Graphical Models - Part I

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

Outline

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

$$p(x_1, x_2, \dots, x_K)$$

  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

	toothache		*¬ toothache*	
	catch	*¬ catch*	*catch*	*¬ catch*
cavity	**.108**	**.012**	**.072**	**.008**
¬ cavity	**.016**	**.064**	**.144**	**.576**

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

$$p(\neg cavity | toothache)$$

Joint Distribution

	toothache		*¬ toothache*	
	catch	*¬ catch*	*catch*	*¬ catch*
cavity	**.108**	**.012**	**.072**	**.008**
¬ cavity	**.016**	**.064**	**.144**	**.576**

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

$$p(\neg cavity | toothache) = \frac{p(\neg cavity, toothache)}{p(toothache)}$$

$$p(\neg cavity | toothache) = \frac{0.016 + 0.064}{0.108 + 0.012 + 0.016 + 0.064} = 0.4$$

Joint Distribution

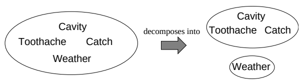
- In general, to answer a query on random variables $\boldsymbol{Q} = Q_1, \ldots, Q_N$ given evidence $\boldsymbol{E} = \boldsymbol{e}$, $\boldsymbol{E} = E_1, \ldots, E_M$, $\boldsymbol{e} = e_1, \ldots, e_M$:

$$\begin{aligned} p(\boldsymbol{Q}|\boldsymbol{E} = \boldsymbol{e}) &= \frac{p(\boldsymbol{Q}, \boldsymbol{E} = \boldsymbol{e})}{p(\boldsymbol{E} = \boldsymbol{e})} \\ &= \frac{\sum_{\boldsymbol{h}} p(\boldsymbol{Q}, \boldsymbol{E} = \boldsymbol{e}, \boldsymbol{H} = \boldsymbol{h})}{\sum_{\boldsymbol{q},\boldsymbol{h}} p(\boldsymbol{Q} = \boldsymbol{q}, \boldsymbol{E} = \boldsymbol{e}, \boldsymbol{H} = \boldsymbol{h})} \end{aligned}$$

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
  $p(A|B) = p(A)$ or $p(B|A) = p(B)$ or $p(A,B) = p(A)p(B)$
- $p(Toothache, Catch, Cavity, Weather) =$
  $p(Toothache, Catch, Cavity)p(Weather)$
  - 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:
  (1) $P(catch|toothache, cavity) = P(catch|cavity)$
- The same independence holds if I haven't got a cavity:
  (2) $P(catch|toothache, \neg cavity) = P(catch|\neg cavity)$
- $Catch$ is conditionally independent of $Toothache$ given $Cavity$: $p(Catch|Toothache, Cavity) = p(Catch|Cavity)$
- Equivalent statements:
  - $p(Toothache|Catch, Cavity) = p(Toothache|Cavity)$
  - $p(Toothache, Catch|Cavity) =$
    $p(Toothache|Cavity)p(Catch|Cavity)$
  - $Toothache \perp\!\!\!\perp Catch|Cavity$

Conditional Independence contd.

- Write out full joint distribution using chain rule:
  $p(Toothache, Catch, Cavity)$
  $= p(Toothache|Catch, Cavity)p(Catch, Cavity)$
  $= p(Toothache|Catch, Cavity)p(Catch|Cavity)p(Cavity)$
  $= p(Toothache|Cavity)p(Catch|Cavity)p(Cavity)$
  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 indepence 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)

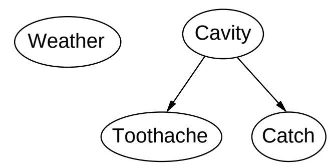
Bayesian Networks

- 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

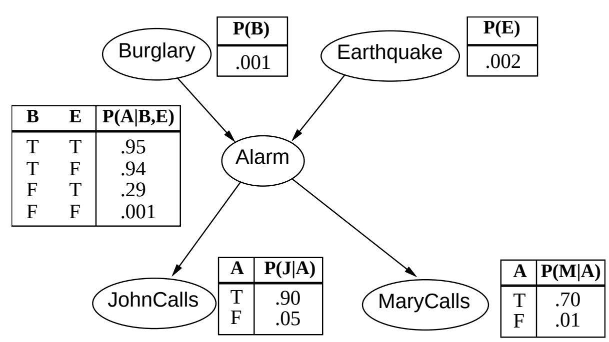


- Topology of network encodes conditional independence assertions:
  - *Weather* is independent of the other variables
  - *Toothache* and *Catch* are conditionally independent given *Cavity*

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.



P(B)
.001

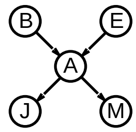
P(E)
.002

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

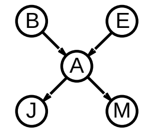
A	P(M|A)
T	.70
F	.01

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:

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

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

$$\begin{aligned} & P(j|a)P(m|a)P(a|\neg b, \neg e)P(\neg b)P(\neg e) \\ = \ & 0.9 \times 0.7 \times 0.001 \times 0.999 \times 0.998 \\ \approx \ & 0.00063 \end{aligned}$$

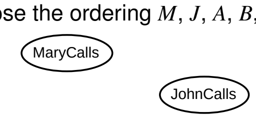
Constructing Bayesian Networks

- 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:

$$\begin{aligned} p(X_1, \ldots, X_n) &= \prod_{i=1}^{n} p(X_i | X_1, \ldots, X_{i-1}) \quad \text{(chain rule)} \\ &= \prod_{i=1}^{n} p(X_i | pa(X_i)) \quad \text{(by construction)} \end{aligned}$$

Example

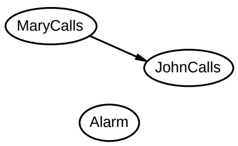
Suppose we choose the ordering M, J, A, B, E



$P(J|M) = P(J)$?

Example

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



$P(J|M) = P(J)$? No
$P(A|J,M) = P(A|J)$? $P(A|J,M) = P(A)$?

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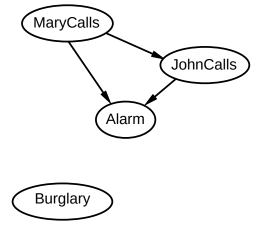
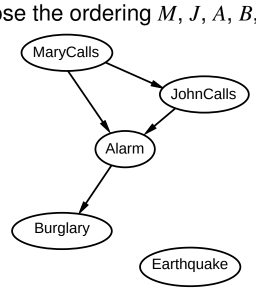


$P(J|M) = P(J)$? No
$P(A|J,M) = P(A|J)$? $P(A|J,M) = P(A)$? No
$P(B|A,J,M) = P(B|A)$?
$P(B|A,J,M) = P(B)$?

Example

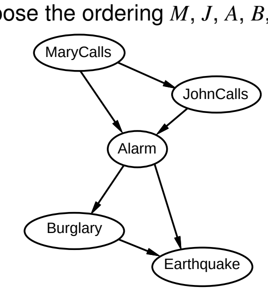
Suppose we choose the ordering M, J, A, B, E



$P(J|M) = P(J)$? No
$P(A|J,M) = P(A|J)$? $P(A|J,M) = P(A)$? No
$P(B|A,J,M) = P(B|A)$? Yes
$P(B|A,J,M) = P(B)$? No
$P(E|B,A,J,M) = P(E|A)$?
$P(E|B,A,J,M) = P(E|A,B)$?

Example

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



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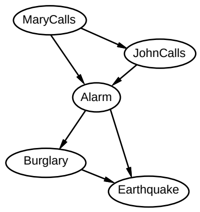
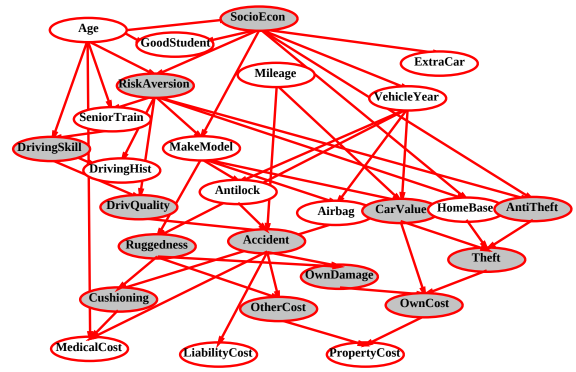
$P(E|B,A,J,M) = P(E|A)$? No
$P(E|B,A,J,M) = P(E|A,B)$? Yes

Example contd.

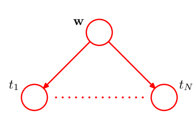


- Deciding conditional independence is hard in noncausal directions
  - (Causal models and conditional independence seem hardwired for humans!)
- Assessing conditional probabilities is hard in noncausal directions
- Network is less compact: $1 + 2 + 4 + 2 + 4 = 13$ numbers needed

Example - Car Insurance



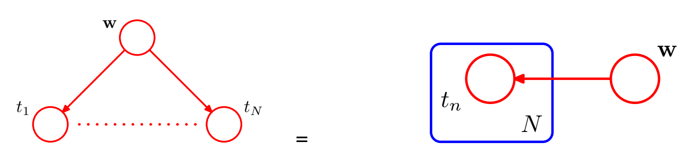
Example - Polynomial Regression



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

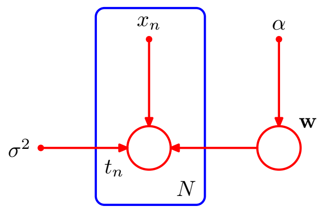
$$p(\boldsymbol{t}, \boldsymbol{w}) = p(\boldsymbol{w}) \prod_{n=1}^{N} p(t_n|\boldsymbol{w})$$

Plates



- A shorthand for writing repeated nodes such as the t_n uses plates

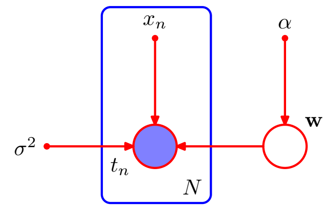
Deterministic Model Parameters



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

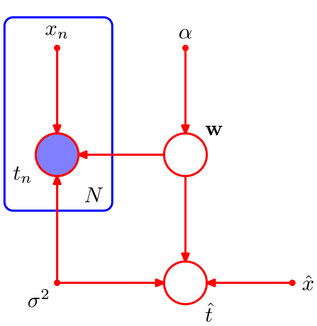
$$p(\boldsymbol{t}, \boldsymbol{w}|\boldsymbol{x}, \alpha, \sigma^2) = p(\boldsymbol{w}|\alpha) \prod_{n=1}^{N} p(t_n|\boldsymbol{w}, x_n, \sigma^2)$$

Observations



- In polynomial regression, we assumed we had a training set of N pairs $(\boldsymbol{x}_n, t_n)$
- Convention is to use shaded nodes for observed random variables

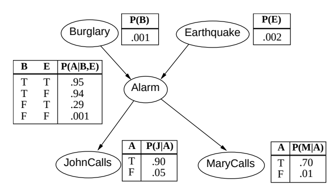
Predictions



- 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:

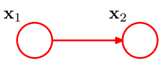


$$p(\boldsymbol{x}|\boldsymbol{\mu}) = \prod_{k=1}^{K} \mu_k^{x_k}$$

- e.g. $p(B) = 0.001^{B_1} 0.999^{B_2}$, 1-of-$K$ representation

Specifying Distributions - Discrete Variables cont.

- With two variables $\boldsymbol{x}_1, \boldsymbol{x}_2$ can have two cases



- Dependent

$$p(\boldsymbol{x}_1, \boldsymbol{x}_2|\boldsymbol{\mu}) = p(\boldsymbol{x}_1|\boldsymbol{\mu})p(\boldsymbol{x}_2|\boldsymbol{x}_1, \boldsymbol{\mu}) = \left(\prod_{k=1}^{K} \mu_{k1}^{x_{1k}}\right)\left(\prod_{k=1}^{K}\prod_{j=1}^{K} \mu_{kj2}^{x_{1k}x_{2j}}\right)$$

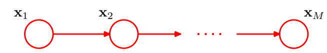
- $K^2 - 1$ free parameters in $\boldsymbol{\mu}$

- Independent

$$p(\boldsymbol{x}_1, \boldsymbol{x}_2|\boldsymbol{\mu}) = p(\boldsymbol{x}_1|\boldsymbol{\mu})p(\boldsymbol{x}_2|\boldsymbol{\mu}) = \left(\prod_{k=1}^{K} \mu_{k1}^{x_{1k}}\right)\left(\prod_{k=1}^{K} \mu_{k2}^{x_{2k}}\right)$$

- $2(K-1)$ free parameters in $\boldsymbol{\mu}$

Chains of Nodes

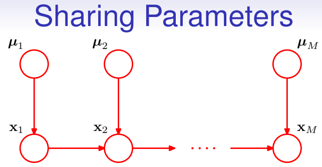


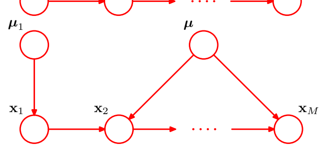
- With M nodes, could form a chain as shown above
- Number of parameters is:

$$\underbrace{(K-1)}_{\boldsymbol{x}_1} + (M-1)\underbrace{K(K-1)}_{others}$$

- Compare to:
  - $K^M - 1$ for fully connected graph
  - $M(K-1)$ for graph with no edges (all independent)

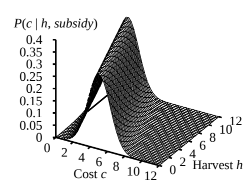
Sharing Parameters





- Another way to reduce number of parameters is sharing parameters (a. k. a. tying of parameters)
- Lower graph reuses same $\boldsymbol{\mu}$ for nodes 2-M
  - $\boldsymbol{\mu}$ 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*:

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

  - 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

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

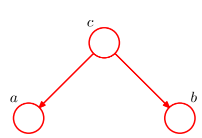
$$p(x_1, \ldots, x_N) = \prod_{i=1}^{N} \mathcal{N}\left(x_i; \sum_{j \in pa_i} w_{ij} x_j + b_i, v_i\right)$$

- Each factor looks like $\exp((x_i - (\boldsymbol{w}_i^T \boldsymbol{x}_{pa_i})^2)$, 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 ($a \perp\!\!\!\perp b|c$) 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

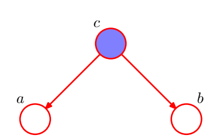


- The graph above means

$$\begin{aligned} p(a, b, c) &= p(a|c)p(b|c)p(c) \\ p(a, b) &= \sum_c p(a|c)p(b|c)p(c) \\ &\neq p(a)p(b) \text{ in general} \end{aligned}$$

- So a and b not independent

A Tale of Three Graphs - Part 1

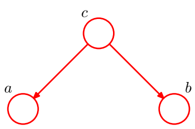


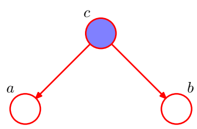
- However, conditioned on c

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

- So $a \perp\!\!\!\perp b|c$

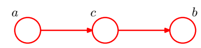
A Tale of Three Graphs - Part 1





- 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

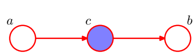


- The graph above means

$$p(a, b, c) = p(a)p(b|c)p(c|a)$$

- Again a and b not independent

A Tale of Three Graphs - Part 2



- However, conditioned on c

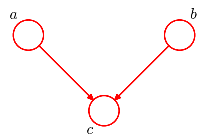
$$\begin{aligned} p(a, b|c) &= \frac{p(a,b,c)}{p(c)} = \frac{p(a)p(b|c)}{p(c)}p(c|a) \\ &= \frac{p(a)p(b|c)}{p(c)} \underbrace{\frac{p(a|c)p(c)}{p(a)}}_{\text{Bayes' Rule}} \\ &= p(a|c)p(b|c) \end{aligned}$$

- 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

A Tale of Three Graphs - Part 3

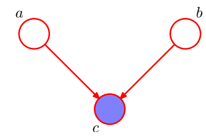


- The graph above means

$$\begin{aligned} p(a,b,c) &= p(a)p(b)p(c|a,b) \\ p(a,b) &= \sum_c p(a)p(b)p(c|a,b) \\ &= p(a)p(b) \end{aligned}$$

- This time a and b are independent

A Tale of Three Graphs - Part 3

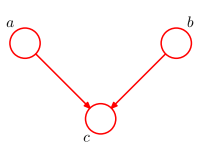


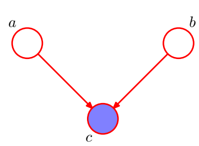
- However, conditioned on c

$$\begin{aligned} p(a,b|c) &= \frac{p(a,b,c)}{p(c)} = \frac{p(a)p(b)p(c|a,b)}{p(c)} \\ &\neq p(a|c)p(b|c) \text{ in general} \end{aligned}$$

- So $a \not\perp\!\!\!\perp b|c$

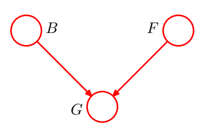
A Tale of Three Graphs - Part 3

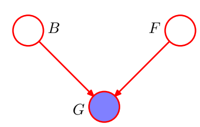


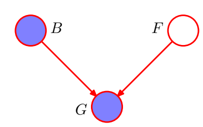


- Frustratingly, the behaviour here is different
  - When c is not observed, path is blocked, a and b independent
  - When c is observed, path is unblocked, a and b not independent
- In this case c is head-to-head with respect to this path
- Situation is in fact more complex, path is unblocked if any descendent of c is observed

Part 3 - Intuition





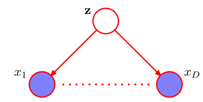


- Binary random variables B (battery charged), F (fuel tank full), G (fuel gauge reads full)
- B and F independent
- But if we observe $G = 0$ (false) things change
  - e.g. $p(F = 0|G = 0, B = 0)$ could be less than $p(F = 0|G = 0)$, as $B = 0$ explains away the fact that the gauge reads empty
  - Recall that $p(F|G, B) = p(F|G)$ is another $F \perp\!\!\!\perp B|G$

D-separation

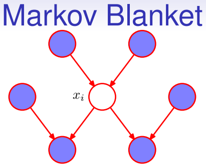
- A general statement of conditional independence
- For sets of nodes A, B, C, check all paths from A to B in graph
- If all paths are blocked, then $A \perp\!\!\!\perp B|C$
- Path is blocked if:
  - Arrows meet head-to-tail or tail-to-tail at a node in C
  - Arrows meet head-to-head at a node, and neither 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

Markov Blanket



- 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 is a method for this