BN learning

Dynamic BN learning

Relational BN learning

The end

# Advances in Learning with Bayesian Networks

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DUKe (Data User Knowledge) research group, LS2N UMR 6004, Nantes, France

### Séminaire IRT SystemX, 19 jan. 2017



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# LS2N - UMR CNRS 6004

1er janvier 2017, fusion de 2 UMR

 IRCCyN (Institut de Recherche en Communications et Cybernétique de Nantes)



- LINA (Laboratoire d'Informatique de Nantes Atlantique)
- 450 personnes (pprox 215 permanents)
- 5 axes thématiques
  - Conception et Conduite de Systèmes
  - Robotique, Procédés, Calcul
  - Signaux, Images, Ergonomie et Langues
  - Science du Logiciel et des Systèmes Distribués
  - Science des Données et de la Décision
- 5 établissements support
  - Ecole Centrale de Nantes
  - Université de Nantes
  - Institut Mines Telecom Atlantique
  - CNRS, INRIA



### **Research group in Data Sciences**

- 16 permanents
- 3 associates
- 12 PhD students
- 2 postdoc/engineers

BN learning

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# DUKe scientific approach

Proposing « agile », « user in the loop » Data-mining / Machine Learning algorithms

User Ke Hg B1 Get (6) Got (2) Dr D1 Pro 30 des Fat Markins Data Knowledge Applications and valorisation Digital Humanity, BioInformatics, **Business Intelligence** 



- Bayesian networks (BNs) are a powerful tool for graphical representation of the underlying knowledge in the data and reasoning with incomplete or imprecise observations.
- BNs have been extended (or generalized) in several ways, as for instance, causal BNs, dynamic BNs, relational BNs, ...





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Initial Model



Dynamic BN learning **BN** learning

Relational BN learning

# **Motivations**



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• complete

8 5 4 3



• complete /incomplete [François 06]



- complete /incomplete [François 06]
- high n,



complete /incomplete [François 06]

```
• high n, n >> p [Ammar 11]
```

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- stream [Yasin 13]

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Relational BN learning

The end

### Wotwations

We would like to learn a BN from data... but which kind of data ?

- complete /incomplete [François 06]
- high *n*, *n* >> *p* [Ammar 11]
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Relational BN learning

The end

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• structured data [Ben Ishak 15, Coutant 15, Chulyadyo 16]





The end

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- complete /incomplete [François 06]
- high *n*, *n* >> *p* [Ammar 11]
- stream [Yasin 13]
- + prior knowledge / ontology [Ben Messaoud 13]
- structured data [Ben Ishak 15, Coutant 15, Chulyadyo 16]
- not so structured data [Elabri]





Even the learning task can differ : generative

- modeling P(X, Y)
- no target variable
- more general model
- better behavior with incomplete data

### **Objectives of this talk**

- how to learn BNs in such various contexts ?
- state of the art : founding algorithms and recent ones
- pointing out our contributions in this field



Even the learning task can differ : generative vs. discriminative

- modeling P(X, Y)
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• modeling P(Y|X)

Relational BN learning

The end

- one target variable Y
- dedicated model

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modeling P(Y|X)
one target variable Y

dedicated model

The end

3N learning

Dynamic BN learning

Relational BN learning

The end

# Outline ...



### BN learning

- Definition
- Parameter learning
- Structure learning
- Dynamic BN learning
  - Definition
  - Learning
- Relational BN learning
  - Definitions
  - Learning with a relational DB
  - Learning with a Graph DB
- The end



Relational BN learning

The end

# **Bayesian network**



### Definition

- G qualitative description of conditional dependences / independences between variables directed acyclic graph (DAG)
- quantitative description of these dependences conditional probability distributions (CPDs)



### Main property

 the global model is decomposed into a set of local conditional models



### Relational BN learning

The end

# **Bayesian network**



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 the global model is decomposed into a set of local conditional models BN learning

Dynamic BN learning

Relational BN learning

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# One model... but two learning tasks

# **BN** = graph G and set of **CPD**s $\Theta$

- parameter learning / G given
- structure learning





### $BN = graph \ G \ and \ set \ of \ CPDs \ \Theta$

- parameter learning / G given
- structure learning





### **BN** = graph G and set of **CPDs** $\Theta$

- parameter learning / G given
- structure learning





### Complete data $\mathcal{D}$

- max. of likelihood (ML) :  $\hat{\theta}^{MV} = \operatorname{argmax} P(\mathcal{D}|\theta)$
- closed-form solution :

$$\hat{P}(X_i = x_k | Pa(X_i) = x_j) = \hat{\theta}_{i,j,k}^{MV} = \frac{N_{i,j,k}}{\sum_k N_{i,j,k}}$$

 $N_{i,j,k}$  = nb of occurrences of  $\{X_i = x_k \text{ and } Pa(X_i) = x_j\}$ 

#### ther approaches

• max. a posteriori (MAP) :  $\hat{\theta}^{MAP}$  = argmax  $P(\theta|D)$ 

• expectation a posteriori (EAP) :  $\hat{\theta}^{EAP} = \mathbb{E}(P(\theta|\mathcal{D}))$  $\hat{\theta}^{MAP}_{i,j,k} = \frac{N_{i,j,k} + \alpha_{i,j,k} - 1}{\sum_{k} (N_{i,j,k} + \alpha_{i,j,k} - 1)}$   $\hat{\theta}^{EAP}_{i,j,k} = \frac{N_{i,j,k}}{\sum_{k} (N_{i,j,k} - 1)}$ 



### Complete data ${\cal D}$

- max. of likelihood (ML) :  $\hat{\theta}^{MV} = \operatorname{argmax} P(\mathcal{D}|\theta)$
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### Other approaches

### $P(\theta) \sim \text{Dirichlet}(\alpha)$

- max. a posteriori (MAP) :  $\hat{\theta}^{MAP}$  = argmax  $P(\theta|D)$
- expectation a posteriori (EAP) :  $\hat{\theta}^{EAP} = \mathsf{E}(P(\theta|\mathcal{D}))$  $\hat{\theta}^{MAP}_{i,j,k} = \frac{N_{i,j,k} + \alpha_{i,j,k} - 1}{\sum_{k} (N_{i,j,k} + \alpha_{i,j,k} - 1)}$   $\hat{\theta}^{EAP}_{i,j,k} = \frac{N_{i,j,k} + \alpha_{i,j,k}}{\sum_{k} (N_{i,j,k} + \alpha_{i,j,k})}$



### Incomplete data

- no closed-form solution
- EM (iterative) algorithm [Dempster, 77], convergence to a local optimum

#### ncremental data

advantages of sufficient statistics

$$\theta_{i,j,k} = \frac{N^{old} \theta_{i,j,k}^{old} + N_{i,j,k}}{N^{old} + N}$$

this Bayesian updating can include a forgetting factor



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Dynamic BN learning

Relational BN learning

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# Parameter learning (discriminative)

### **Complete data**

- no closed-form
- iterative algorithms such as gradient descent

### Incomplete data

- no closed-form
- iterative algorithms + EM :-(



Dynamic BN learning

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The end

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- no closed-form
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### **Incomplete data**

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### Size of the "solution" space

- the number of possible DAGs with *n* variables is super-exponential w.r.t *n* [Robinson, 77] NS(5) = 29281  $NS(10) = 4.2 \times 10^{18}$
- an exhaustive search is impossible for realistic n !

One thousand millenniums  $= 3.2 \times 10^{13} \mbox{ seconds}$ 

### Identifiability

- data can only help finding (conditional) dependences / independences
- Markov Equivalence : several graphs describe the same dependence statements
- causal Sufficiency : do we know all the explaining variables ?



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Dynamic BN learning

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# Structure learning (generative / complete)

### **Constraint-based methods**

- BN = independence model
   ⇒ find CI in data in order to build the DAG
  - ex : IC [Pearl & Verma, 91], PC [Spirtes et al., 93]
- problem : reliability of CI statistical tests (ok for n < 100)

### **Score-based methods**

- BN = probabilistic model that must fit data as well as possible
- problem : size of search space (ok for n < 1000)

### Hybrid/ local search methods

- local search / neighbor identification (statistical tests)
- global (score) optimization
- usually for scalability reasons (ok for high n)

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Relational BN learning

The end

# Structure learning (generative / complete)

### **Constraint-based methods**

- BN = independence model
- problem : reliability of CI statistical tests (ok for n < 100)

### **Score-based methods**

 BN = probabilistic model that must fit data as well as possible ⇒ search the DAG space in order to maximize a scoring function

ex : Maximum Weighted Spanning Tree [Chow & Liu, 68], Greedy Search [Chickering, 95], evolutionary approaches [Larranaga et al., 96] [Wang & Yang, 10]

• problem : size of search space (ok for n < 1000)

Hybrid/ local search methods



Relational BN learning

The end

# Structure learning (generative / complete)

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- ex : MMHC algorithm [Tsamardinos et al., 06]



### **Specific structures**

- naive Bayes, augmented naive Bayes
- multi-nets
- ...





The end

#### Structure learning

- usually, the structure is learned in a generative way
- the parameters are then tuned in a discriminative way

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#### Specific structures

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#### Structure learning

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Dynamic BN learning

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The end

## **Structure learning**

#### Incomplete data

- hybridization of previous structure learning methods and EM
- ex : Structural EM [Friedman, 97]
  ≃ Greedy Search + EM
- problem : convergence



Dynamic BN learning

Relational BN learning

The end

## **Structure learning**

#### n >> p

- robustness and complexity issues
- application of Perturb & Combine principle
- ex : mixture of randomly perturbed trees [Ammar & Leray, 11]

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Dynamic BN learning

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The end

## **Structure learning**

# Incremental learning and data streams

- Bayesian updating is easy for parameters
- Bayesian updating is complex for structure learning
- and other constraints related to data streams (limited storage, ...)
- ex : incremental MMHC [Yasin and Leray, 13]

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Dynamic BN learning

Relational BN learning

The end

## **Structure learning**

#### Integration of prior knowledge

- in order to reduce search space : white list, black list, node ordering [Campos & Castellano, 07]
- interaction with ontologies [Ben Messaoud et al., 13]

$\mathbf{\nabla}$
ΥΥ

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M.P.H

Outline ...

Relational BN learning

The end

Definition

**Dynamic BN learning** 

- Parameter learning
- Structure learning

## **Dynamic BN learning**

- Definition
- Learning
- Definitions
- Learning with a relational DB
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Dynamic BN learning

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The end

## Dynamic Bayesian networks (DBNs)

## k slices temporal BN (k-TBN) [Murphy, 02]

- prior graph  $G_0$  + transition graph  $G_{\rightarrow}$
- for example : 2-TBNs model [Dean & Kanazawa, 89]



 k-TBN with only temporal edges [Dojer, 06][Vinh et al, 12]



(a) Prior network (b) Transition network

Dynamic BN learning

Relational BN learning

The end

## Dynamic Bayesian networks (DBNs)

### k slices temporal BN (k-TBN) [Murphy, 02]

- prior graph  $G_0$  + transition graph  $G_{\rightarrow}$
- for example : 2-TBNs model [Dean & Kanazawa, 89]

#### Simplified k-TBN

 k-TBN with only temporal edges [Dojer, 06][Vinh et al, 12]



(c) Transition network with only inter time-slice arcs



Dynamic BN learning

Relational BN learning

The end

## DBN structure learning (generative)

#### Score-based methods

- dynamic Greedy Search [Friedman et al., 98], genetic algorithm [Gao et al., 07], dynamic Simulated Annealing [Hartemink, 05], ...
- for k-TBN (G<sub>0</sub> and G<sub> $\rightarrow$ </sub> learning)
- but not scalable (high n)

#### Hybrid methods

- [Dojer, 06] [Vinh et al., 12] for simplified k-TBN, but often limited to k = 2 for scalability
- dynamic MMHC for "unsimplified" 2-TBNs with high n [Trabelsi et al., 13]



Dynamic BN learning

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Outline ...

The end

Definition

- Parameter learning
- Structure learning
- - Definition

Dynamic BN learning

- Learning
- **Relational BN learning** 
  - Definitions
  - Learning with a relational DB
  - Learning with a Graph DB





#### Flat data

- No relational model
- Learning probabilistic dependencies between variables

Dynamic BN learning

Relational BN learning

The end

## **Motivations**



## Flat data

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## Relational DB

- Relational schema is given
- Learning prob. dep. between variables, but more complex !

Dynamic BN learning

Relational BN learning

The end

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- Relational schema is given
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## Graph DB

- Relational schema ?
- Learning prob. dep. between variables ?

Dynamic BN learning

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## **Relational schema**



#### relational schema ${\cal R}$

#### classes + attributes

- reference slots (e.g. *Vote.Movie*, *Vote.User*)
- inverse reference slots (e.g. *User*.*User*<sup>-1</sup>)
- slot chain = a sequence of (inverse) reference slots

Dynamic BN learning

Relational BN learning

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Dynamic BN learning

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  - ex: *Vote.User.User*<sup>-1</sup>.*Movie*: all the movies voted by a particular user

Dynamic BN learning

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## **Relational skeleton**



#### Instance ${\mathcal I}$

- set of objects for each class
- with a value for each reference slot and each attribute
- == a "populated" database

### Relational skeleton $\sigma_{\mathcal{R}}$

 Instance without attribute values



Relational BN learning

The end

## **Probabilistic Relational Models**

## [Koller & Pfeffer, 98]

#### Definition

- A PRM  $\Pi$  associated to  $\mathcal{R}$ :
  - a qualitative dependency structure S (with possible long slot chains and aggregation functions)
  - a set of parameters  $\theta_{\mathcal{S}}$





#### Aggregators

- Vote.User.User<sup>-1</sup>.Movie.genre  $\rightarrow$  Vote.rating
- movie rating from one user can be dependent with the genre of all the movies voted by this user
  - how to describe the dependency with an unknown number of parents ?
  - solution : using an aggregated value, e.g.  $\gamma = \textit{MODE}$



Another probabilistic relational model [Heckerman & Meek, 04]



Dynamic BN learning

The end

## Learning from a relational datatase

#### **PRM/DAPER** learning

- finding the probabilistic dependencies and the probability tables from an instantiated database
- relational schema is known. but ...
- several situations / PRM extensions



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## Learning from a relational datatase

#### Attribute uncertainty

- Input : relational skeleton (all the objects and relations), some attributes
- Objective : predict only missing attributes



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## Learning from a relational datatase

#### **Reference uncertainty**

- Input : partial relational skeleton (all the objects, but some relations are missing)
- Objective : predict missing attributes and "foreign keys"



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The end

## Learning from a relational datatase

#### Existence uncertainty

- Input : partial relational skeleton (all the entity objects, but some relationship objects are missing)
- Objective : predict existence of relationships between entity objects





## **PRM/DAPER** learning with AU

#### **Relational variables**

- finding new variables by exploring the relational schema
- ex: student.reg.grade, registration.course.reg.grade, registration.student reg.course.reg.grade, ...
- $\Rightarrow$  adding another dimension in the search space
- $\Rightarrow$  limitation to a given maximal slot chain length

#### **Constraint-based methods**

- relational PC [Maier et al., 10] relational CD [Maier et al., 13]
- odon't deal with aggregation functions

#### Score-based methods

• Greedy search [Getoor et al., 07]



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#### Need for partitionning

- The missing foreign key is considered as a random variable
- We need to partition the similar "target" objects in order to obtain a generic model

#### How to partition

- $\bullet$  With object attributes [Getoor et al.] = clustering
- With relational information = graph partitionning
- With both : [Coutant et al., 15]





#### Definition

- Data is described in a graph, with nodes and relationships
- Attributes can be associated to both





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#### Definition

- Scalability / large data (no join operation, only graph traversal)
- Schema-free, no relational schema



Dynamic BN learning

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## Graph database



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## Learning from a Graph database



#### Our assumptions

- Data is "organized" / stored by approx. following some meta/ER model.
- Use of labels in order to "type" nodes and relationships
- Otherwise, we can't do anything !

[Elabri, in progress]
Dynamic BN learning

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#### ER identification from data

- E=node labels, R=relationship labels
- choosing only the most frequent signature (E<sub>i</sub> × E<sub>i</sub>) for each R





The end



#### ER identification from data

- E=node labels, R=relationship labels
- choosing only the most frequent signature  $(E_i \times E_j)$  for each R







Dynamic BN learning

Relational BN learning

The end

# **DAPER** learning

#### **DAPER** structure learning

Once ER model is identified, we can learn the probabilistic dependencies :

- Attribute uncertainty : predicting attribute value only
- Reference uncertainty : predicting the target node for an existing relation ?
- Existence uncertainty : predicting a relationship between two existing nodes ?



Dynamic BN learning

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Outline ....

Relational BN learning

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Dynamic BN learning

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- Parameter learning
- Structure learning

- Definition
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- Bayesian networks = powerful tool for knowledge representation and reasoning with data
- Our contributions about BN learning in several contexts



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- Dealing with all the problems in the same time :-)
- Interacting with some probabilistic & logic frameworks
- Implementation in our software platform PILGRIM



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Relational BN learning

The end

# One buzzword for the road

## BN Learning wrt. 7 Vs of Big Data

**BN** learning

- Volume : scalable algorithms and map-reduce implementations
- Variety : flat data, SQL, graph databases, ...
- Velocity/Variability : incremental anytime learning, non stationary data
- Visualization : for user interaction
- Veracity : does the user give accurate data ?
- Value : of data ...



Dynamic BN learning

Relational BN learning

The end

## References



#### One starting point

[Koller & Friedman, 09]
Probabilistic Graphical Models:
Principles and Techniques. MIT
Press.

#### **Our publications**

http://tinyurl.com/PhLeray

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