# Bayesian network internals 

Inference algorithms, time series \& distributed learning with Big Data


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Profile
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- PhD Imperial College - Bayesian networks
- Machine learning - 15 years
- Implementation
- Application
- Numerous techniques
- Algorithm programming even longer
- Scala, C\#, Java, C++
- Graduate scheme - mathematician (BAE Systems)
- Artificial Intelligence / ML research program 8 years (GE/USAF)
- BP trading \& risk analytics - big data + machine learning
- Also: NYSE stock exchange, hedge fund, actuarial consultancy, international newspaper


## What is a Bayesian network?

## What is a Bayesian network?

- DAG - directed acyclic graph
- Nodes, links, probability distributions
- Each node requires a probability distribution conditioned on its parents (if any)


## Example - Asia network



## Example - Waste network



## Example - the bat (40,000 links)



## Example - static \& temporal



## Insight, prediction \& diagnostics



## What is inference?

## Inference

- Asking a question given things you already know
- Encompasses prediction, reasoning \& diagnostics
- Given a number of symptoms, which diseases are most likely?
- How likely is it that a component will fail, given the current state of the system?
- Given recent behaviour of 2 stock, how will they behave together for the next 5 time steps?
- Handles missing data


## Exact \& approximate

- Exact inference
- Applicable to a large range of problems, but not all
- May not be possible when combinations/paths get large
- Correct answer subject to rounding errors
- Approximate inference
- Wider class of problems
- Deterministic / non deterministic
- No guarantee of correct answer


## Exact inference

- We will discuss exact inference
- Many concepts apply to both



## Probability notation

- $P(A)$
- $\mathrm{P}(\mathrm{A} \mid \mathrm{B})$ - Conditional probability (probability of $A$ given $B$ )
- $P(A, B)$ - Joint probability (probability of $A$ and $B$ )
- $P($ Head | Tail)
- variables on the left are referred to as head, and variables on the right are referred to as tail
- $P(A, B)=P(A \mid B) P(B)=P(B \mid A) P(A)=>$
- $P(A \mid B)=P(B \mid A) P(A) / P(B)$
- This is Bayes theorem
- Used during inference


## Joint probability

- E.g. P(Raining, Windy)
- Sums to 1

| Raining | Windy = False | Windy = True |
| :--- | :--- | :--- |
| False | 0.64 | 0.16 |
| True | 0.1 | 0.1 |

## Marginalization

## P(Raining, Windy)

| Raining | Windy $=$ False | Windy $=$ True | Sum |
| :--- | :--- | :--- | :--- |
| False | 0.64 | 0.16 | 0.8 |
| True | 0.1 | 0.1 | 0.2 |


| P(Raining) | Raining = False | Raining = True |
| :--- | :--- | :--- |
|  | 0.8 | 0.2 |

For discrete variables we sum, whereas for continuous variables we integrate

## Marginalization - multiple variables

## P(A,B,C,D)

| B | C | D | $\mathrm{A}=$ True | $\mathrm{A}=$ False |
| :--- | :--- | :--- | :--- | :--- |
| True | True | True | 0.0036 | 0.0054 |
| True | True | False | 0.0098 | 0.0252 |
| True | False | True | 0.0024 | 0.0486 |
| True | False | False | 0.0042 | 0.1008 |
| False | True | True | 0.0256 | 0.0864 |
| False | True | False | 0.0432 | 0.1728 |
| False | False | True | 0.0064 | 0.2016 |
| False | False | False | 0.0048 | 0.2592 |

## $P(A, C)$

| C | $\mathrm{A}=$ True | $\mathrm{A}=$ False |
| :--- | :--- | :--- |
| True | 0.0822 | 0.2898 |
| False | 0.0178 | 0.6102 |

Marginal probability $P(A, C)$ created by marginalizing $B$ and $D$ from the joint probability $P(A, B, C, D)$

## Multiplication

## $\mathrm{P}(\mathrm{B}, \mathrm{D} \mid \mathrm{A}, \mathrm{C})$

| B | C | D | $\mathrm{A}=$ True | $\mathrm{A}=$ False |
| :--- | :--- | :--- | :--- | :--- |
| True | True | True | 0.0438 | 0.0186 |
| True | True | False | 0.1192 | 0.0870 |
| True | False | True | 0.1348 | 0.0796 |
| True | False | False | 0.2360 | 0.1652 |
| False | True | True | 0.3114 | 0.2981 |
| False | True | False | 0.5255 | 0.5963 |
| False | False | True | 0.3596 | 0.3304 |
| False | False | False | 0.2697 | 0.4248 |
|  |  |  |  |  |

## P(A,B,C,D)

| B | C | D | A = True | A = False |
| :--- | :--- | :--- | :--- | :--- |
| True | True | True | 0.0036 | 0.0054 |
| True | True | False | 0.0098 | 0.0252 |
| True | False | True | 0.0024 | 0.0486 |
| True | False | False | 0.0042 | 0.1008 |
| False | True | True | 0.0256 | 0.0864 |
| False | True | False | 0.0432 | 0.1728 |
| False | False | True | 0.0064 | 0.2016 |
| False | False | False | 0.0048 | 0.2592 |
|  |  |  |  |  |

## Instantiation - (evidence)

## $P(A=$ False, $B, C, D)$

| B | C | D | A $=$ True | A = False |
| :--- | :--- | :--- | :--- | :--- |
| True | True | True | 0.0036 | 0.0 |
| True | True | False | 0.0098 | 0.0 |
| True | False | True | 0.0024 | 0.0 |
| True | False | False | 0.0042 | 0.0 |
| False | True | True | 0.0256 | 0.0 |
| False | True | False | 0.0432 | 0.0 |
| False | False | True | 0.0064 | 0.0 |
| False | False | False | 0.0048 | 0.0 |

## $P(B, C, D)$

| C | D | B=True | B=False |
| :--- | :--- | :--- | :--- |
| True | True | 0.0036 | 0.0256 |
| True | False | 0.0098 | 0.0432 |
| False | True | 0.0024 | 0.0064 |
| False | False | 0.0042 | 0.0048 |



## Joint probability - Bayesian network

- If we multiply all the distributions of a Bayesian network together, we get the joint distribution over all variables
- What can we do with the joint?
- Any evidence e is information we know (e.g. D=True)

$$
P(\mathbf{X}, \mathbf{e})=\sum_{\mathbf{U} \backslash \mathbf{x}} P(\mathbf{U}, \mathbf{e})=\sum_{\mathbf{U} \backslash \mathbf{x}} \prod_{i} P\left(\mathbf{U}_{i} \mid p a\left(\mathbf{U}_{i}\right)\right) \mathbf{e}
$$

## Just use the joint over all variables?

- We could perform the same tasks if memory and time were not an issue.
- The problem?
- Exponential increases in size with discrete variables
- The answer?
- Bayesian network inference


## Distributive law

$$
\text { if } A \notin \mathbf{X}, A \in \mathbf{Y}, \text { then } \sum_{A} \phi_{\mathbf{X}} \phi_{\mathbf{Y}}=\phi_{\mathbf{X}} \sum_{A} \phi_{\mathbf{Y}}
$$

This simply means that if we want to marginalize out the variable A we can perform the calculations on the subset of distributions that contain A

## Consider calculating $P(A \mid D=$ True $)$



$$
\begin{aligned}
& P(A \mid \mathrm{e}) \propto \sum_{B, C, D} P(A) P(B \mid A) P(C \mid B) P(D \mid C) e_{D} \\
& P(A \mid \mathbf{e}) \propto P(A) \sum_{B} P(B \mid A) \sum_{C} P(C \mid B) \sum_{D} P(D \mid C) e_{D}
\end{aligned}
$$

## Elimination order

- The order in which marginalization is performed is called an elimination order.
- Many different possible orders
- NP hard
- A number of algorithms exist to determine orderings that work well in practise
- E.g. pick the variable(s) that result in the smallest distribution to be marginalized at each step
- Multiple variables can be eliminated at each step.

$$
P(A \mid \mathbf{e}) \propto P(A) \sum_{B} P(B \mid A) \sum_{C} P(C \mid B) \sum_{D} P(D \mid C) e_{D}
$$

## Junction trees

- What if we want to predict all variables, not just A?
- We could use the previous procedure known as Variable Elimination multiple times.
- Or we can use a junction tree (join tree)
- Simply the tree formed by eliminating all variables in the same way as before


## Asia network

$$
P(\mathbf{U})=
$$

Dyspnea (D)

$$
\begin{aligned}
& \text { Dyspne } \\
& \text { True }
\end{aligned}
$$

False
$56.40 \%$
囲 ○

| Node | Distribution |
| :---: | :---: |
| $A$ | $P(A)$ |
| $T$ | $P(T \mid A)$ |
| $S$ | $P(S)$ |
| $L$ | $P(L \mid S)$ |
| $B$ | $P(B \mid S)$ |
| $O$ | $P(O \mid T, L)$ |
| $X$ | $P(X \mid O)$ |
| $D$ | $P(D \mid O, B)$ |

$$
\begin{array}{r}
P(A) P(S) P(T \mid A) P(L \mid S) \times \\
P(B \mid S) P(O \mid T, L)(X \mid O) P(D \mid B, O)
\end{array}
$$

## Elimination



Domain graph after elimination of $A$

## Elimination



Domain graph after elimination of $A$


Domain graph after elimination of $T$

## Elimination



Domain graph after elimination of $T$
Domain graph after elimination of $X$

## Elimination



Domain graph after elimination of $D$
Domain graph after elimination of $X$

## Elimination


7.: Domain graph after elimination of $S$. The dotted line is a required fill-in.

Domain graph after elimination of $D$

## The complete elimination order is... $\{A\},\{T\},\{X\},\{D\},\{S\},\{L, B, O\}$

## Junction trees



Collect computations

- Collect towards the root $\{\mathrm{L}, \mathrm{B}, \mathrm{O}\}$ - similar to variable elimination
- Distribute from the root $\{L, B, O\}$ back to the leaves - allows us to calculate all marginals- $P(A), P(X), P(B), P(L)$ etc...


## Relevance - Bayes ball algorithm



# Inference with time series <br> -Dynamic Bayesian networks 

## Dynamic Bayesian networks



## Unrolling



We could unroll, and use standard methods

## Distributions that understand time

## $P(X 1[t], X 2[t] \mid X 1[t-1], X 2[t-1])$

|  |  | X1[t] | X2[t] |
| :---: | :---: | :---: | :---: |
| - | Intercept | 3.076214646583... | -1.58979124120... |
|  | Covariance ( $\mathrm{X} 1[\mathrm{t}]$ ) | 4.142028922619... | -1.63113437658... |
|  | Covariance ( $\mathrm{X} 2[\mathrm{t}]$ ) | -1.63113437658... | 2.023002098810... |
|  | Weight (X1[t-1]) | 0.995368300968... | -0.00816950459... |
|  | Weight ( $\times 2[t-1]$ ) | 0.026861977953... | 0.942548514594... |

Note that X1 appears in the same distribution twice, but at different times

## Time aware distributions

- Marginalization \& multiplication is well defined
- We can use all the existing algorithms
- We can construct queries like...
- P(X1@t=4)
- Returns probabilities for discrete, mean \& variance for continuous
- P(X1@t=4, X2@t=4)
- Joint time series prediction (funnel)
- P(X1@t=2, X1@t=3)
- Across different times
- P(A, X1@t=2)
- Mixed static \& temporal
- Log-likelihood of a multivariate time series
- Anomaly detection



## Different types of scalability

Data size
Big data?

Network size,
Rephil > 1M nodes

Connectivity
(discrete -> exponential)

## Inference

(distributed)

Apache Spark

## RDD Objects


路


rdd1.join(rdd2)
.groupby(...)
.filter(...)

## Apache Spark

- RDD (Resilient distributed dataset)
- Can be in memory
- Code automatically converted to DAG execution engine
- Serialization of variables


## Distributed architecture

1. Distribute Bayesian network to worker nodes
2. Calculate the sufficient statistics per partition

- This often requires an inference algorithm per thread/partition

3. Aggregate the sufficient statistics (reduce)
4. Update the Bayesian network based on the new statistics
5. Return to 1 until convergence

## Distributed parameter learning

|  |  | Node 1 |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| $\times$ | $\checkmark$ | x | $\checkmark$ | $\times$ | r |
| 10.2 | 12.5 | 3.4 | 3.2 | 2.0 | 4.0 |
| 14.5 | 3.2 | 6.6 | 1.6 | 8.1 | 3.4 |
| 15.6 | 8.2 | 5.5 | 4.3 | 2.2 | 7.7 |
| 9.2 | 12.2 | 12.4 | 8.9 | 15.1 | 1.2 |
| 15.8 | 9.2 | -1.1 | -2.4 | 4.6 | 4.5 |
| 4.5 | 2.1 | 4.5 | 4.2 | 2.4 | 1.9 |
| ... | ... | ... | -. | ..- | .-. |
| $\Sigma$ stats |  | $\Sigma$ stats |  | $\Sigma$ stats |  |


| Node 2 |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| $x$ | Y | $\times$ | $\checkmark$ | $\times$ | r |
| 10.2 | 12.5 | 3.4 | 3.2 | 2.0 | 4.0 |
| 14.5 | 3.2 | 6.6 | 1.6 | 8.1 | 3.4 |
| 15.6 | 8.2 | 5.5 | 4.3 | 2.2 | 7.7 |
| 9.2 | 12.2 | 12.4 | 8.9 | 15.1 | 1.2 |
| 15.8 | 9.2 | -1.1 | -2.4 | 4.6 | 4.5 |
| 4.5 | 2.1 | 4.5 | 4.2 | 2.4 | 1.9 |
| ... | ... | ... | .. | ..- | - |
| $\sum$ stats |  | $\Sigma$ stats |  | $\Sigma$ stats |  |


| Node 3 |  |  |  |
| :---: | :---: | :---: | :---: |
| $\times$ | Y | $\times$ | r |
| 10.2 | 12.5 | 3.4 | 3.2 |
| 14.5 | 3.2 | 6.6 | 1.6 |
| 15.6 | 8.2 | 5.5 | 4.3 |
| 9.2 | 12.2 | 12.4 | 8.9 |
| 15.8 | 9.2 | ${ }^{-1.1}$ | -2.4 |
| 4.5 | 2.1 | 4.5 | 4.2 |
| .-. | ... | ..- | ... |
| $\Sigma$ stats |  |  |  |



```
 stats \Sigma stats \Sigma stats \Sigma stats
 stats \Sigma stats \Sigma stats \Sigma stats
```


## Distributed parameter learning



## Example - distributed learning

```
val SC = new SparkContext(conf)
// hard code some test data. Normally you would read data from your cluster.
val data = createRDD.cache()
// A network could be loaded from a file or stream
// we create it manually here to keep the example self contained
val network = createNetwork
val parameterLearningOptions = new ParameterLearningOptions
// Bayes Server supports multi-threaded learning
// which we want to turn off as Spark takes care of this
parameterLearningOptions.setMaximumConcurrency(1)
/// parameterLearningOptions.setMaximumIterations(...) // this can be useful to limit the number of iterations
val config = new MemoryNameValues // we could also use broadcast variables
val output = ParameterLearning.learnDistributed(network, parameterLearningOptions,
    new BayesSparkDistributer[Seq[(Double, Double)]](
        data,
        config,
        (ctx, iterator) => new TimeSeriesEvidenceReader(ctx.getNetwork, iterator)
    ))
```


## Distributed time series prediction

```
// make some time series predictions into the future
val predictions = Prediction.predict[TimeSeries](
    network,
    testData,
    Seq(
        PredictVariable("X1", Some(PredictTime(5, Absolute))), PredictVariance("X1", Some(PredictTime(5, Absolute))),
        PredictVariable("X2", Some(PredictTime(5, Absolute))), PredictVariance("X2", Some(PredictTime(5, Absolute))),
        PredictVariable("X1", Some(PredictTime(6, Absolute))), PredictVariance("X1", Some(PredictTime(6, Absolute))),
        PredictVariable("X2", Some(PredictTime(6, Absolute))), PredictVariance("X2", Some(PredictTime(6, Absolute))),
        PredictLogLikelihood() // this value can be used for Time Series anomaly detection
    ),
    (network, iterator) => new TimeSeriesReader(network, iterator))
predictions.foreach(println)
```


## Thank you

