Graphical Models - Part I

CMPT 419/726
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Feb. 10, 2020

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

Probabilistic Models

Bayesian Networks

Markov Random Fields

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

- **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

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

• Can answer query such as

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

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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

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

$$
p(Q|E = e) = \frac{p(Q, E = e)}{p(E = e)} = \frac{\sum_h p(Q, E = e, H = h)}{\sum_{q,h} p(Q = q, E = e, H = h)}
$$
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 (*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:
  \[ P(\text{catch}|\text{toothache}, \text{cavity}) = P(\text{catch}|\text{cavity}) \]
- The same independence holds if I haven’t got a cavity:
  \[ P(\text{catch}|\text{toothache}, \neg\text{cavity}) = P(\text{catch}|\neg\text{cavity}) \]
- \textit{Catch} is \textbf{conditionally independent} of \textit{Toothache} given \textit{Cavity}: $p(Catch|Toothache, Cavity) = p(Catch|Cavity)$
- Equivalent statements:
  - $p(\text{Toothache}|\text{Catch, Cavity}) = p(\text{Toothache}|\text{Cavity})$
  - $p(\text{Toothache}, \text{Catch}|\text{Cavity}) = p(\text{Toothache}|\text{Cavity})p(\text{Catch}|\text{Cavity})$
  - \textit{Toothache} \ Jeffrey \text{Catch}|\text{Cavity}
Conditional Independence contd.

- Write out full joint distribution using chain rule:
  \[ p(\text{Toothache}, \text{Catch}, \text{Cavity}) \]
  \[ = p(\text{Toothache}|\text{Catch}, \text{Cavity})p(\text{Catch}, \text{Cavity}) \]
  \[ = p(\text{Toothache}|\text{Catch}, \text{Cavity})p(\text{Catch}|\text{Cavity})p(\text{Cavity}) \]
  \[ = p(\text{Toothache}|\text{Cavity})p(\text{Catch}|\text{Cavity})p(\text{Cavity}) \]
  \[ 2 + 2 + 1 = 5 \text{ independent numbers} \]

- 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 2 types of graph (can be combined)
  - Directed graphs: Bayesian networks
  - Undirected graphs: Markov Random Fields
  - Factor graphs (won’t cover)
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 ∼ “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
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, ?? 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:

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

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

\[
P(j | a)P(m | a)P(a | \neg b, \neg e)P(\neg b)P(\neg e)
\]

\[
= 0.9 \times 0.7 \times 0.001 \times 0.999 \times 0.998
\]

\[
\approx 0.00063
\]
Constructing Bayesian Networks

- Need a method such that a series of locally testable assertions of conditional independence guarantees the required global semantics

1. Choose an ordering of variables $X_1, \ldots, X_n$
2. For $i = 1$ to $n$
   - add $X_i$ to the network
   - select parents from $X_1, \ldots, X_{i-1}$ such that
     $$p(X_i|pa(X_i)) = p(X_i|X_1, \ldots, X_{i-1})$$

- This choice of parents guarantees the global semantics:

$$p(X_1, \ldots, X_n) = \prod_{i=1}^{n} p(X_i|X_1, \ldots, X_{i-1})$$ \hspace{1cm} \text{(chain rule)}$$

$$= \prod_{i=1}^{n} p(X_i|pa(X_i))$$ \hspace{1cm} \text{(by construction)}$$
Example

Suppose we choose the ordering $M, J, A, B, E$

$P(J|M) = P(J)\, ? \, \text{No}$
$P(B|A, J, M) = P(B|A)\, ? \, \text{Yes}$
$P(B|A, J, M) = P(B)\, ? \, \text{No}$
$P(E|B, A, J, M) = P(E|A)\, ? \, \text{No}$
$P(E|B, A, J, M) = P(E|A, B)\, ? \, \text{Yes}$
Example contd.

- Deciding conditional independence is hard in noncausal directions
  - (Causal models and conditional independence seem hardwired for humans!)
- Assessing conditional probabilities is hard in noncausal directions
- Network is less compact: $1 + 2 + 4 + 2 + 4 = 13$ numbers needed
Example - Car Insurance
Example - Polynomial Regression

• Bayesian polynomial regression model
• Observations $t = (t_1, ..., t_N)$
• Vector of coefficients $\mathbf{w}$
• Inputs $x$ and noise variance $\sigma^2$ were assumed fixed, not stochastic and hence not in model
• Joint distribution:

$$p(t, \mathbf{w}) = p(\mathbf{w}) \prod_{n=1}^{N} p(t_n|\mathbf{w})$$
Plates

- A shorthand for writing repeated nodes such as the $t_n$ uses plates
Deterministic Model Parameters

- Can also include deterministic parameters (not stochastic) as small nodes
- Bayesian polynomial regression model:

\[
p(t, w | x, \alpha, \sigma^2) = p(w | \alpha) \prod_{n=1}^{N} p(t_n | w, x_n, \sigma^2)
\]
In polynomial regression, we assumed we had a training set of $N$ pairs $(x_n, t_n)$

Convention is to use shaded nodes for observed random variables.
Suppose we wished to predict the value $\hat{t}$ for a new input $\hat{x}$

The Bayesian network used for this inference task would be this one
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

  \[
  p(x_1, x_2 | \mu) = p(x_1 | \mu)p(x_2 | x_1, \mu) = \left( \prod_{k=1}^{K} \mu_{k1}^{x_{1k}} \right) \left( \prod_{k=1}^{K} \prod_{j=1}^{K} \mu_{kj2}^{x_{1k}x_{2j}} \right)
  \]

  - \( K^2 - 1 \) free parameters in \( \mu \)

  - Independent

  \[
  p(x_1, x_2 | \mu) = p(x_1 | \mu)p(x_2 | \mu) = \left( \prod_{k=1}^{K} \mu_{k1}^{x_{1k}} \right) \left( \prod_{k=1}^{K} \mu_{k2}^{x_{2k}} \right)
  \]

  - \( 2(K - 1) \) free parameters in \( \mu \)
Chains of Nodes

- With $M$ nodes, could form a chain as shown above.
- Number of parameters is:
  \[
  \frac{(K - 1)}{x_1} + \frac{(M - 1)K(K - 1)}{\text{others}}
  \]
- 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**

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

- e.g. With one parent *Harvest*:

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

- 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

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

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

• Each factor looks like \( \exp\left( (x_i - \mathbf{w}_i^T \mathbf{x}_{pa_i})^2 \right) \), this product will be another quadratic form

• With no links in graph, end up with diagonal covariance matrix

• With fully connected graph, end up with full covariance matrix
Conditional Independence in Bayesian Networks

- 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 $\approx$ “directly 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
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 $a \perp b | c$
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
A Tale of Three Graphs - Part 2

- However, conditioned on $c$

\[
p(a, b|c) = \frac{p(a, b, c)}{p(c)} = \frac{p(a)p(b|c)}{p(c)}p(c|a)
\]
\[
= \frac{p(a)p(b|c)}{p(c)} \frac{p(a|c)p(c)}{p(a)} \quad \text{Bayes’ rule}
\]
\[
= p(a|c)p(b|c)
\]

- So $a \independent b|c$
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.
A Tale of Three Graphs - Part 3

- 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 $c$

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

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

So $a \perp b | c$
A Tale of Three Graphs - Part 3

- Frustratingly, 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 descendent of $c$ is observed
Part 3 - Intuition

- 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 $F \perp B|G$
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 $A \perp B | C$
- 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:

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

- 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 $p(x_i | p a_i)$ 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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