Graphical Models - Part I

Oliver Schulte - CMPT 726

Bishop PRML Ch. 8, some slides from Russell and Norvig
AIMA2e
Outline

Probabilistic Models

Bayesian Networks

Markov Random Fields

Inference
Outline

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Bayesian Networks

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Inference
Probabilistic Models

• We now turn our focus to probabilistic models for pattern recognition
  • Probabilities express beliefs about uncertain events, useful for decision making, combining sources of information

• Key quantity in probabilistic reasoning is the joint distribution

\[ p(x_1, x_2, \ldots, x_K) \]

where \( x_1 \) to \( x_K \) are all variables in model

• Address two problems
  • Inference: answering queries given the joint distribution
  • Learning: deciding what the joint distribution is (involves inference)

• All inference and learning problems involve manipulations of the joint distribution
Reminder - Three Tricks

- Bayes’ rule:

\[ p(Y|X) = \frac{p(X|Y)p(Y)}{p(X)} = \alpha p(X|Y)p(Y) \]

- Marginalization:

\[ p(X) = \sum_y p(X, Y = y) \text{ or } p(X) = \int p(X, Y = y)dy \]

- Product rule:

\[ p(X, Y) = p(X)p(Y|X) \]

- All 3 work with extra conditioning, e.g.:

\[ p(X|Z) = \sum_y p(X, Y = y|Z) \]

\[ p(Y|X, Z) = \alpha p(X|Y, Z)p(Y|Z) \]
Joint Distribution

Consider model with 3 boolean random variables: cavity, catch, toothache

Can answer query such as

\[ p(\neg\text{cavity}|\text{toothache}) \]
### Joint Distribution

Consider model with 3 boolean random variables: \( \textit{cavity}, \textit{catch}, \textit{toothache} \)

Can answer query such as

\[ p(\neg \textit{cavity}|\textit{toothache}) \]

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- Consider model with 3 boolean random variables: cavity, catch, toothache
- Can answer query such as

\[
p(\neg\text{cavity}|\text{toothache}) = \frac{p(\neg\text{cavity}, \text{toothache})}{p(\text{toothache})}
\]

\[
p(\neg\text{cavity}|\text{toothache}) = \frac{0.016 + 0.064}{0.108 + 0.012 + 0.016 + 0.064} = 0.4
\]
Joint Distribution

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- Consider model with 3 boolean random variables: cavity, catch, toothache
- Can answer query such as

\[ p(¬cavity | toothache) = \frac{p(¬cavity, toothache)}{p(toothache)} \]

\[ p(¬cavity | toothache) = \frac{0.016 + 0.064}{0.108 + 0.012 + 0.016 + 0.064} = 0.4 \]
Joint Distribution

- In general, to answer a query on random variables $Q = Q_1, \ldots, Q_N$ given evidence $E = e, E = E_1, \ldots, E_M$, $e = e_1, \ldots, e_M$:

$$p(Q|E = e) = \frac{p(Q,E = e)}{p(E = e)}$$

$$= \frac{\sum_h p(Q,E = e, H = h)}{\sum_q, h p(Q = q, E = e, H = h)}$$
Problems

- The joint distribution is large
  - e.g., with $K$ boolean random variables, $2^K$ entries
- Inference is slow, previous summations take $O(2^K)$ time
- Learning is difficult, data for $2^K$ parameters
- Analogous problems for continuous random variables
Reminder - Independence

- **A and B are independent** iff
  \[ p(A|B) = p(A) \quad \text{or} \quad p(B|A) = p(B) \quad \text{or} \quad p(A, B) = p(A)p(B) \]

- \[ p(\text{Toothache}, \text{Catch}, \text{Cavity}, \text{Weather}) = p(\text{Toothache}, \text{Catch}, \text{Cavity})p(\text{Weather}) \]
  - 32 entries reduced to 12 (\text{Weather} takes one of 4 values)

- Absolute independence powerful but rare

- Dentistry is a large field with hundreds of variables, none of which are independent. What to do?
Reminder - Conditional Independence

- \( p(Toothache, Cavity, Catch) \) has \( 2^3 - 1 = 7 \) independent entries
- If I have a cavity, the probability that the probe catches in it doesn’t depend on whether I have a toothache:
  \[
  (1) \quad P(\text{catch}|\text{toothache}, \text{cavity}) = P(\text{catch}|\text{cavity})
  \]
- The same independence holds if I haven’t got a cavity:
  \[
  (2) \quad P(\text{catch}|\text{toothache}, \neg\text{cavity}) = P(\text{catch}|\neg\text{cavity})
  \]
- Catch is conditionally independent of Toothache given Cavity: \( p(\text{Catch}|\text{Toothache}, \text{Cavity}) = p(\text{Catch}|\text{Cavity}) \)
- Equivalent statements:
  - \( p(\text{Toothache}|\text{Catch}, \text{Cavity}) = p(\text{Toothache}|\text{Cavity}) \)
  - \( p(\text{Toothache}, \text{Catch}|\text{Cavity}) = p(\text{Toothache}|\text{Cavity})p(\text{Catch}|\text{Cavity}) \)
  - Toothache \( \perp \perp \) Catch|Cavity
Write out full joint distribution using chain rule:

\[ p(\text{Toothache}, \text{Catch}, \text{Cavity}) = p(\text{Toothache}|\text{Catch}, \text{Cavity})p(\text{Catch}, \text{Cavity}) \]
\[ = p(\text{Toothache}|\text{Catch}, \text{Cavity})p(\text{Catch}|\text{Cavity})p(\text{Cavity}) \]
\[ = p(\text{Toothache}|\text{Cavity})p(\text{Catch}|\text{Cavity})p(\text{Cavity}) \]

2 + 2 + 1 = 5 independent numbers

In many cases, the use of conditional independence greatly reduces the size of the representation of the joint distribution.
Graphical Models

- Graphical Models provide a visual depiction of probabilistic model
- Conditional independence assumptions can be seen in graph
- Inference and learning algorithms can be expressed in terms of graph operations
- We will look at 3 types of graph (can be combined)
  - Directed graphs: Bayesian networks
  - Undirected graphs: Markov Random Fields
  - Factor graphs
Outline

Probabilistic Models

Bayesian Networks

Markov Random Fields

Inference
Bayesian Networks

- A simple, graphical notation for conditional independence assertions and hence for compact specification of full joint distributions
- Syntax:
  - a set of nodes, one per variable
  - a directed, acyclic graph (link \(\approx\) “directly influences”)
  - a conditional distribution for each node given its parents:
    \[
    p(X_i|pa(X_i))
    \]
- In the simplest case, conditional distribution represented as a **conditional probability table** (CPT) giving the distribution over \(X_i\) for each combination of parent values
Example

- Topology of network encodes conditional independence assertions:
  - Weather is independent of the other variables
  - Toothache and Catch are conditionally independent given Cavity
Example

• I’m at work, neighbor John calls to say my alarm is ringing, but neighbor Mary doesn’t call. Sometimes it’s set off by minor earthquakes. Is there a burglar?
• Variables: Burglar, Earthquake, Alarm, JohnCalls, MaryCalls
• Network topology reflects causal knowledge:
  • A burglar can set the alarm off
  • An earthquake can set the alarm off
  • The alarm can cause Mary to call
  • The alarm can cause John to call

• (Causal models and conditional independence seem hardwired for humans!)
Example contd.

| B  | E  | P(A|B,E) |
|----|----|----------|
| T  | T  | .95      |
| T  | F  | .94      |
| F  | T  | .29      |
| F  | F  | .001     |

| A  | P(J|A) |
|----|-------|
| T  | .90   |
| F  | .05   |

| A  | P(M|A) |
|----|-------|
| T  | .70   |
| F  | .01   |
Compactness

- A CPT for Boolean $X_i$ with $k$ Boolean parents has $2^k$ rows for the combinations of parent values.
- Each row requires one number $p$ for $X_i = true$ (the number for $X_i = false$ is just $1 - p$).
- If each variable has no more than $k$ parents, the complete network requires $O(n \cdot 2^k)$ numbers.
- i.e., grows linearly with $n$, vs. $O(2^n)$ for the full joint distribution.
- For burglary net, $1 + 1 + 4 + 2 + 2 = 10$ numbers (vs. $2^5 - 1 = 31$).
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- For burglary net, ?? numbers:
  - $1 + 1 + 4 + 2 + 2 = 10$ numbers (vs. $2^5 - 1 = 31$).
Global Semantics

- **Global semantics** defines the full joint distribution as the product of the local conditional distributions:

\[
P(x_1, \ldots, x_n) = \prod_{i=1}^{n} P(x_i | pa(X_i))
\]

E.g., \( P(j \land m \land a \land \neg b \land \neg e) = \)
Global Semantics

- **Global semantics** defines the full joint distribution as the product of the local conditional distributions:

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e.g., \( P(j \land m \land a \land \neg b \land \neg e) = \)

\[
P(j|a)P(m|a)P(a|\neg b, \neg e)P(\neg b)P(\neg e) = 0.9 \times 0.7 \times 0.001 \times 0.999 \times 0.998 \\ \approx 0.00063
\]
Example - Car Insurance

http://aispace.org/bayes
Specifying Distributions - Discrete Variables

- Earlier we saw the use of conditional probability tables (CPT) for specifying a distribution over discrete random variables with discrete-valued parents.
- For a variable with no parents, with $K$ possible states:

$$ p(x|\mu) = \prod_{k=1}^{K} \mu_k^{x_k} $$

- e.g. $p(B) = 0.001^B_1 0.999^B_2$, 1-of-$K$ representation
Specifying Distributions - Discrete Variables cont.

- With two variables $x_1, x_2$ can have two cases

  ![Diagram](image)

  - Dependent
    
    $$p(x_1, x_2 | \mu) = p(x_1 | \mu)p(x_2 | x_1, \mu)$$
    
    $$= \left( \prod_{k=1}^{K} \mu_{x_{1k}}^{x_1} \right) \left( \prod_{k=1}^{K} \prod_{j=1}^{K} \mu_{x_{1k}x_{2j}}^{x_{1k}x_{2j}} \right)$$
    
    - $K^2 - 1$ free parameters in $\mu$

  - Independent
    
    $$p(x_1, x_2 | \mu) = p(x_1 | \mu)p(x_2 | \mu)$$
    
    $$= \left( \prod_{k=1}^{K} \mu_{x_{1k}}^{x_1} \right) \left( \prod_{k=1}^{K} \mu_{x_{2k}}^{x_2} \right)$$
    
    - $2(K - 1)$ free parameters in $\mu$
Chains of Nodes

- With $M$ nodes, could form a chain as shown above
- Number of parameters is:
  \[
  (K - 1) + (M - 1)K(K - 1)
  \]
  \[
  \underbrace{x_1}_{\text{x}_1} + \underbrace{\text{others}}_{\text{others}}
  \]
- Compare to:
  - $K^M - 1$ for fully connected graph
  - $M(K - 1)$ for graph with no edges (all independent)
Another way to reduce number of parameters is sharing parameters (a. k. a. tying of parameters)

- Lower graph reuses same $\mu$ for nodes $2-M$
  - $\mu$ is a random variable in this network, could also be deterministic
- $(K - 1) + K(K - 1)$ parameters
Specifying Distributions - Continuous Variables

- One common type of conditional distribution for continuous variables is the linear-Gaussian

\[ p(x_i | pa_i) = \mathcal{N} \left( x_i; \sum_{j \in pa_i} w_{ij}x_j + b_i, v_i \right) \]

- e.g. With one parent Harvest:

\[ p(c|h) = \mathcal{N} \left( c; -0.5h + 5, 1 \right) \]

- For harvest \( h \), mean cost is \(-0.5h + 5\), variance is 1
Linear Gaussian

• Interesting fact: if all nodes in a Bayesian Network are linear Gaussian, joint distribution is a multivariate Gaussian.
• Converse is true as well, see Ch.2.3.

\[ p(x_i|pa_i) = \mathcal{N}\left(x_i; \sum_{j \in pa_i} w_{ij} x_j + b_i, v_i\right) \]

\[ p(x_1, \ldots, x_N) = \prod_{i=1}^{N} \mathcal{N}\left(x_i; \sum_{j \in pa_i} w_{ij} x_j + b_i, v_i\right) \]

• Each factor looks like \( \exp((x_i - (w^T x_{pa_i})^2) \), this product will be another quadratic form of the components of \( x \).
• With no links in graph, end up with diagonal covariance matrix
• With fully connected graph, end up with full covariance matrix
• Recall again that $a$ and $b$ are conditionally independent given $c$ \(a \perp b | c\) if
  • \(p(a|b,c) = p(a|c)\) or equivalently
  • \(p(a,b|c) = p(a|c)p(b|c)\)

• Before we stated that links in a graph are \(\approx\) “direct influences”

• We now develop a correct notion of links, in terms of the conditional independences they represent
  • This will be useful for general-purpose inference methods
  • It provides a fast solution to the relevance problem: determine whether $X$ is relevant to $Y$ given knowledge of $Z$. 

Conditional Independence in Bayesian Networks
A Tale of Three Graphs - Part 1

The graph above means

\[ p(a, b, c) = p(a|c)p(b|c)p(c) \]

\[ p(a, b) = \sum_c p(a|c)p(b|c)p(c) \]

\[ \neq p(a)p(b) \text{ in general} \]

So \( a \) and \( b \) not independent
However, conditioned on $c$

$$p(a, b|c) = \frac{p(a, b, c)}{p(c)} = \frac{p(a|c)p(b|c)p(c)}{p(c)} = p(a|c)p(b|c)$$

So $a \perp \perp b|c$
A Tale of Three Graphs - Part 1

- Note the path from $a$ to $b$ in the graph
  - When $c$ is not observed, path is open, $a$ and $b$ not independent
  - When $c$ is observed, path is blocked, $a$ and $b$ independent
- In this case $c$ is tail-to-tail with respect to this path
A Tale of Three Graphs - Part 2

- The graph above means

\[ p(a, b, c) = p(a)p(b|c)p(c|a) \]

- Again, \( a \) and \( b \) not independent
• However, conditioned on $c$

\[
p(a, b|c) = \frac{p(a, b, c)}{p(c)} = \frac{p(a)p(b|c)}{p(c)}p(c|a)
\]

\[
= \frac{p(a)p(b|c)}{p(c)} \cdot \frac{p(c|a)}{p(a)}
\]

\[
= p(a|c)p(b|c)
\]

• So $a \perp\!\!\!\!\!\!\!\perp b|c$
A Tale of Three Graphs - Part 2

- As before, the path from $a$ to $b$ in the graph
  - When $c$ is not observed, path is open, $a$ and $b$ not independent
  - When $c$ is observed, path is blocked, $a$ and $b$ independent
- In this case $c$ is head-to-tail with respect to this path
The graph above means

\[ p(a, b, c) = p(a)p(b)p(c|a, b) \]

\[ p(a, b) = \sum_{c} p(a)p(b)p(c|a, b) \]

\[ = p(a)p(b) \]

This time \(a\) and \(b\) are independent.
A Tale of Three Graphs - Part 3

- However, conditioned on $c$

  $p(a, b|c) = \frac{p(a, b, c)}{p(c)} = \frac{p(a)p(b)p(c|a, b)}{p(c)}$

  $\neq p(a|c)p(b|c)$ in general

- So $a$ is dependent on $b$ given $c$
The behaviour here is different
- When $c$ is not observed, path is blocked, $a$ and $b$ independent
- When $c$ is observed, path is unblocked, $a$ and $b$ not independent

In this case $c$ is head-to-head with respect to this path

Situation is in fact more complex, path is unblocked if any descendant of $c$ is observed
• Binary random variables $B$ (battery charged), $F$ (fuel tank full), $G$ (fuel gauge reads full)

• $B$ and $F$ independent

• But if we observe $G = 0$ (false) things change
  • e.g. $p(F = 0|G = 0, B = 0)$ could be less than $p(F = 0|G = 0)$, as $B = 0$ explains away the fact that the gauge reads empty
  • Recall that $p(F|G, B) = p(F|G)$ is another $F \perp \perp B|G$
D-separation

- A general statement of conditional independence
- For sets of nodes $A, B, C$, check all paths from $A$ to $B$ in graph
- If all paths are blocked, then $A \perp\!\!\!\!\!\!\!\perp B | C$
- Path is blocked if:
  - Arrows meet head-to-tail or tail-to-tail at a node in $C$
  - Arrows meet head-to-head at a node, and neither node nor any descendent is in $C$
Naive Bayes

- Commonly used *naive Bayes* classification model
- Class label $z$, features $x_1, \ldots, x_D$
- Model assumes features independent given class label
  - *Tail-to-tail* at $z$, blocks path between features
What is the minimal set of nodes which makes a node $x_i$ conditionally independent from the rest of the graph?

- $x_i$’s parents, children, and children’s parents (co-parents)

Define this set $MB$, and consider:

\[
p(x_i | x_{\{j \neq i\}}) = \frac{p(x_1, \ldots, x_D)}{\int p(x_1, \ldots, x_D) dx_i} = \frac{\prod_k p(x_k | pa_k)}{\int \prod_k p(x_k | pa_k) dx_i}
\]

- All factors other than those for which $x_i$ is $x_k$ or in $pa_k$ cancel
Learning Parameters

- When all random variables are observed in training data, relatively straight-forward
  - Distribution factors, all factors observed
  - e.g. Maximum likelihood used to set parameters of each distribution $p(x_i|pa_i)$ separately
- When some random variables not observed, it’s tricky
  - This is a common case
  - Expectation-maximization (later) is a method for this
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