Soft Computing

Lecture Notes on Machine Learning

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Unsupervised Learning
– Bayesian Networks –
Beyond Independence . . .

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- It makes computation possible
- It yields optimal classifiers when satisfied
- It gives good enough generalization to our Bayes Classifiers
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These models are often referred also as **Graphical Models**
Bayesian Networks Intro

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Similar to Naïve Bayes we will make some independence assumptions, but not as strong as the assumption of all variables being independent.
Bayesian Networks

A Bayesian Network is a compact representation of the joint probability distribution of a set of variables by explicitly indicating the assumptions of conditional independence through the following:

- A Directed Acyclic Graph (DAG)
  - Nodes - random variables
  - Edges - direct influence
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A Bayesian Network is a compact representation of the joint probability distribution of a set of variables by explicitly indicating the assumptions of conditional independence through the following:

- A Directed Acyclic Graph (DAG)
  - Nodes - random variables
  - Edges - direct influence
- Set of Conditional Probability Distributions (CPD) for “influenced” variables

\[
\begin{align*}
S, B & \quad S, \sim B & \sim S, B & \sim S, \sim B \\
C & 0.4 & 0.1 & 0.8 & 0.2 \\
\sim C & 0.6 & 0.9 & 0.2 & 0.8
\end{align*}
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Conditional Independence

We say $X_1$ is conditionally independent of $X_2$ given $X_3$ if the probability of $X_1$ is independent of $X_2$ given some knowledge about $X_3$:

$$P(X_1|X_2, X_3) = P(X_1|X_3)$$
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The same can be said for a set of variables: $X_1, X_2, X_3$ is independent of $Y_1, Y_2, Y_3$ given $Z_1, Z_2, Z_3$:

$$P(X_1, X_2, X_3|Y_1, Y_2, Y_3, Z_1, Z_2, Z_3) = P(X_1, X_2, X_3|Z_1, Z_2, Z_3)$$
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Example: Martin and Norman toss the same coin. Let be $A$ “Norman’s outcome”, and $B$ “Martin’s outcome”. Assume the coin might be biased; in this case $A$ and $B$ are not independent: observing that $B$ is Heads causes us to increase our belief in $A$ being Heads.
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Variables $A$ and $B$ are both dependent on $C$, “the coin is biased towards Heads with probability $\theta$”. Once we know for certain the value of $C$ then any evidence about $B$ cannot change our belief about $A$.

$$P(A|B, C) = P(A|C)$$
The Sprinkler Example: Modeling

The event “grass is wet” ($W=true$) has two possible causes: either the water Sprinkler is on ($S=true$) or it is Raining ($R=true$).

\[
\begin{array}{c|cc}
C & P(S=true) & P(S=false) \\
\hline
true & 0.5 & 0.5 \\
false & 0.9 & 0.1 \\
\end{array}
\]

\[
\begin{array}{c|cc}
P(C=true) & P(C=false) \\
\hline
0.5 & 0.5 \\
\end{array}
\]

\[
\begin{array}{c|cc}
P(R=true) & P(R=false) \\
\hline
0.8 & 0.2 \\
false & 0.2 & 0.8 \\
\end{array}
\]

\[
\begin{array}{c|cc}
P(W=true) & P(W=false) \\
\hline
true true & 0.99 & 0.01 \\
true false & 0.9 & 0.1 \\
false true & 0.9 & 0.1 \\
false false & 0 & 1 \\
\end{array}
\]
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The strength of this relationship is shown in the tables. For example, on second row, \(P(W = \text{true}|S = \text{true}, R = \text{false}) = 0.9\), and, since each row sums up to one, \(P(W = \text{false}|S = \text{true}, R = \text{false}) = 1 - 0.9 = 0.1\).
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The $C$ node has no parents, its Conditional Probability Table (CPT) simply specifies the prior probability that it is $Cloudy$ (in this case, 0.5).
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Using the chain rule we get the joint probability of nodes in the graph

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P(C, S, R, W) = P(W | C, S, R) P(R | C, S) P(S | C) P(C)
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In general, with \( N \) binary nodes and being \( k \) the maximum node fan-in, the full joint requires \( O(2^N) \) parameters while the factored one \( O(N \cdot 2^k) \).
The Sprinkler Example: Making Inference

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<table>
<thead>
<tr>
<th>C</th>
<th>P(S=true)</th>
<th>P(S=false)</th>
</tr>
</thead>
<tbody>
<tr>
<td>true</td>
<td>0.5</td>
<td>0.5</td>
</tr>
<tr>
<td>false</td>
<td>0.9</td>
<td>0.1</td>
</tr>
</tbody>
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<table>
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<th>P(R=true)</th>
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<tbody>
<tr>
<td>true</td>
<td>0.8</td>
<td>0.2</td>
</tr>
<tr>
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<td>0.2</td>
<td>0.8</td>
</tr>
</tbody>
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<table>
<thead>
<tr>
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</tr>
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<tbody>
<tr>
<td>true</td>
<td>true</td>
<td>0.99</td>
<td>0.01</td>
</tr>
<tr>
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<td>false</td>
<td>0.9</td>
<td>0.1</td>
</tr>
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Use Bayes’ rule to compute the posterior probability of each explanation:

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P(S|W) = \frac{P(S, W)}{P(W)} = \sum_{c, r} P(C, S, R, W)/P(W) = 0.430
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\(P(W)\) is a normalizing constant, equal to the probability (likelihood) of the data; the likelihood ratio is \(0.7079/0.4298 = 1.647\).
The Sprinkler Example: Explaining Away

In Sprinkler Example the two causes “compete” to “explain” the observed data. Hence $S$ and $R$ become conditionally dependent given that their common child, $W$, is observed.

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In College population, being Brainy makes you less likely to be Sporty and vice versa, because either property alone is sufficient to explain evidence on $C$

$$P(S = 1|C = 1, B = 1) \leq P(S = 1|C = 1)$$
Bottom-up and Top-down Reasoning

Looking at the simple Sprinkler Example we can already see the two kinds of reasoning we can make with Bayesian Networks:

- “bottom up” reasoning: we had evidence of an effect (Wet Grass), and inferred the most likely cause; it goes from effects to causes and it is a common task in expert systems or diagnostic;
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The most interesting property of Bayesian Networks is that they can be used to reason about causality on a solid mathematical basis:

**Question:** Can we distinguish causation from mere correlation? So we don’t need to make experiments to infer causality.

**Answer:** Yes, “sometimes”, but we need to measure the relationships between at least three variables.

For details refer to [Causality: Models, Reasoning and Inference](#), Judea Pearl, 2000.
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- $C$ is a “bridge”: nodes upstream and downstream of $C$ are dependent iff $C$ is hidden, because conditioning breaks the graph at that point.
Undirected Bayesian Networks

Undirected graphical models, also called Markov Random Fields (MRFs) or Markov Networks, are more popular with the Physics and Computer Vision communities, and have a simpler definition of independence:

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When converting a directed graph to an undirected graph, we must add links between “unmarried” parents who share a common child (i.e., “moralize” the graph) to prevent reading incorrect independences.
Graphical Models with Real Values

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  *We’ll see just a few of them ... don’t worry!*
Inference in Bayes Nets: Variable Elimination

We can sometimes use the factored representation of Joint Probability to do marginalisation efficiently. The key idea is to “push sums in” as far as possible when summing (marginalizing) out irrelevant terms:

\[
p(W) = \sum_c \sum_s \sum_r P(C, S, R, W)
\]

\[
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Inference in Bayes Nets: Variable Elimination

We can sometimes use the factored representation of Joint Probability to do marginalisation efficiently. The key idea is to “push sums in” as far as possible when summing (marginalizing) out irrelevant terms:

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As we perform the innermost sums we create new terms to be summed:

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Complexity is bounded by the size of the largest term. Finding the optimal order is NP-hard, although greedy algorithms work well in practice.
Inference in Bayes Nets: Local Message Passing (I)

If the underlying undirected graph of the BN is acyclic (i.e., a tree), we can use a local message passing algorithm:

- Suppose we want $P(X_i|E)$ where $E$ is some set of evidence variables
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- Let’s Split $E$ into two parts:
  - $E_i^-$ assignments to variables in the subtree rooted at $X_i$;
  - $E_i^+$ the rest of $E$.
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$$P(X_i|E) = P(X_i|E_i^-, E_i^+)$$

$$= \frac{P(E_i^-|X_i, E_i^+)P(X_i|E_i^+)}{P(E_i^-|E_i^+)}$$

$$= \frac{P(E_i^-|X_i)P(X_i|E_i^+)}{P(E_i^-|E_i^+)}$$

$$= \alpha \pi(X_i) \lambda(X_i)$$

With $\alpha$ independent from $X_i$, $\pi(X_i) = P(X_i|E_i^+)$, $\lambda(X_i) = P(E_i^-|X_i)$. 

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  - $X_i \in E$: then $\lambda(X_i) = 1$ if $X_i$ matches $E$, 0 otherwise;
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\lambda(X_i) = P(E_i^- | X_i) = \sum_j P(E_i, X_c = j | X_i)
$$

$$
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  \]

- **if $X_i$ has a set of children $C$ since $X_i$ d-separates them**
  \[
  \lambda(X_i) = P(E_i^- | X_i) = \prod_{X_j \in C} \lambda_j(X_j) = \prod_{X_j \in C} \left( \sum_{X_j} P(X_j | X_i) \lambda(X_j) \right)
  \]
  where $\lambda_j(X_j)$ is the contribution to $P(E_i^- | X_i)$ of subtree rooted at $X_j$. 

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We can now compute the rest of our inference: $\pi(X_i) = P(X_i | E_i^+)$

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\pi(X_i) = P(X_i|E_i^+) = \sum_j P(X_i, X_p = j|E_i^+) \\
= \sum_j P(X_i|X_p = j, E_i^+)P(X_p = j|E_i^+) \\
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Inference in Bayes Nets: Local Message Passing (III)

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\]

Having defined \( \pi_i(X_p = j) \) equal to \( \frac{P(X_p = j|E)}{\lambda_i(X_p = j)} \) we can now compute all \( \pi(X_i)s \) and then all the \( P(X_i|E)s \)!
Inference in Bayes Nets: Local Message Passing (IV)

In the message passing algorithm, we can thing nodes as autonomous processors passing $\lambda$ and $\pi$ messages to their neighbors.
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If we want $P(A, B|C)$ instead of just marginal distributions $P(A|C)$ and $P(B|C)$?

- Apply the chain rule:
  
  \[ P(A, B|C) = P(A|B, C)P(B|C); \]

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- Apply Local Message Passing twice.

This technique can be generalized to polytrees:
Inference in Bayes Nets: Message Passing with Cycles

The Local Message Passing algorithm can deal also with cycles:

- Clustering variables together:
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4. Randomly choose a sample \( w, w = \text{true} \) with prob \( P(W|s, r) \)

The sample \( c, s, r, w \) is a sample from the joint distribution of \( C, S, R, W \).
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- When $N$ is big enough we have:
  - $P(E_2) \approx N_c / N$
  - $P(E_1, E_2) \approx N_s / N$
  - $P(E_1 | E_2) = P(E_1, E_2) / P(E_2) \approx N_s / N_c$
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We should use **Likelihood Sampling**!
Inference in Bayes Nets: Simulation & Sampling (III)

We can exploit a simple idea to improve our sampling strategy

- Suppose in $E_2$ we have the constraint $X_i = v$
- We are about generating a random value with $P(X_i = v|\text{parents}) = w$;
- Generate always $X_i = v$ but weight the final answer by $w$. 
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This turns into the following algorithm (initialize $N_c = 0$ and $N_s = 0$):

1. Generate a random assignment for all variables matching $E_2$;
2. Define $w$ to be the probability that this assignment would have been generated instead of an unmatching assignment ($w$ is the product of all likelihood factors involved in its generation);
3. $N_c = N_c + w$;
4. if our sample matches $E_1$ the $N_s = N_s + w$;
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Again the ratio $N_s/N_c$ estimates our query $P(E_1|E_2)$
Bayesian Networks Applications

They originally arose to add probabilities in expert systems; a famous example is the reformulation of the Quick Medical Reference model.

- Top layer represents hidden disease;
- Bottom layer represents observed symptoms;
- QMR-DT is so densely connected that exact inference is impossible.

The goal is to infer the posterior probability of each disease given all the symptoms (which can be present, absent or unknown).
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The most widely used Bayes Nets are embedded in Microsoft’s products:
- Answer Wizard in Office 95;
- Office Assistant in Office 97;
- Over 30 Technical Support Troubleshooters.

Check the Economist article (22/3/01) about Microsoft’s application of BNs.
Learning Bayesian Networks

In order to define a Bayesian Network we need to specify:

- The graph topology (structure)
- The parameters of each Conditional Probability Density.
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We can specify both of them with the help of experts or it is possible to learn both of these from data; however remember that:

- Learning the structure is much harder than learning parameters
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This gives rise to 4 approaches:

<table>
<thead>
<tr>
<th>Structure/Observability</th>
<th>Full</th>
<th>Partial</th>
</tr>
</thead>
<tbody>
<tr>
<td>Known</td>
<td>Maximum Likelihood Estimation</td>
<td>EM (or gradient ascent)</td>
</tr>
<tr>
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<td>EM + search through model space</td>
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Learning: Known Structure & Full Observability

Learning has to find the values of the parameters of each Conditional Probability Distribution which maximizes the likelihood of the training data:

$$\mathcal{L} = \sum_{i=1}^{m} \sum_{r=1}^{R} \log P(X_i | Pa(X_i), D_r)$$

Log-likelihood decomposes according to the structure of the graph; we can maximize the contribution of each node independently.
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Example: For the *WetGrass* node, from a set of training data, we can just count the number of times the “grass is wet” when it is “raining” and the “sprinkler” is on, \( N(W = 1, S = 1, R = 1) \), and so on:

$$
P(W | S, R) = \frac{N(W, S, R)}{N(S, R)} = \frac{N(W, S, R)}{N(W, S, R) + N(W, S, R)}
$$
Learning: Known Structure & Partial Observability

When some of the nodes are hidden, we can use the *Expectation Maximization* (EM) algorithm to find a (locally) optimal estimate:

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Given the expected counts, maximize parameters, and recompute the expected counts iteratively. EM converges to a likelihood local maximum.
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**Example**: in the case of *WetGrass* node, we replace the observed counts of the events with the number of times we expect to see each event:

\[
P(W|S, R) = \frac{E[N(W, S, R)]}{E[N(S, R)]}
\]

where \( E[N(x)] \) is the expected number of times \( x \) occurs in the training set, given the current guess of the parameters: \( E[N(.|)] = \sum_k P(.|D_k) \).
Learning: Unknown Structure & Full Observability (I)

The maximum likelihood model $G_{MLE}$ will be a complete graph:

- It has the largest number of parameters and can fit the data the best
- This is a joint distribution, it will overfit for sure!
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taking logs, we find:

$$\log P(G|D) = \log P(D|G) + \log P(G) + c.$$
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Last term $c = -\log P(\mathcal{D})$ does not depend on $G$. We could use structure prior $P(G)$ to penalizes overly complex models, however, this is not necessary since the marginal likelihood term

$$P(\mathcal{D}|G) = \int_{\theta} P(\mathcal{D}|G, \theta)$$

has already a similar effect; it embodies the Bayesian Occam’s razor.
Learning: Unknown Structure & Full Observability (II)

The goal of structure learning is to learn a DAG that best explains the data:

- it is an NP-hard problem, since the number of DAGs on $M$ variables is super-exponential in $M$
  - there are 543 DAGs on 4 nodes;
  - there are $O(10^{18})$ DAGSs on 10 nodes.
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  - there are 543 DAGs on 4 nodes;
  - there are $O(10^{18})$ DAGSs on 10 nodes.
- if we know the ordering of the nodes, we can learn the parent set for each node independently
  - there are at most $\sum_{k=0}^{M} \binom{M}{k} = 2^M$ sets of possible parents.
Learning: Unknown Structure & Full Observability (II)

The goal of structure learning is to learn a DAG that best explains the data:

- it is an NP-hard problem, since the number of DAGs on $M$ variables is super-exponential in $M$
  - there are 543 DAGs on 4 nodes;
  - there are $O(10^{18})$ DAGSs on 10 nodes.

- if we know the ordering of the nodes, we can learn the parent set for each node independently
  - there are at most $\sum_{k=0}^{M} \binom{M}{k} = 2^M$ sets of possible parents.

We can start with an initial guess of the model structure, and then perform local search, evaluating the score of neighboring structures and move to the best one, until we reach a local optimum.
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- use the Tabu Search algorithm;
- use Genetic Algorithms to find a global optimum;
- use multiple restarts to try to find the global optimum, and to learn an ensemble of models.
Here come the tough part! We have that

- the structure is unknown;
- there are hidden variables and/or missing data.
Learning: Unknown Structure & Partial Observability

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This is usually intractable; we can use an approximation of the posterior called Bayesian Information Criterion (BIC):

\[ \log P(D|G) \approx \log P(D|G, \hat{\Theta}_G) - \frac{N}{2} \log R \]

where \( R \) is the number of samples, \( \hat{\Theta}_G \) is the ML estimate of model parameters, and \( N \) is the dimension of the model:
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- in the fully observable case, dimension of a model is the number of free parameters; in models with hidden variables, it might be less;
- BIC score decomposes into a sum of local terms, but local search is still expensive, because we need to run EM at each step to compute $\hat{\Theta}_G$. We can do local search inside the M-Step (Structural EM).