Bayesian network internals Inference algorithms, time series & distributed learning with Big Data

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Introduction



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?

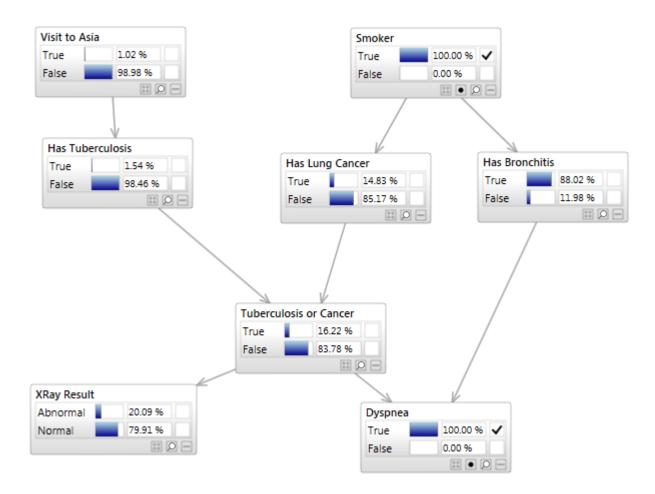


What is a Bayesian network?

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

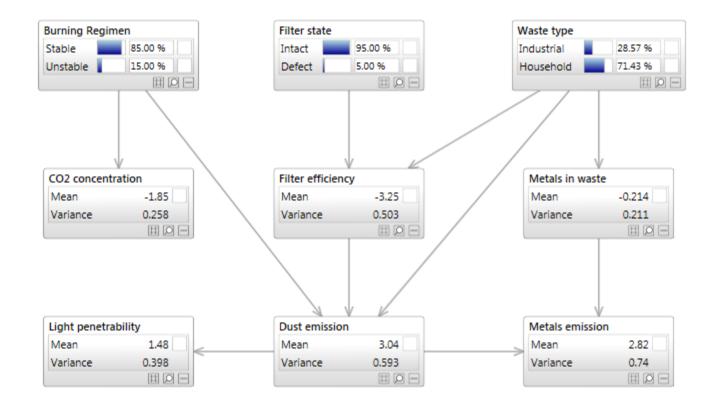


Example – Asia network



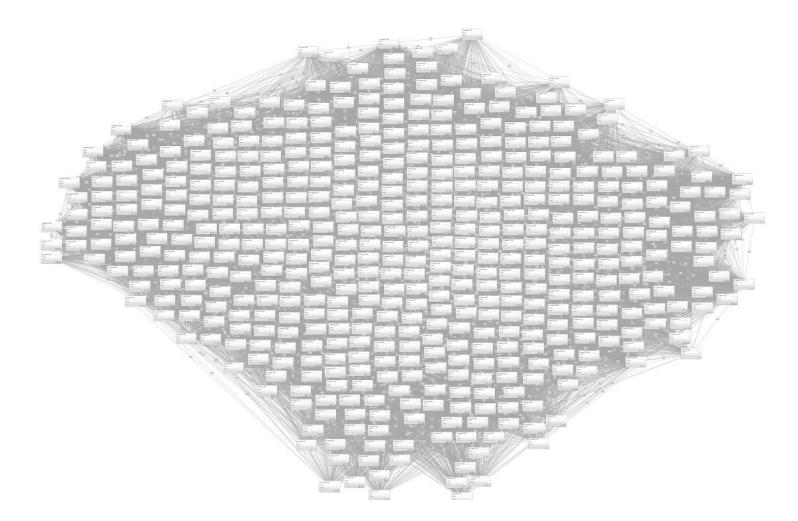


Example – Waste network



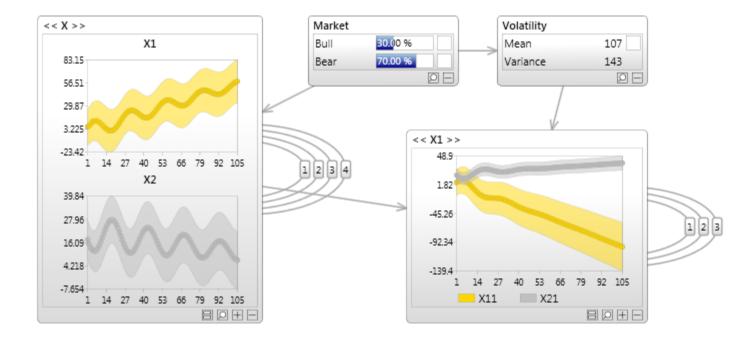


Example – the bat (40,000 links)



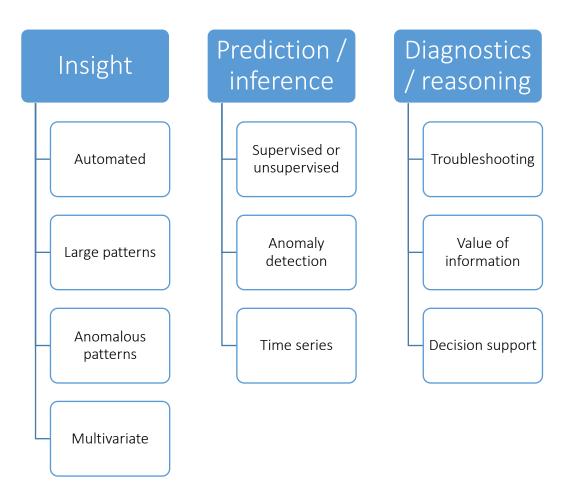


Example – static & temporal





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



Probability notation

- P(A)
- P(A|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 | B)P(B) = P(B | A)P(A) =>
 - P(A | B) = P(B | 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 = FalseRaining = True0.80.2

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



Marginalization – multiple variables

P(A,B,C,D)

В	С	D	A = True	A = False				
True	True	True	0.0036	0.0054				
True	True	False	0.0098	0.0252	P(A,C)			
True	False	True	0.0024	0.0486		С	A = True	A = False
True	False	False	0.0042	0.1008		True	0.0822	0.2898
False	True	True	0.0256	0.0864	-	False	0.0178	0.6102
False	True	False	0.0432	0.1728				
False	False	True	0.0064	0.2016				
False	False	False	0.0048	0.2592				

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



Multiplication

P(B,D | A, C)

В	С	D	A = True	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,C)

С	A = True	A = False
True	0.0822	0.2898
False	0.0178	0.6102

P(A,B,C,D)

В	С	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)

В	С	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)

С	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



Bayesian network inference



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)

$$P(\mathbf{X}, \mathbf{e}) = \sum_{\mathbf{U} \setminus \mathbf{X}} P(\mathbf{U}, \mathbf{e}) = \sum_{\mathbf{U} \setminus \mathbf{X}} \prod_{i} P(\mathbf{U}_i | pa(\mathbf{U}_i)) \mathbf{e}$$

U = universe of variablesX = variables being predictede = evidence on any variables



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

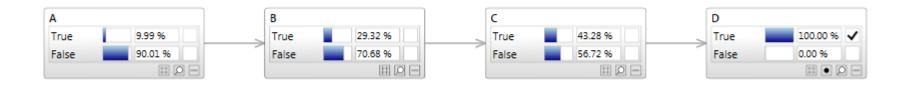
$$if A \notin \mathbf{X}, A \in \mathbf{Y}, then \sum_{A} \phi_{\mathbf{X}} \phi_{\mathbf{Y}} = \phi_{\mathbf{X}} \sum_{A} \phi_{\mathbf{Y}}$$

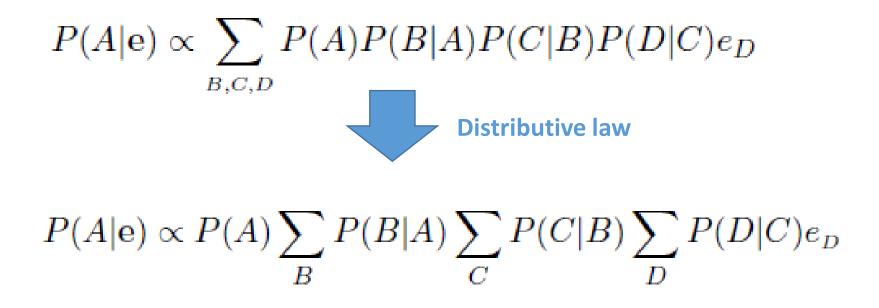
This simply means that if we want to marginalize out the variable A we can perform the calculations on the subset of distributions that contain A

 ϕ is a probability distribution over the variables in the subscript



Consider calculating P(A|D=True)







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.

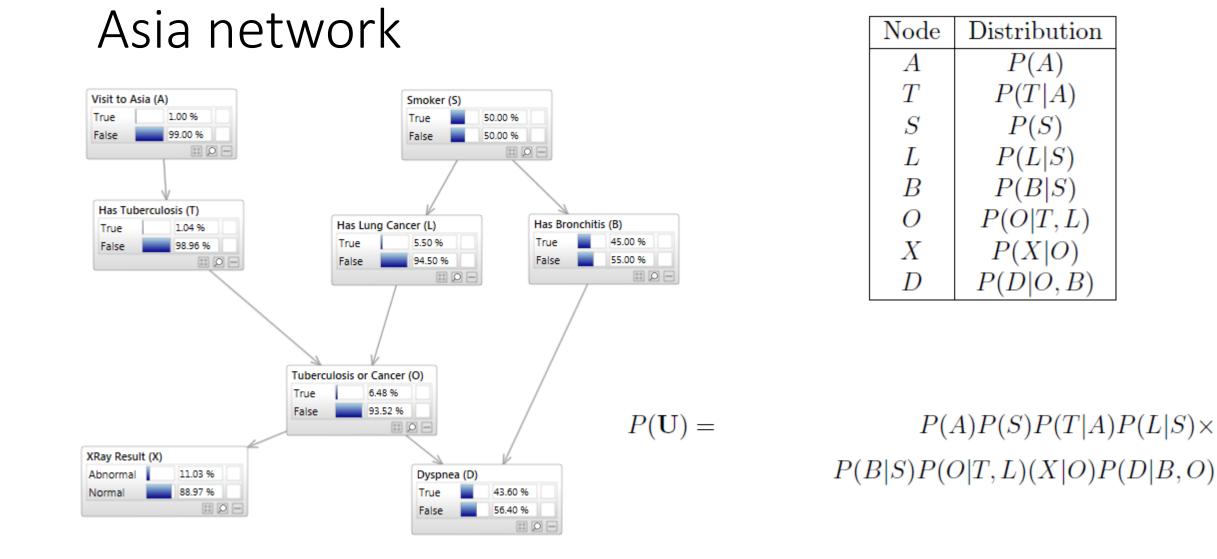
$$P(A|\mathbf{e}) \propto P(A) \sum_{B} P(B|A) \sum_{C} P(C|B) \sum_{D} P(D|C) e_{D}$$



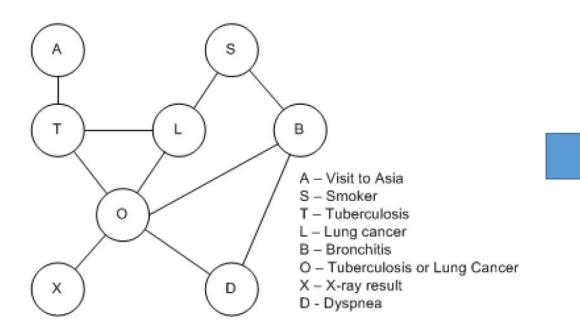
Junction trees

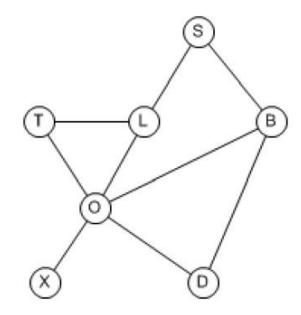
- What if we want to predict all variables, not just A?
- We could use the previous procedure known as Variable Elimination multiple times.
- Or we can use a junction tree (join tree)
 - Simply the tree formed by eliminating all variables in the same way as before





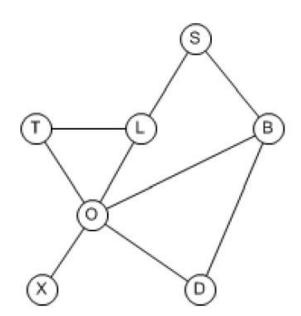


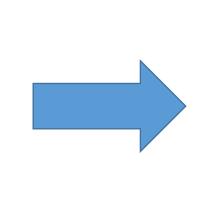


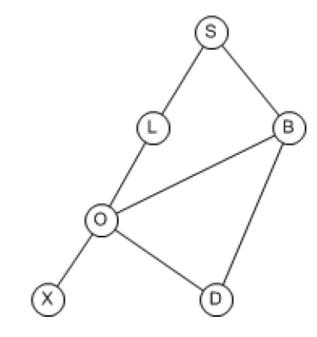


Domain graph after elimination of A





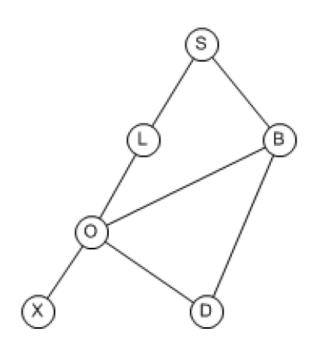


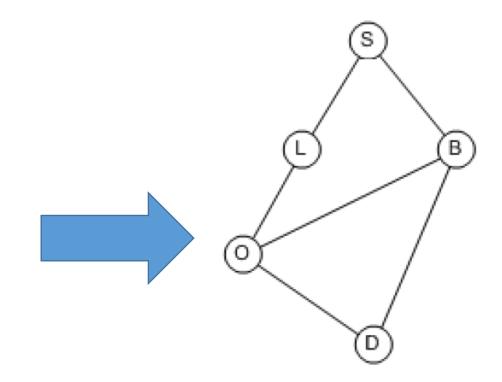


Domain graph after elimination of A

Domain graph after elimination of ${\cal T}$



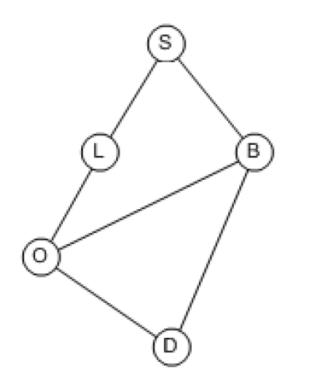


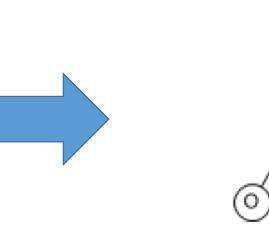


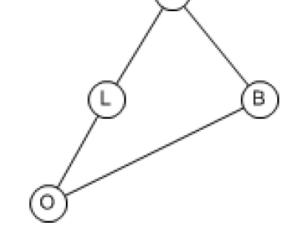
Domain graph after elimination of T

Domain graph after elimination of X





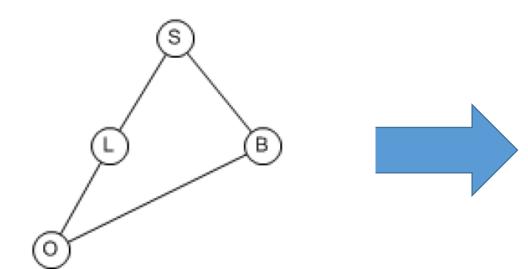


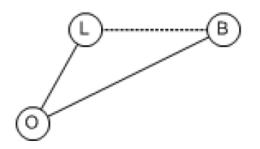


Domain graph after elimination of ${\cal D}$

Domain graph after elimination of \boldsymbol{X}





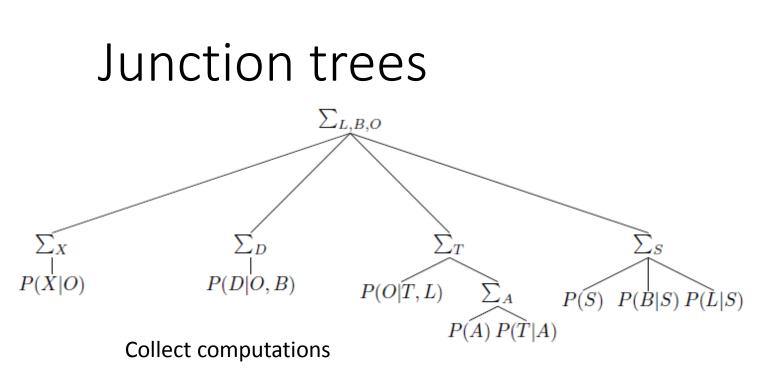


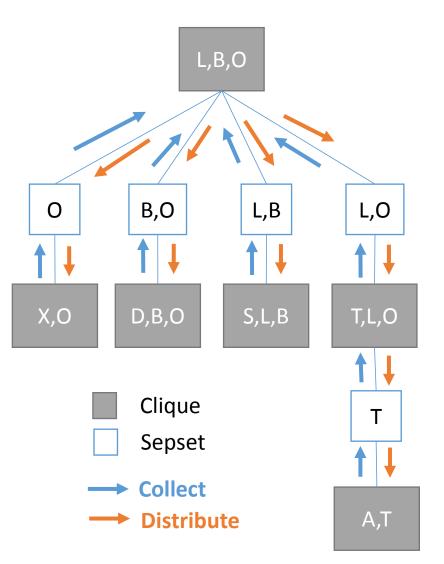
7.: Domain graph after elimination of S. The dotted line is a required fill-in.

Domain graph after elimination of D

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

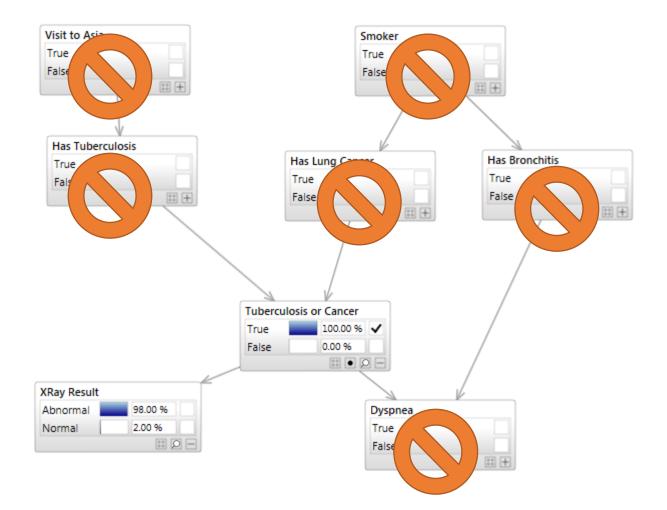






- Collect towards the root {L,B,O} similar to variable elimination
- Distribute from the root {L,B,O} back to the leaves allows us to calculate all marginals– P(A), P(X), P(B), P(L) etc...

Relevance – Bayes ball algorithm

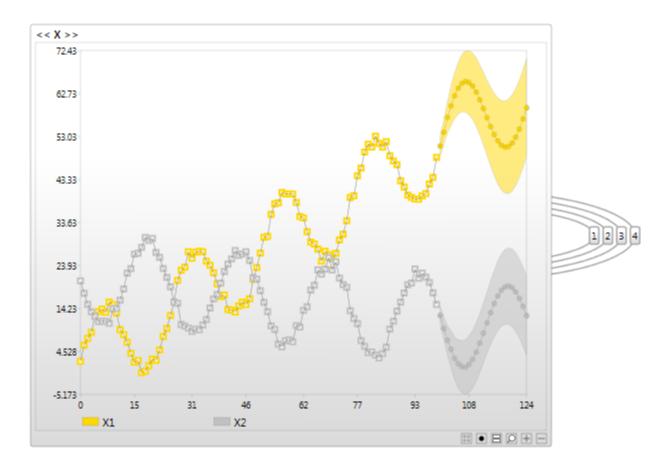




Inference with time series -Dynamic Bayesian networks

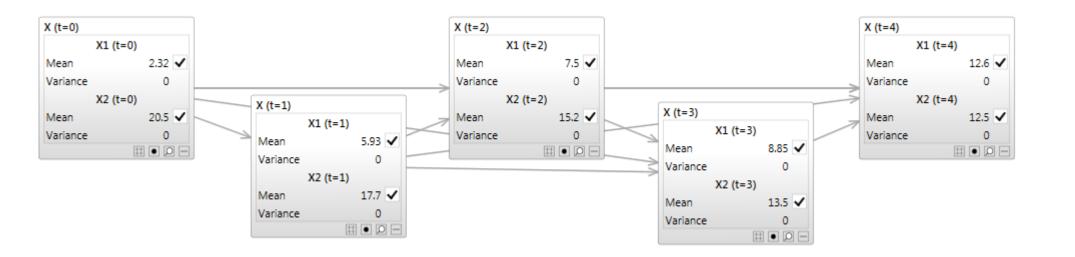


Dynamic Bayesian networks









- - -

We could unroll, and use standard methods



Distributions that understand time

P(<mark>X1[t]</mark>, X2[t] | <mark>X1[t-1]</mark>, X2[t-1])

		X1[t]	X2[t]			
•	Intercept	3.076214646583	-1.58979124120			
	Covariance (X1[t])	4.142028922619	-1.63113437658			
	Covariance (X2[t])	-1.63113437658	2.023002098810			
	Weight (X1[t-1])	0.995368300968	-0.00816950459			
	Weight (X2[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



Distributed parameter learning



Different types of scalability

Data size

Big data?

Connectivity (discrete -> exponential)

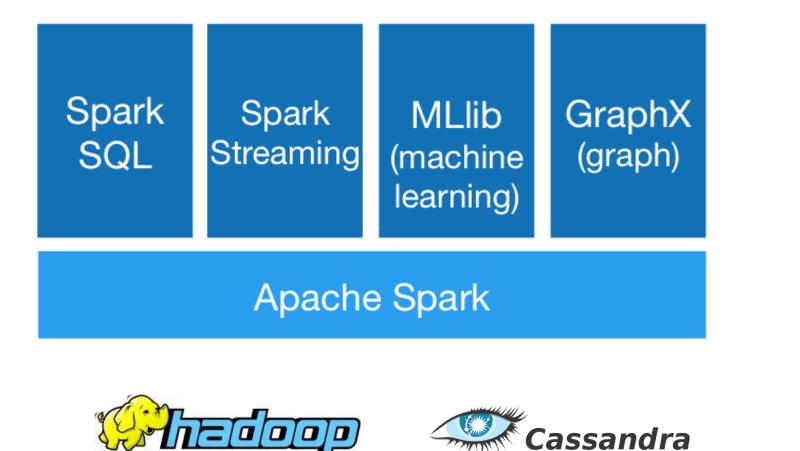
Network size, <u>Rephil > 1M nodes</u>

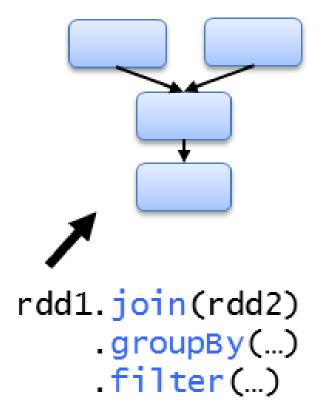
Inference (distributed)





RDD Objects







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					Г	Node 2							Node 3				
x	Y	X	Y	x	Y		x	Y	x	Y	x	Υ		X	Y	x	Υ
10.2	12.5	3.4	3.2	2.0	4.0		10.2	12.5	3.4	3.2	2.0	4.0		10.2	12.5	3.4	3.2
14.5	3.2	6.6	1.6	8.1	3.4		14.5	3.2	6.6	1.6	8.1	3.4		14.5	3.2	6.6	1.6
15.6	8.2	5.5	4.3	2.2	7.7		15.6	8.2	5.5	4.3	2.2	7.7		15.6	8.2	5.5	4.3
9.2	12.2	12.4	8.9	15.1	1.2		9.2	12.2	12.4	8.9	15.1	1.2		9.2	12.2	12.4	8.9
15.8	9.2	-1.1	-2.4	4.6	4.5		15.8	9.2	-1.1	-2.4	4.6	4.5		15.8	9.2	-1.1	-2.4
4.5	2.1	4.5	4.2	2.4	1.9		4.5	2.1	4.5	4.2	2.4	1.9		4.5	2.1	4.5	4.2
∑ st	∑ stats ∑ stats ∑ stat		tats	∑ stats		∑ stats		∑ stats			∑ stats		∑ stats				
Σ stats Σ stats Σ stats Σ stats Σ stats Σ stats Σ stats Σ stats Σ stats Σ 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

