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# Learning from partly observable time- dependent graphs

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# Learning from partly observable time-dependent graphs

Jan Ramon

TDLSG workshop @ ECML/PKDD 2017

Skopje, September 18th, 2017

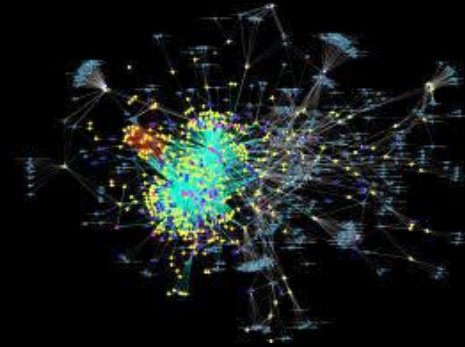


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# Types of time-dependent graphs

- Fixed structure, evolving attributes
  - E.g. Gene regulatory network
    - Node: gene
    - Arc: regulation
    - Attribute: expression level
- Fixed attributes, evolving structure
  - E.g. Citation network
    - Node: article
    - Arc: citation
- Evolving attributes, evolving structure
  - E.g. Social network

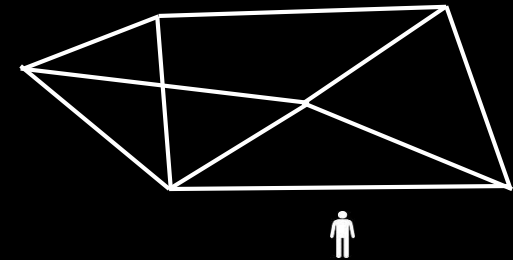
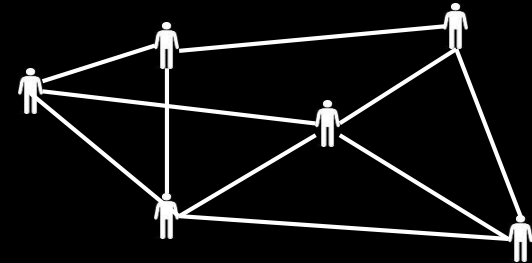


# Observability

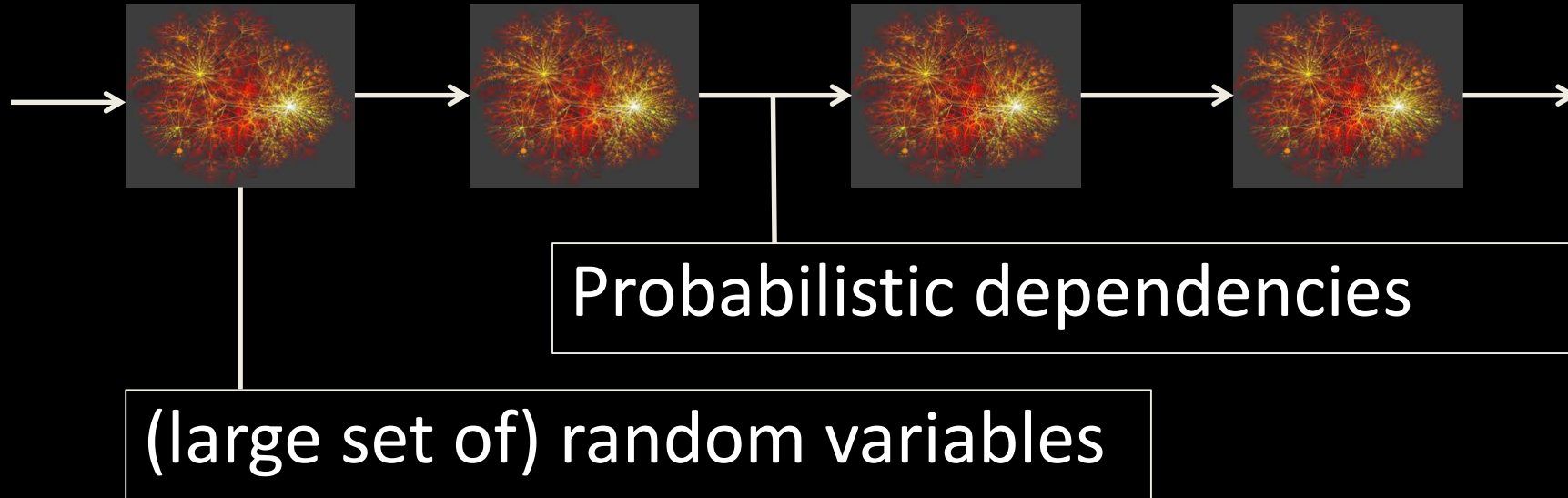
- Collecting actual information
  - is expensive
    - Communication costs
    - Bothering people to record everything
  - Isn't privacy-friendly
  - May be technically infeasible
    - If observations require destructive measurements

# Some observation settings

- Nodes as observers
  - Observe/query/inform neighborhood
  - Limited information about distant nodes
  - E.g. Node in communication network
  - E.g. Car in road network
- External observer
  - Overview of graph structure
  - Only limited observation of local details
  - E.g. Service provider in communication network
  - E.g. Government/maintainer monitoring road network



# Dynamic probabilistic models



- TD-graph can be modeled with probabilistic relational model (MLN, ProbLog, PRM, RBN, ...)
- But existing inference techniques can't exploit all structure easily

# Exploitable structure

- Uniformity of network
  - closeby vertices are/behave similar(ly)
- Continuity
  - Values don't change
- Information flow
  - Also: causality
  - (but not easily conditional independence)



# Case studies

- Case study 1: Local observation
- Case study 2: Unobservable history
- Case study 3: Destructive measurement

# Case study: Traversal time learning in connected cars

- Networks:

- Traffic

- Static structure: Road network
    - Time-dependent attribute: traffic load



- Communication

- Time-dependent structure: cars communicate if they are close together (sufficiently close to exchange useful traffic experience)

# Traffic data

- Car collects data:
  - Car sensors (windows, seats, fuel, ...)
  - Real-time data: acceleration, ...
  - GPS localisation
  - Video data
- Infrastructure collects data:
  - Is parking space used?
  - Speed of traffic
- Databases:
  - Maps, navigation data
  - Ride organization (agenda, ride sharing, ...)

# Case study: Traversal time learning in connected cars

- Tasks:
  - Understand behavior of other traffic users
  - Understand & maintain car
  - Determine best route (possibly avoiding congestions)
  - Find free parking slots
  - Learn about unusual traffic situations
  - Update world map
  - ...

# Case study: Traversal time learning in connected cars

- Two main problems:
  - Learn regularities in the system
  - Collect real-time information sufficiently quickly
    - Learn to communicate, prioritize, ...
- Here:
  - Learn traversal time of road segments
  - Privacy-friendly

# Centralized vs. decentralized

- Privacy
  - Central server can track location of users
- Risk of failure of central service
- Communication & computation cost
  - Amount of applications increases
  - Data volume increases

# Constraints

- Each car has a local model of the traffic in its neighborhood
- Cars can only communicate with nearby cars
- Need to respect privacy
- Semi-stream: the car memory is large, but cars hear all broadcasts at most once

# Model

- Road segments  $e \in E$ 
  - have average traversal time  $\bar{d}_{e,\tau}$  in time-of-days  $\tau$ .
- Users (cars)  $u \in U$ 
  - prefer to take  $w_z^u \bar{d}_{e,\tau}$  time for a unit distance on roads of type  $z$  (highway, local road, ...)
- Actual traversal  $i$  of  $x_i^e \in E$  by  $x_i^u \in U$  at time  $x_i^t$  takes time  $x_i^d$ , assumed close to  $w_z^u \bar{d}_{e,\tau} + c_i$ , where  $c_i$  is the additional time due to congestion



# Objective function

$$L(w, c) = \sum_i (x_i^u - w_z^u \bar{d}_{e,\tau} - c_i)^2$$
$$+ \lambda_1 \sum_{i,j} (c_i - c_j)^2 \exp\left(-\left(x_i^t - x_j^t\right)^2 - d(x_i^e, x_j^e)\right)$$
$$+ \lambda_2 \sum_i c_i^2$$

Accurate predictions

Traffic situation is often similar in nearby places and at nearby times

Try to explain things with few congestions

# Algorithm

- Keep knowledge alive:
  - Broadcast learned average traversal times and current congestions, newcomers in area will learn it, those leaving can forget.
- Decentralized: Not just any optimization algorithm
- EM strategy:
  - Estimate  $c_i$  from difference between predicted and observed traversal time and from neighborhood
  - Estimate  $w_z^u$  by averaging difference between broadcasted average and personal average.
  - Improve  $\bar{d}_{e,\tau}$  incrementally from new observations

# Learnability

- Static: Converges rather quickly
  - Quadratic program
  - Each step decreases loss
  - (Wider broadcast is helpful)
- Time-dependent:
  - Target may drift
  - Can converge (and predict well) if target moves sufficiently slowly

# Privacy

- Broadcast only
  - Congestion  $c_i$
  - Road traversal time average  $\bar{d}_{e,\tau}$
- But not
  - Personal deviation in speed  $w_z^u$
- Apply protocol to broadcast training example  $(x_i^e, x_i^t, x_i^d)$  without revealing identity  $x_i^u$ 
  - Challenge: ensure trust in broadcasted messages (e.g., making traceable in case of misinformation)

# Case study: Homophilic preferential attachment

- Preferential attachment  $\rightarrow$  powerlaw graphs
  - Very simple
  - Very popular
  - No data
- E.g. Social networks
- Can we parameterize the generative process to understand better?
  - Parameterized preferential attachment  $PA_{\theta}$
  - Newly arrived node selects neighbors  $v$  with probability  $PA_{\theta}(v)$



# Homophilic preferential attachment

## Problem statement

- We only see the end-result, nobody kept a log
- Can we still estimate  $\theta$  ?
- Simple case: homophily
  - Each vertex  $v$  has feature vector  $x^v \in F$  with distribution  $p_f(\cdot)$
  - Probability of selecting neighbor  $v$  for  $u$  is proportional to  $\sum_i \theta_i x_i^u x_i^v$ .

# Learning homophilic weights

- Known history (order in which nodes arrive):
  - Regression
  - Given newcomer features, existing node features and edge (1) / no-edge (0)
- Undirected graph:
  - Can't reconstruct attachment examples directly
  - Probabilistic approach
  - Assume order of node arrivals is random

# Homophilic preferential attachment

## Solution by minimizing loss

$$L(w) = \sum_{x \in F} \sum_{y \in F} \left( E_{x,y} - \frac{p_f(x)p_f(y) \sum_i w_i x_i y_i}{\sum_{z \in F} p_f(z) \sum_i w_i x_i z_i} \right)$$



# Learnability

- Yes, one can learn from a snapshot
  - Need  $O(\epsilon^{-2} p_{min}^2)$  examples
- Extensions:
  - Including degree, patterns, ...
  - Becomes quickly more complex

# Case study: biological regulatory networks

- Network:
  - Nodes: genes
  - Arcs: regulations
- More activated genes (high expression level) generate more transcription factors that (up or down) regulate other genes.



$$v_{g,t} = f(v_{pa(g,1),t-1}, v_{pa(g,2),t-1}, \dots)$$

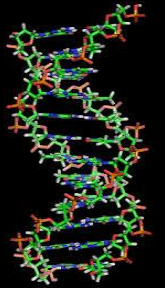
where  $pa(g, i)$  is  $i$ -th parent of gene  $g$  and  $v_{g,t}$  is expression level of gene  $g$  at time  $t$ .

# Learning task

- Given:
  - Input (experimental setup), output (measurement) pairs
- Learn:
  - The network
    - structure  $pa$
    - combination functions  $f$
- Active learning operators:
  - Can choose experiment

# Biological regulatory networks

- Hardness:
  - In principle turing complete (see also DNA computing)
  - Hence, learning network from (only) input and output is hard.
- Experiments:
  - Destructive
  - May measure output at selected point in time
  - May modify the network (gene knock out)



# Biological regulatory networks

- Program induction?
  - Learning programs from input-output pairs is hard
  - But what if we can also get input-output pairs of programs obtained by deleting lines in the original program?
- Approach:
  - Hill climbing through model space
    - In each iteration evaluate minor changes to model
  - Exploit domain knowledge
- Results:
  - Can't expect to learn exactly the same network
  - With sufficient domain knowledge, improvements on prior models can be made

# Case studies

Setting	Observation	Exploit	
Traffic	Neighborhood Semi-stream Multi-agent	Continuity Collaboration (info flow) (regularity of network)	Stochastic gradient
Preferential attachment	Global Only present Single world	Regularity of network (and Large Scale)	Analysis & optimization
Regulatory network	Selected variable Selected time Repeatable	Experimental options (info flow)	Hill climbing

# Discussion – Generic approaches?

- Several types of settings for time-dependent networks.
  - Wide range in learnability
- generic probabilistic model solvers can't (yet) exploit the various structures. How does this map to lifted inference?
- Meta-learning from 3 case studies:
  - Network regularity (i.e. High network entropy) is important in determining learnability

# Discussion - Complexity

- What makes learning from time-dependent large-scale partially-observed graphs hard?
  - No network regularity
  - Long sequences without good observations (as in (PO)MDPs) (making information flow harder to exploit)
  - Discrete / non-continuous / combinatorial evolution



# Conclusions

- TD graph is often not fully observable
- LS can help to collect sufficient information
- Often domain-specific solutions needed

# Future directions

- More in-depth study of learnability
  - Exploit network regularity?
- More generic approach?
  - Can we automatically understand structure, information flow, ...?
- Tagging: only “TDG” may not be sufficient
  - Can we isolate frequently recurring (sub)problems?

Questions?

