X in A     Z in C     Y in B
```
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**

  X in A \hspace{1cm} \hspace{1cm} Y in B

  ![Diagram](attachment:diagram.png)

  Z or any of its descendants not in C

Independences in BBNs

- Earthquake and Burglary are independent given MaryCalls

  ![Diagram](attachment:bbn.png)
Independences in BBNs

• Earthquake and Burglary are independent given MaryCalls \( F \)
• Burglary and MaryCalls are independent (not knowing Alarm) \(?\)

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 \(?\)
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 \( ? \)
Full joint distribution in BBNs

Rewrite the full joint probability using the product rule:

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

---

Full joint distribution in BBNs

Rewrite the full joint probability using the product rule:

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

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

---
Full joint distribution in BBNs

Rewrite the full joint probability using the product rule:

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

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

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

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Full joint distribution in BBNs

Rewrite the full joint probability using the product rule:

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

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

---
Rewrite the full joint probability using the product rule:

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

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

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

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

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

---

Rewrite the full joint probability using the product rule:

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

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

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

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

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

\[ P(A = T \mid B = T, E = T)P(B = T, E = T) \]
Rewrite the full joint probability using the product rule:

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

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

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

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

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

\[
P(A = T \mid B = T, E = T)P(B = T, E = T)
\]

\[
P(B = T)P(E = T)
\]
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: binary (True, False) variables

# of parameters of the full joint: 

\[
2^5 = 32
\]

One parameter depends on the rest:

\[
2^5 - 1 = 31
\]

# of parameters of the BBN:

?
Bayesian belief network: parameters count

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<td>P(B)</td>
<td>0.999</td>
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<td>P(E)</td>
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<td>F</td>
<td>0.05</td>
<td>0.95</td>
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|        | P(A|B,E) |
|--------|---------|
|        | T   | T   | T   | F   |
|        | 0.95 | 0.05 | 0.94 | 0.06 |
|        | F   | T   | T   | F   |
|        | 0.29 | 0.71 | 0.001 | 0.999 |

|        | P(J|A) |
|--------|------|
|        | T   | F   |
|        | T   | 0   | 0   |
|        | F   | 0   | 0   |

|        | P(M|A) |
|--------|------|
|        | T   | F   |
|        | T   | 0.7 | 0.3 |
|        | F   | 0.01 | 0.99 |

Total: 20

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

# of parameters of the full joint:

\[ 2^5 = 32 \]

One parameter depends on the rest:

\[ 2^5 - 1 = 31 \]

# of parameters of the BBN:

\[ 2^3 + 2(2^2) + 2(2) = 20 \]

One parameter in every conditional depends on the rest:

?
Bayesian belief network: free parameters

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
  
  - # of parameters of the full joint:
    \[
    2^5 = 32
    \]
  - One parameter depends on the rest:
    \[
    2^5 - 1 = 31
    \]
  - # of parameters of the BBN:
    
    \[
    2^3 + 2(2^2) + 2(2) = 20
    \]
  - One parameter in every conditional depends on the rest:
    
    \[
    2^2 + 2(2) + 2(1) = 10
    \]
BBNs examples

- In various areas:
  - Intelligent user interfaces (Microsoft)
  - Troubleshooting, diagnosis of a technical device
  - Medical diagnosis:
    - Pathfinder CPSC
    - Munin
    - QMR-DT
  - Collaborative filtering
  - Military applications
  - Insurance, credit applications

Diagnosis of car engine

- Diagnose the engine start problem

[Diagram of a car engine diagnosis process]
Car insurance example

- Predict claim costs (medical, liability) based on application data

(ICU) Alarm network
CPCS

- Computer-based Patient Case Simulation system (CPCS-PM) developed by Parker and Miller (at University of Pittsburgh)
- 422 nodes and 867 arcs

Naïve Bayes model

A special (simple) Bayesian belief network

- Defines a generative classifier model
- Model of $P(x, y) = P(x | y) P(y)$
  - Class variable $y$
    - $p(y)$
  - Attributes are independent given $y$
    - $p(x | y = i) = \prod_{j=1}^{d} p(x_j | y = i)$

Learning:

- Parameterize models of $p(y)$ and all $p(x_j | y = i)$
- ML estimates of the parameters
Naïve Bayes model

A special (simple) Bayesian belief network
- Defines a generative classifier model
- Model of $P(x, y) = P(x | y) P(y)$

Classification: given $x$ select the class
- Select the class with the maximum posterior
- Calculation of a posterior is an example of BBN inference

$$p(y = i | x) = \frac{p(y = i) p(x | y = i)}{\sum_{u=1}^{k} p(y = u) p(x | y = u)} = \frac{p(y = i) \prod_{j=1}^{d} p(x_j | y = i)}{\sum_{u=1}^{k} p(y = u) \prod_{j=1}^{d} p(x_j | y = u)}$$

Remember: we can calculate the probabilities from the full joint

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:
- Learning of the parameters of BBN
- Values for all variables are observable
Estimation 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 local parent-variable conditionals.

- **Example:** Assume A,E,B are binary with True, False values

  Learning of $P(A|B,E) = 4$ estimation problems

  

  ![Diagram](image)

  

  $P(A|B=T,E=T)$
  $P(A|B=T,E=F)$
  $P(A|B=F,E=T)$
  $P(A|B=F,E=F)$

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

---

Estimates of parameters of BBN

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

    $$P(D | \Theta, \xi) = \prod_{a=1}^{N} P(D_a | \Theta, \xi)$$

  - **Parameter independence**

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

  Parameters of each conditional (one for every assignment of values to parent variables) can be learned independently.
Learning of BBN parameters. Example.

Example:

\[
\begin{array}{c|c|c}
\text{Pneumonia} & \text{T} & \text{F} \\
\hline
? & ? & ? \\
\end{array}
\]

\[
\begin{array}{c|c|c}
\text{Paleness} & \text{T} & \text{F} \\
\hline
\text{Pn} & ? & ? \\
\end{array}
\]

\[
\begin{array}{c|c|c}
\text{Fever} & \text{T} & \text{F} \\
\hline
\text{HWBC|Pneum} & ? & ? \\
\end{array}
\]

\[
\begin{array}{c|c|c}
\text{Cough} & \text{T} & \text{F} \\
\hline
\text{P(Cough|Pneum)} & ? & ? \\
\end{array}
\]

\[
\begin{array}{c|c|c}
\text{High WBC} & \text{T} & \text{F} \\
\hline
\text{P(HWBC|Pneum)} & ? & ? \\
\end{array}
\]

Learning of BBN parameters. Example.

Data D (different patient cases):

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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:** \( P(\text{Fever} | \text{Pneumonia} = T) \)
• **Problem:** How to pick the data to learn?

---

Learning of BBN parameters. Example.

**Learn:** \( P(\text{Fever} | \text{Pneumonia} = T) \)

**Step 1:** Select data points with Pneumonia=T

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</tbody>
</table>

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Learning of BBN parameters. Example.

**Learn:** \( P(\text{Fever} | \text{Pneumonia} = T) \)

**Step 1:** Ignore the rest

\[
\begin{array}{cccccc}
\text{Pal} & \text{Fev} & \text{Cou} & \text{HWB} & \text{Pneu} \\
F & F & T & T & T \\
F & F & T & F & T \\
F & T & T & T & T \\
T & T & T & T & T \\
F & T & F & T & T
\end{array}
\]

Learning of BBN parameters. Example.

**Learn:** \( P(\text{Fever} | \text{Pneumonia} = T) \)

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

\[
\begin{array}{cccccc}
\text{Pal} & \text{Fev} & \text{Cou} & \text{HWB} & \text{Pneu} \\
F & F & T & T & T \\
F & F & T & F & T \\
F & T & T & T & T \\
T & T & T & T & T \\
F & T & F & T & T
\end{array}
\]
Learning of BBN parameters. Example.

Learn: $P(Fever \mid Pneumonia = T)$
Step 2: Ignore the rest

Fever
F F T T T

Learning of BBN parameters. Example.

Learn: $P(Fever \mid Pneumonia = T)$
Step 3a: Learning the ML estimate

Fever
F F T T T

$P(Fever \mid Pneumonia = T)$

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<tbody>
<tr>
<td>Pneumonia</td>
<td>0.6</td>
<td>0.4</td>
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</table>
Learning of BBN parameters. Bayesian learning.

**Learn:** \( P(Fever \mid Pneumonia = T) \)

**Step 3b:** Learning the Bayesian posterior

Assume the prior

\[
\theta_{Fever \mid Pneumonia= T} \sim Beta(3, 4)
\]

**Posterior:**

\[
\theta_{Fever \mid Pneumonia= T} \sim Beta(6, 6)
\]

\[
\theta_{MAP}^{Fever \mid Pneumonia= T} = \frac{6 - 1}{6 + 6 - 2} = 0.5
\]

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<tbody>
<tr>
<td>Pneumonia</td>
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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:**

\( P(Fever \mid Pneumonia = T) \)

**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 local conditionals the same way as we learned the parameters of a biased coin or a die