Graph Mining & Multi-Relational Learning Tools and Applications Part II

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Bird's eye view

Task \ Tool	1.1 PR/HITS	1.1 PPR	1.2 METIS/ SVD	1.3 OddBall+	1.4 BP	2.1 FM	2.1 Tensor	2.2 HIN	2.3 SRL
1.1 Node Ranking	👍								
1.1' Link Prediction		👍							
1.2 Comm. Detection			👍						
1.3 Anomaly Detection				👍					
1.4 Propagation					👍				

Part 1: Plain Graphs

Part 2: Complex Graphs

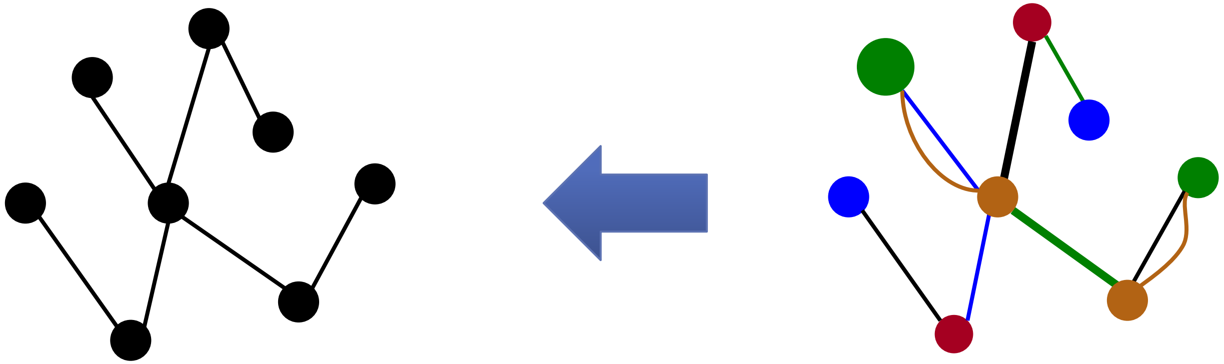
Bird's eye view

- Part 2: Complex and Heterogeneous Graphs
  - P 2.1: Factorization Methods
  - P 2.2: Heterogeneous Information Networks
  - P 3.3: Statistical Relational Learning

Complex Networks

What Plain Graphs Tools Capture

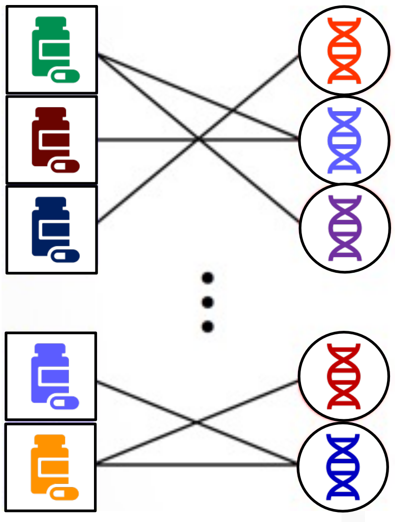
Complex Networks



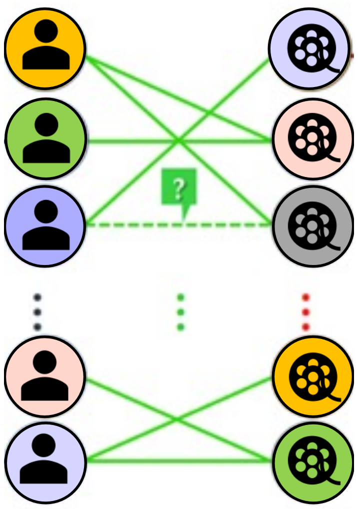
Complex Network (Many Related Terms)

- Plain Graphs + Extra Information on?
  - Nodes?
    - Multi-typed Networks
  - Edges?
    - Multi-layer Networks
    - Multi-dimensional Networks
    - Multi-modal Networks
  - Both?
    - Attributed Networks
    - Multiplex Networks
    - Multi Relational Networks
    - Heterogenous Information Networks
    - Complex Networks
  - …

Common Bipartite Structure



Drug-Target Interactions



Recommender Systems

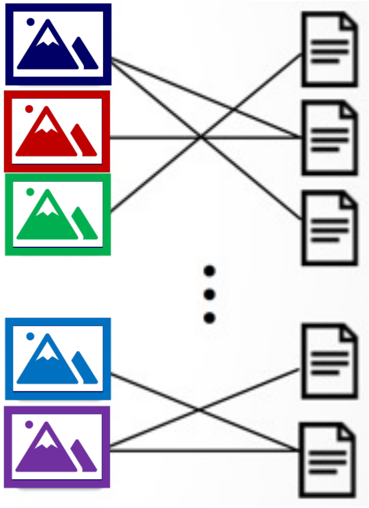
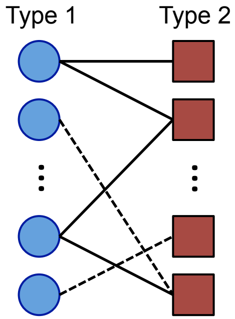


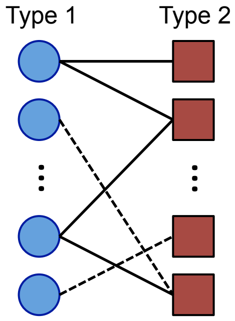
Image Captioning

Complex Bipartite Network

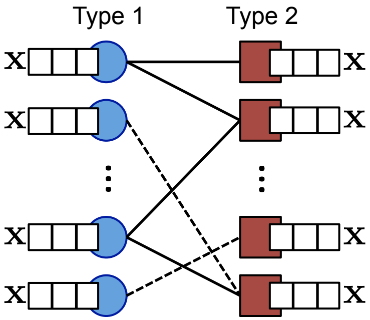


Two types of nodes
and relation of interest

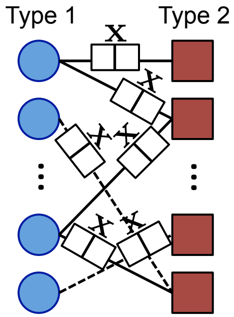
Complex Bipartite Network



Two types of nodes
and relation of interest

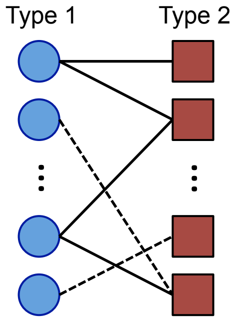


Additional features
for nodes

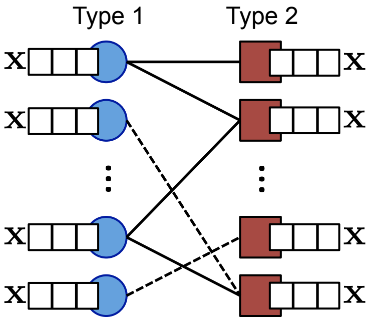


Additional features
for the relation

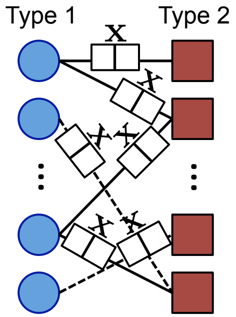
Complex Bipartite Network



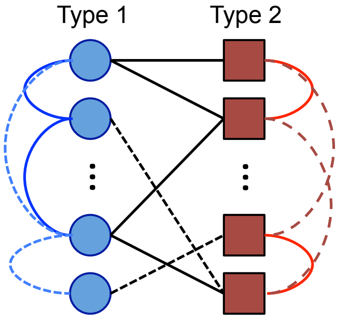
Two types of nodes and relation of interest



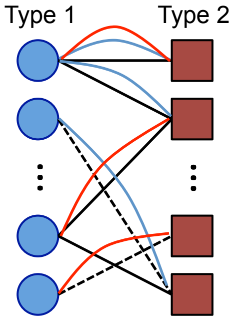
Additional features for nodes



Additional features for the relation

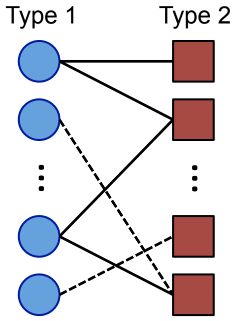


Additional relations for nodes

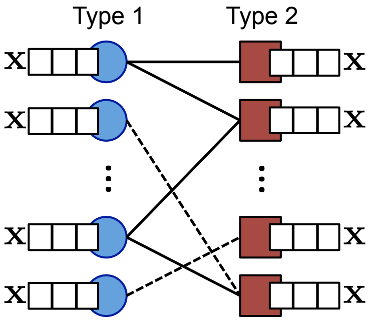


Additional relations for the relation

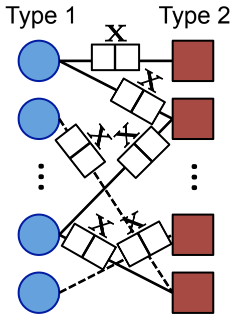
Complex Bipartite Network



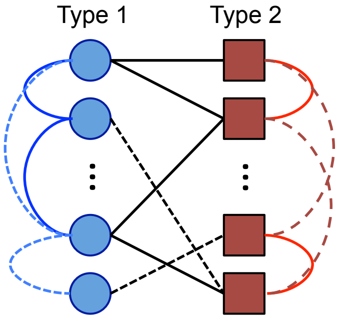
Two types of nodes
and relation of interest



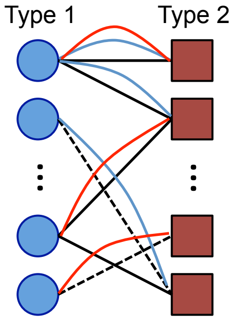
Additional features
for nodes



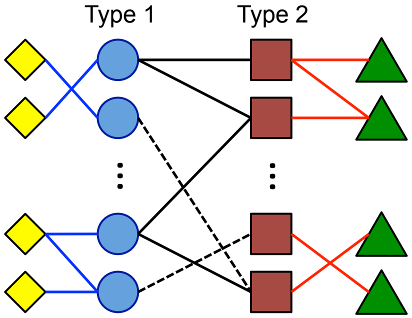
Additional features
for the relation



Additional relations
for nodes

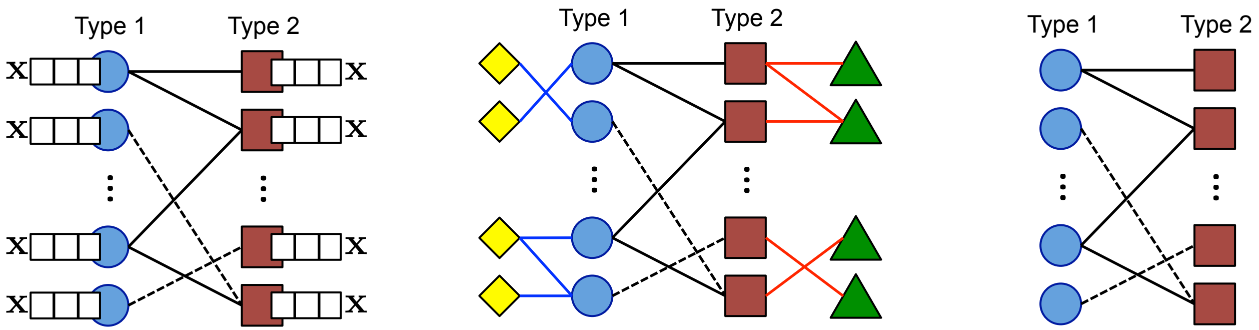


Additional relations
for the relation



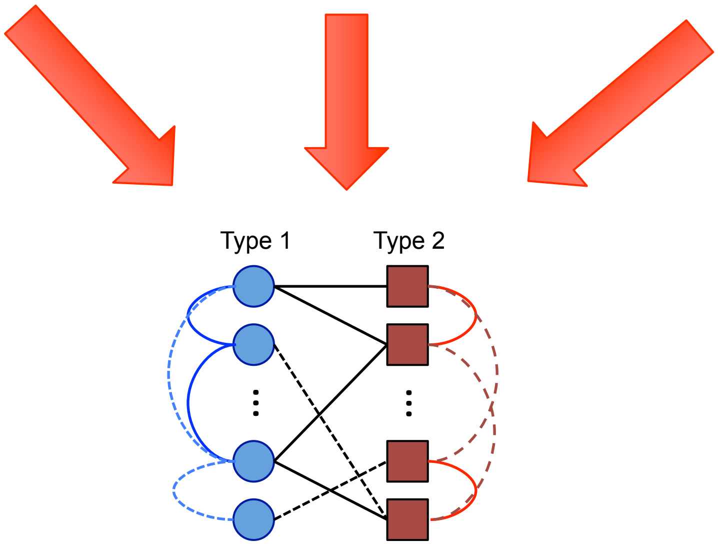
Additional relations
with external nodes

Complex Bipartite Network



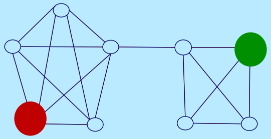
Euclidean Distance

Jaccard/Cosine Similarity



Bird's eye view

- Part 2: Complex and Heterogeneous Graphs
  - P 2.1: Factorization Methods
    - P 2.1.1: Factorization Machines
    - P 2.1.2: Tensor Methods
  - P 2.2: Heterogeneous Information Networks
  - P 3.3: Statistical Relational Learning

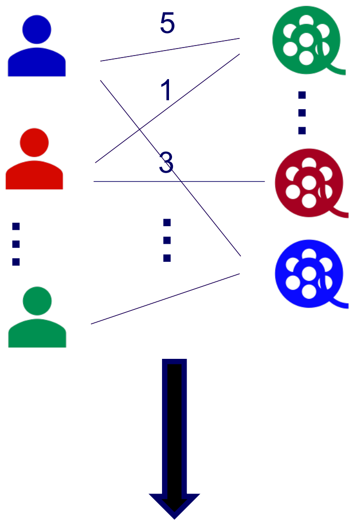


Question:

- Q: How can we add extra information to a bipartite-graph for link predication / recommender systems?

- A: Factorization Machines is one way!

Bipartite Graph

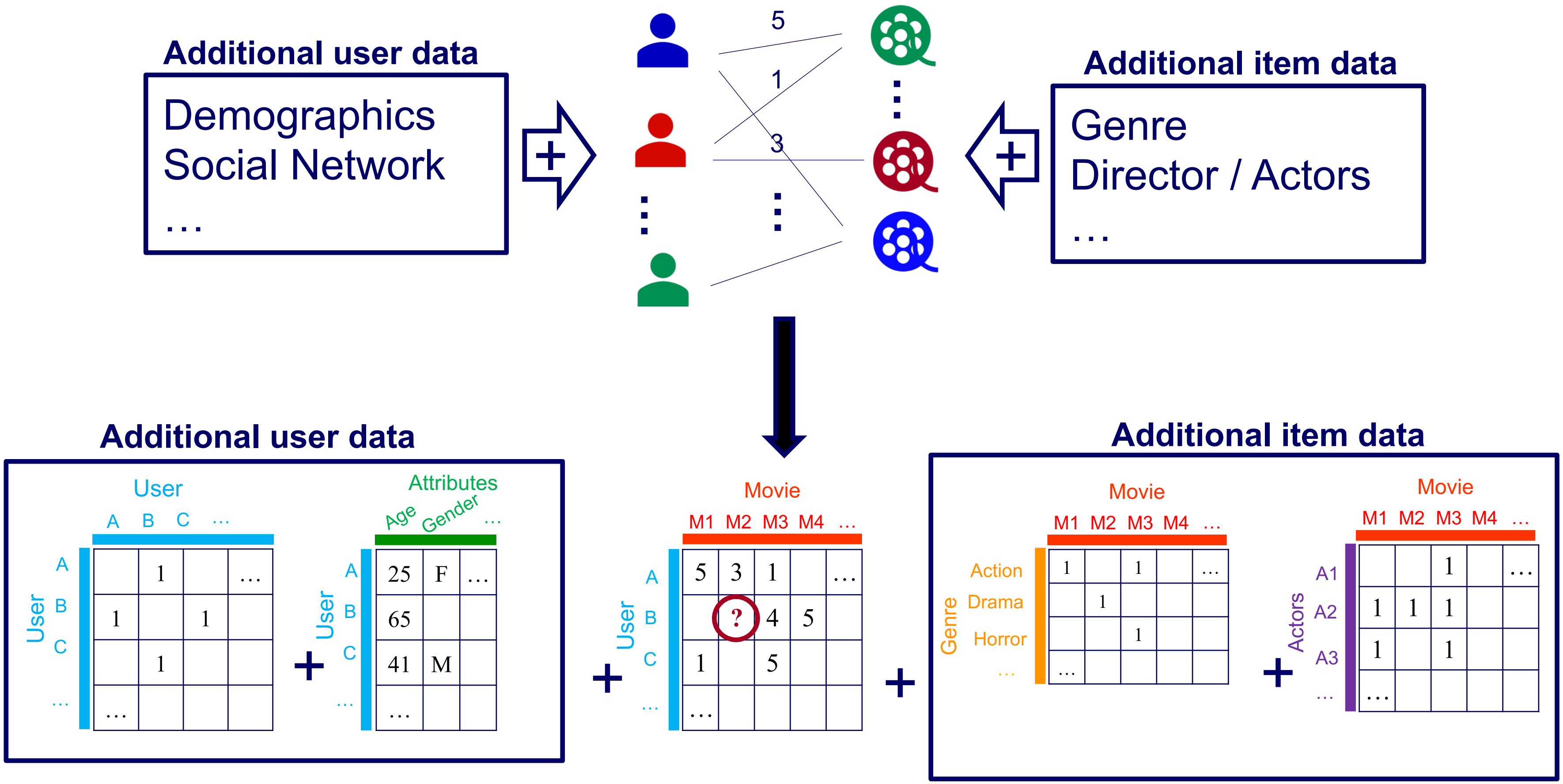


Movie

		M1	M2	M3	M4	…
User	A	5	3	1		…
	B		?	4	5	
	C	1		5		
	…	…				

→ SVD / Matrix Factorization

How to include additional data?



Additional user data

Demographics
Social Network
…

Additional item data

Genre
Director / Actors
…

Additional user data

User	A	B	C	…
A		1		…
B	1		1	
C		1		
…	…			

+

User	Age	Gender	…
A	25	F	…
B	65		
C	41	M	
…	…		

+

User	M1	M2	M3	M4	…
A	5	3	1		…
B		?	4	5	
C	1		5		
…	…				

+

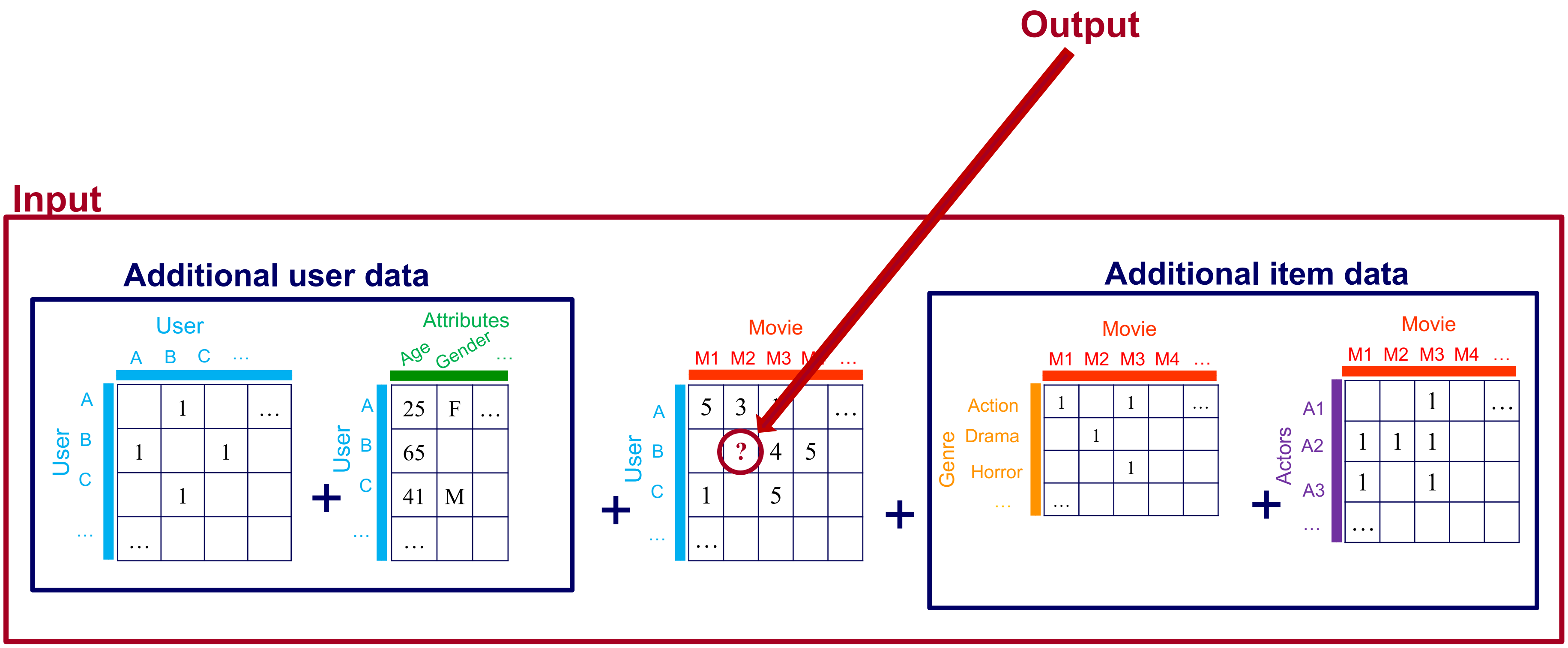
Additional item data

Genre	M1	M2	M3	M4	…
Action	1		1		…
Drama		1			
Horror			1		
…	…				

+

Actors	M1	M2	M3	M4	…
A1			1		…
A2	1	1	1		
A3	1		1		
…	…				

How to include additional data?



Output

Input

Additional user data

User	A	B	C	…
A		1		…
B	1		1	
C		1		
…	…			

+

User	Age	Gender	…
A	25	F	…
B	65		
C	41	M	
…	…		

+

User	M1	M2	M3	M4	…
A	5	3	1		…
B		?	4	5	
C	1		5		
…	…				

+

Additional item data

Genre	M1	M2	M3	M4	…
Action	1		1		…
Drama		1			
Horror			1		
…	…				

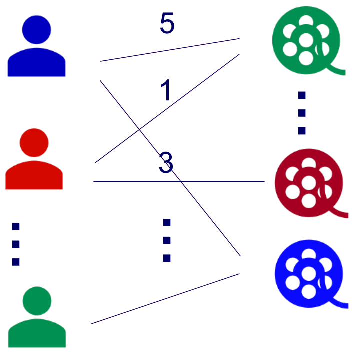
+

Actors	M1	M2	M3	M4	…
A1			1		…
A2	1	1	1		
A3	1		1		
…	…				

How to include additional data?

Additional user data

Demographics
Social Network
…



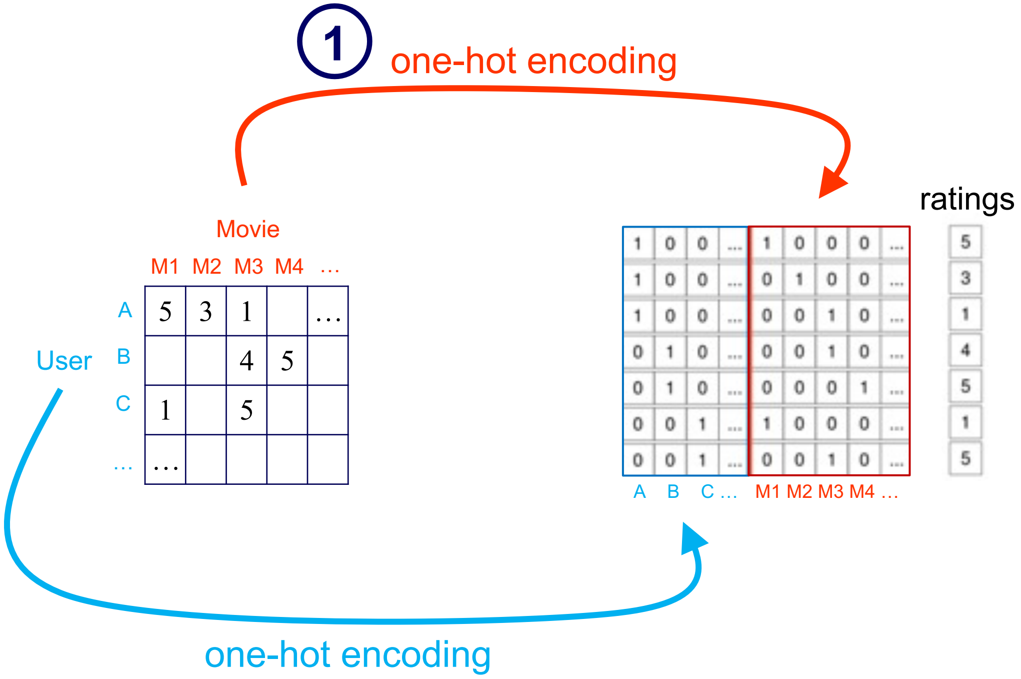
Additional item data

Genre
Director / Actors
…

One answer: Factorization Machines

1. One-hot encoding
2. Pairwise Interactions
3. Latent factor representation

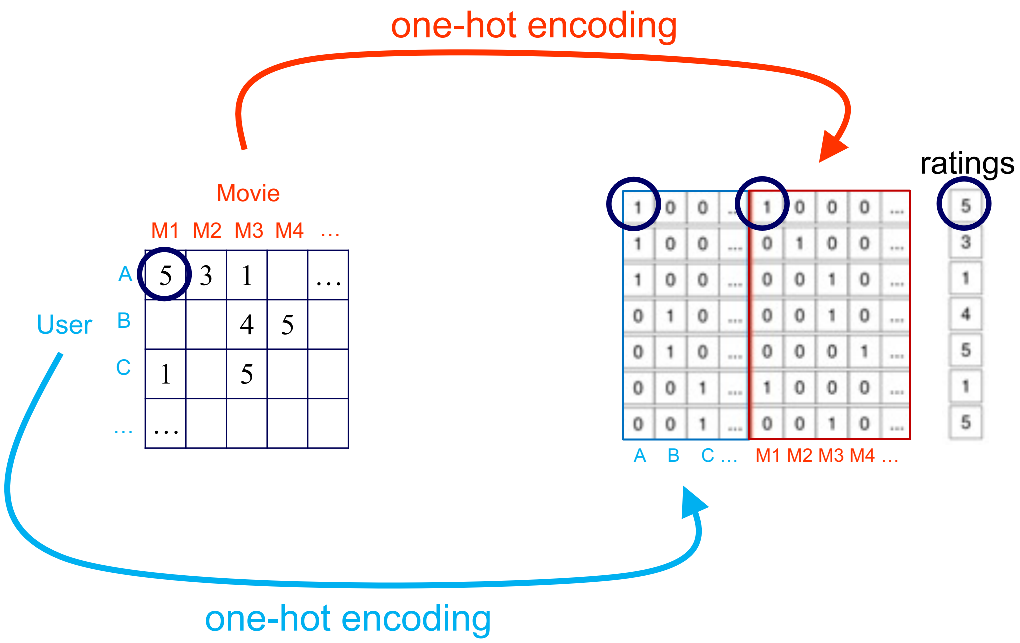
Data Representation in FM



User	M1	M2	M3	M4	…
A	5	3	1		…
B			4	5	
C	1		5		
…	…				

A	B	C	…	M1	M2	M3	M4	…	ratings
1	0	0	…	1	0	0	0	…	5
1	0	0	…	0	1	0	0	…	3
1	0	0	…	0	0	1	0	…	1
0	1	0	…	0	0	1	0	…	4
0	1	0	…	0	0	0	1	…	5
0	0	1	…	1	0	0	0	…	1
0	0	1	…	0	0	1	0	…	5

Data Representation in FM



one-hot encoding

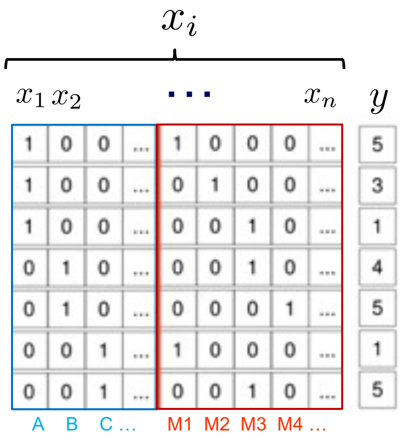
Movie

User	M1	M2	M3	M4	…
A	5	3	1		…
B			4	5	
C	1		5		
…	…				

A	B	C	…	M1	M2	M3	M4	…	ratings
1	0	0	...	1	0	0	0	...	5
1	0	0	...	0	1	0	0	...	3
1	0	0	...	0	0	1	0	...	1
0	1	0	...	0	0	1	0	...	4
0	1	0	...	0	0	0	1	...	5
0	0	1	...	1	0	0	0	...	1
0	0	1	...	0	0	1	0	...	5

one-hot encoding

Factorization Machines

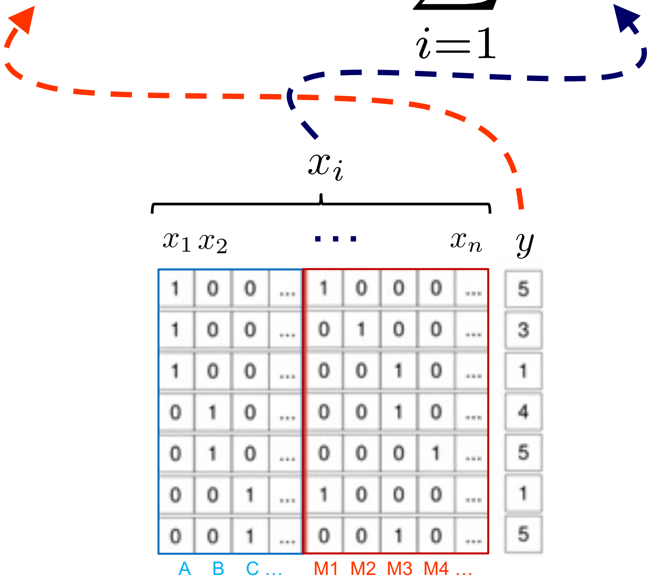

x_i
x_1 x_2
$\cdots$
x_n
y

A	B	C	…	M1	M2	M3	M4	…	y
1	0	0	...	1	0	0	0	...	5
1	0	0	...	0	1	0	0	...	3
1	0	0	...	0	0	1	0	...	1
0	1	0	...	0	0	1	0	...	4
0	1	0	...	0	0	0	1	...	5
0	0	1	...	1	0	0	0	...	1
0	0	1	...	0	0	1	0	...	5

Details

Factorization Machines

$$\hat{y}\left(\mathbf{x}\right) = \overbrace{w_0}^{\text{Global bias}} + \sum_{i=1}^{n} \overbrace{w_i}^{\text{Regression coefficient of i-th variable.}} x_i$$



A	B	C	...	M1	M2	M3	M4	...	y
1	0	0	...	1	0	0	0	...	5
1	0	0	...	0	1	0	0	...	3
1	0	0	...	0	0	1	0	...	1
0	1	0	...	0	0	1	0	...	4
0	1	0	...	0	0	0	1	...	5
0	0	1	...	1	0	0	0	...	1
0	0	1	...	0	0	1	0	...	5

Details

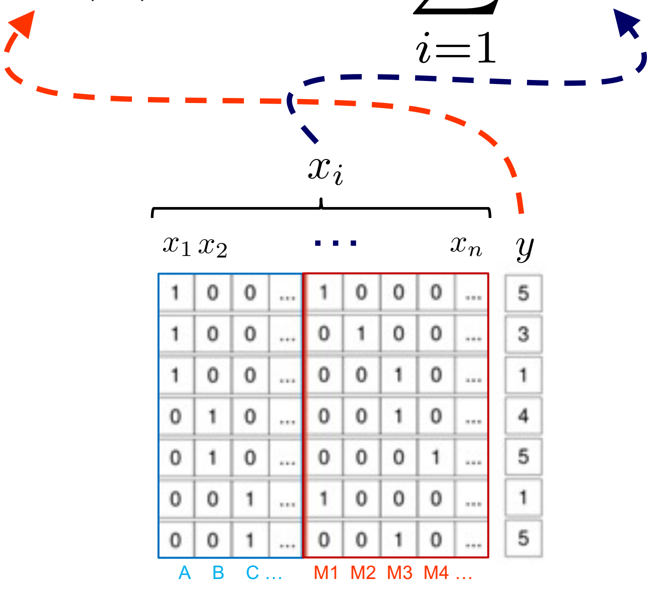
Factorization Machines

Linear Regression

Regression coefficient
of i-th variable.

Global bias

$$\hat{y}(\mathbf{x}) = \overbrace{w_0} + \sum_{i=1}^{n} \overbrace{w_i} x_i$$



A	B	C ...		M1	M2	M3	M4 ...		y
1	0	0	...	1	0	0	0	...	5
1	0	0	...	0	1	0	0	...	3
1	0	0	...	0	0	1	0	...	1
0	1	0	...	0	0	1	0	...	4
0	1	0	...	0	0	0	1	...	5
0	0	1	...	1	0	0	0	...	1
0	0	1	...	0	0	1	0	...	5

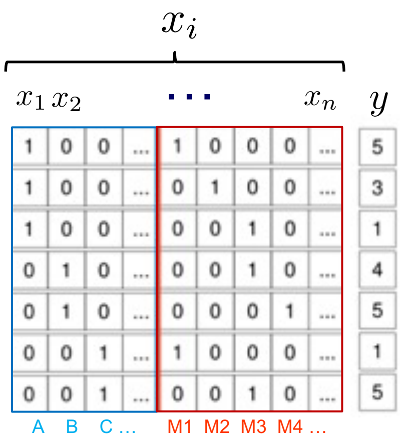
Details

Factorization Machines

2

$$\hat{y}\left(\mathbf{x}\right) = \overbrace{w_0}^{\text{Global bias}} + \sum_{i=1}^{n} \overbrace{w_i}^{\text{Regression coefficient of i-th variable.}} x_i + \sum_{i=1}^{n} \sum_{j=i+1}^{n} \overbrace{w_{ij}}^{\text{Pairwise interactions}} x_i x_j$$

1



x_i
x_1 x_2 $\cdots$ x_n

A	B	C	...	M1	M2	M3	M4	...	y
1	0	0	...	1	0	0	0	...	5
1	0	0	...	0	1	0	0	...	3
1	0	0	...	0	0	1	0	...	1
0	1	0	...	0	0	1	0	...	4
0	1	0	...	0	0	0	1	...	5
0	0	1	...	1	0	0	0	...	1
0	0	1	...	0	0	1	0	...	5

Details

Factorization Machines

$$\hat{y}\left(\mathbf{x}\right) = \overbrace{w_0}^{\text{Global bias}} + \sum_{i=1}^{n} \overbrace{w_i}^{\text{Regression coefficient of i-th variable.}} x_i + \sum_{i=1}^{n} \sum_{j=i+1}^{n} \underbrace{\overbrace{w_{ij}}^{\text{Pairwise interactions (2)}}}_{\text{Impractical to compute}} x_i x_j$$

1

x_i

x_1	x_2	$\cdots$						x_n	y
1	0	0	...	1	0	0	0	...	5
1	0	0	...	0	1	0	0	...	3
1	0	0	...	0	0	1	0	...	1
0	1	0	...	0	0	1	0	...	4
0	1	0	...	0	0	0	1	...	5
0	0	1	...	1	0	0	0	...	1
0	0	1	...	0	0	1	0	...	5
A	B	C ...		M1	M2	M3	M4 ...		

Impractical to compute

Details

Factorization Machines

Regression coefficient
of i-th variable.

Global bias

Pairwise interactions ②

$$\hat{y}\left(\mathbf{x}\right) = \overbrace{w_0} + \sum_{i=1}^{n} \overbrace{w_i} x_i + \sum_{i=1}^{n} \sum_{j=i+1}^{n} \underbrace{\overbrace{w_{ij}}} x_i x_j$$

①

x_i

x_1 x_2 $\cdots$ x_n y

A	B	C ...		M1	M2	M3	M4 ...		y
1	0	0	...	1	0	0	0	...	5
1	0	0	...	0	1	0	0	...	3
1	0	0	...	0	0	1	0	...	1
0	1	0	...	0	0	1	0	...	4
0	1	0	...	0	0	0	1	...	5
0	0	1	...	1	0	0	0	...	1
0	0	1	...	0	0	1	0	...	5

$$w_{ij} \approx \hat{w}_{ij} = \underbrace{\left\langle \mathbf{v}_{\mathbf{x}_i}, \mathbf{v}_{\mathbf{x}_j} \right\rangle}$$ ③

Latent factor for
each column

Details

Factorization Machines

$$\hat{y} = w_0 + \sum_{i=1}^{n} w_i x_i + \sum_{i=1}^{n} \sum_{j=i+1}^{n} \overbrace{\langle \mathbf{v}_{\mathbf{x}_i}, \mathbf{v}_{\mathbf{x}_j} \rangle}^{w_{ij}} x_i x_j$$

Regression →

$$\min \sum_{E} (y - \hat{y})^2 + \lambda_1 ||\mathbf{w}_i||^2 + \lambda_2 ||\mathbf{V}_{\mathbf{x}}||^2$$

X

y

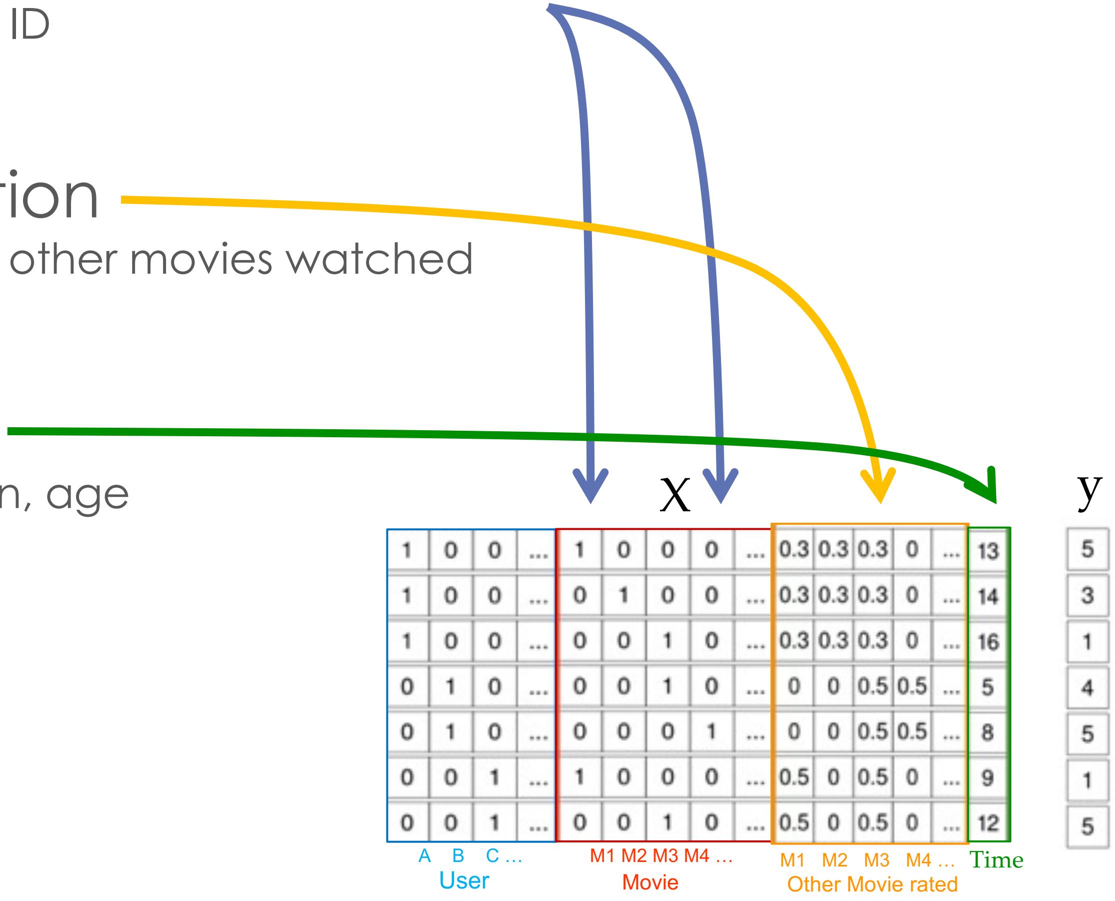
User				Movie					Time					y
A	B	C	…	M1	M2	M3	M4	…	1am	2am	3am	4am	…	
1	0	0	...	1	0	0	0	...	0	0	0	0	...	5
1	0	0	...	0	1	0	0	...	1	0	0	0	...	3
1	0	0	...	0	0	1	0	...	0	1	0	0	...	1
0	1	0	...	0	0	1	0	...	0	0	0	0	...	4
0	1	0	...	0	0	0	1	...	0	0	1	0	...	5
0	0	1	...	1	0	0	0	...	0	0	0	0	...	1
0	0	1	...	0	0	1	0	...	1	0	0	0	...	5

Data Representation in FM

- Categorical Information (One-hot encoding)
  e.g., User and item ID

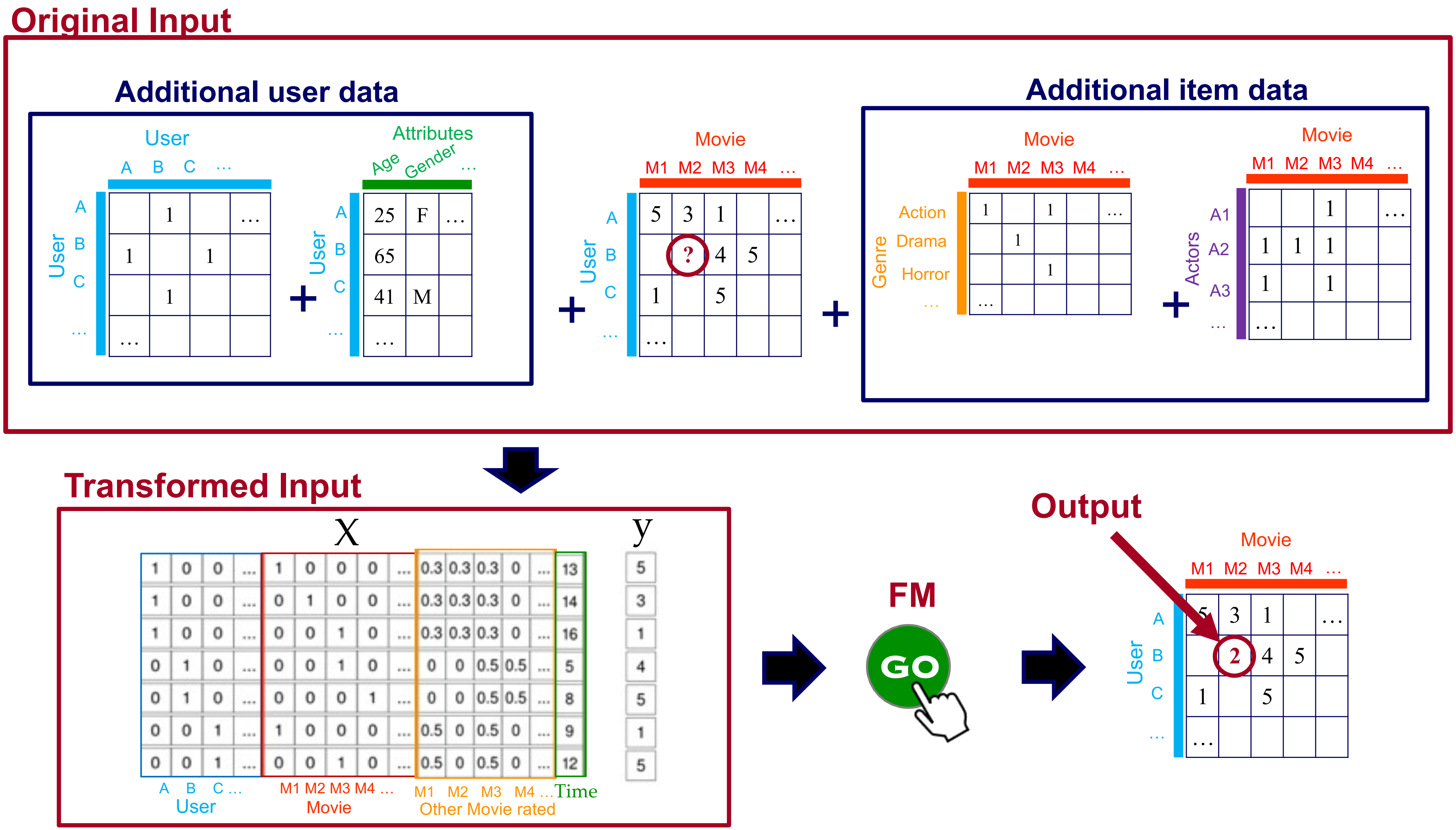
- Set Information
  e.g., list of friends, other movies watched

- Continuous
  e.g., time, location, age



x															y
User				Movie					Other Movie rated					Time	
A	B	C	…	M1	M2	M3	M4	…	M1	M2	M3	M4	…		
1	0	0	...	1	0	0	0	...	0.3	0.3	0.3	0	...	13	5
1	0	0	...	0	1	0	0	...	0.3	0.3	0.3	0	...	14	3
1	0	0	...	0	0	1	0	...	0.3	0.3	0.3	0	...	16	1
0	1	0	...	0	0	1	0	...	0	0	0.5	0.5	...	5	4
0	1	0	...	0	0	0	1	...	0	0	0.5	0.5	...	8	5
0	0	1	...	1	0	0	0	...	0.5	0	0.5	0	...	9	1
0	0	1	...	0	0	1	0	...	0.5	0	0.5	0	...	12	5

Take Away



Original Input

Additional user data

User

User	A	B	C	…
A		1		…
B	1		1	
C		1		
…	…			

+

Attributes

User	Age	Gender	…
A	25	F	…
B	65		
C	41	M	
…	…		

+

Movie

User	M1	M2	M3	M4	…
A	5	3	1		…
B		?	4	5	
C	1		5		
…	…				

+

Additional item data

Movie

Genre	M1	M2	M3	M4	…
Action	1		1		…
Drama		1			
Horror			1		
…	…				

+

Movie

Actors	M1	M2	M3	M4	…
A1			1		…
A2	1	1	1		
A3	1		1		
…	…				

Transformed Input

X

User A	User B	User C	User …	Movie M1	Movie M2	Movie M3	Movie M4	Movie …	Other Movie rated M1	Other Movie rated M2	Other Movie rated M3	Other Movie rated M4	Other Movie rated …	Time	y
1	0	0	...	1	0	0	0	...	0.3	0.3	0.3	0	...	13	5
1	0	0	...	0	1	0	0	...	0.3	0.3	0.3	0	...	14	3
1	0	0	...	0	0	1	0	...	0.3	0.3	0.3	0	...	16	1
0	1	0	...	0	0	1	0	...	0	0	0.5	0.5	...	5	4
0	1	0	...	0	0	0	1	...	0	0	0.5	0.5	...	8	5
0	0	1	...	1	0	0	0	...	0.5	0	0.5	0	...	9	1
0	0	1	...	0	0	1	0	...	0.5	0	0.5	0	...	12	5

FM

GO

Output

Movie

User	M1	M2	M3	M4	…
A	5	3	1		…
B		2	4	5	
C	1		5		
…	…				

Software Tools

- SageMaker Factorization Machines: https://docs.aws.amazon.com/sagemaker/latest/dg/fact-machines.html
- libFM: http://www.libfm.org/

References

- Rendle, Steffen
  Factorization machines with libfm
  ACM Transactions on Intelligent Systems and Technology (TIST), 2012

Bird’s eye view

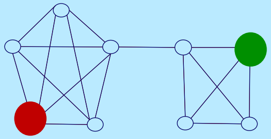
Tool Task	1.1 PR/HITS	1.1 PPR	1.2 METIS/ SVD	1.3 OddBall+	1.4 BP	2.1 FM	2.1 Tensor	2.2 HIN	2.3 SRL
1.1 Node Ranking*	👍					(👍)			
1.1’ Link Prediction		👍				👍			
1.2 Comm. Detection			👍						
1.3 Anomaly Detection				👍					
1.4 Propagation					👍				

Part 1: Plain Graphs ⟷ **Part 2: Complex Graphs**

(* or Node Classification)

Bird’s eye view

- Part 2: Complex and Heterogeneous Graphs
  - – P 2.1: Factorization Methods
    - P 2.1.1: Factorization Machines
    - P 2.1.2: Tensor Methods
  - – P 2.2: Heterogeneous Information Networks
  - – P 3.3: Statistical Relational Learning

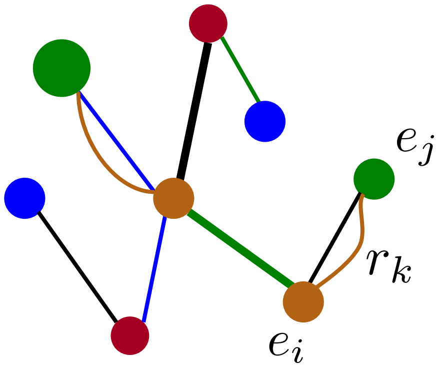


Question:

- Q: How can we add extra information to a graph and find communities?
- A: Tensors are one way!

Multi-relational network

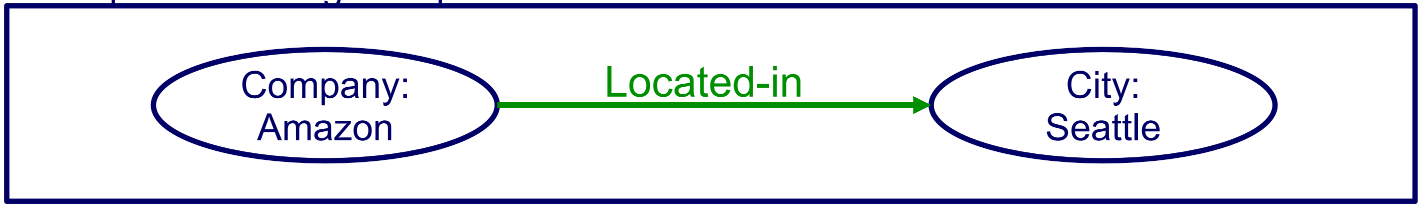
How to represent?



n: entities (e)

m: relations (r)

Example: Knowledge Graph

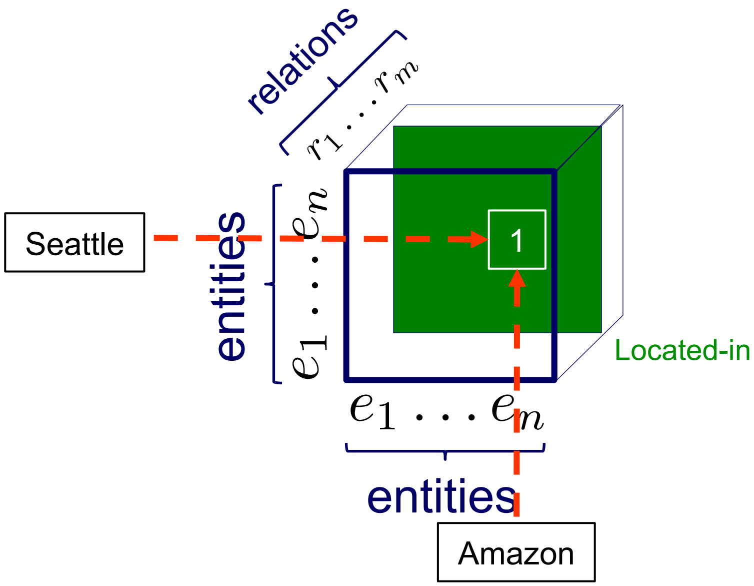


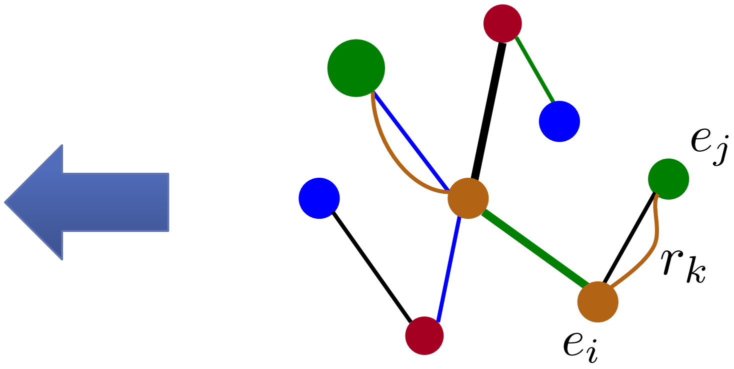
Company: Amazon

Located-in

City: Seattle

Multi-relational network





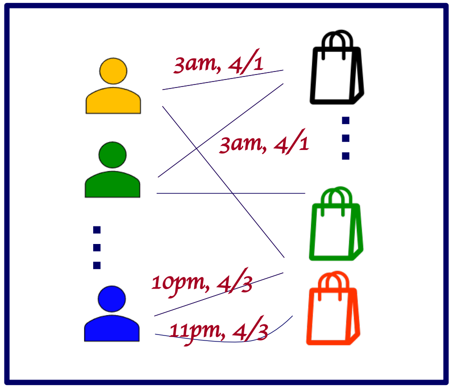
n: entities (e)
m: relations (r)

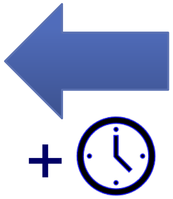
Tensor

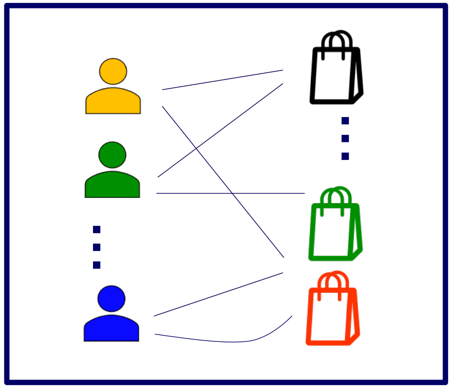
Time-evolving networks

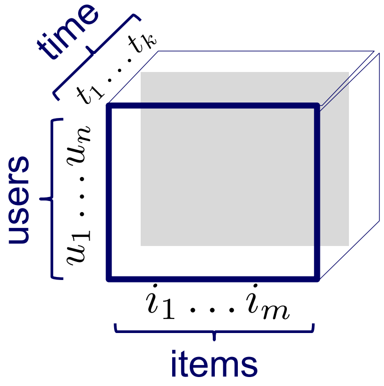
who – buys – what - when

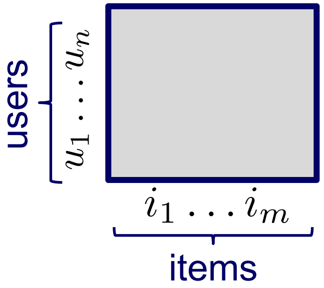
who – buys – what











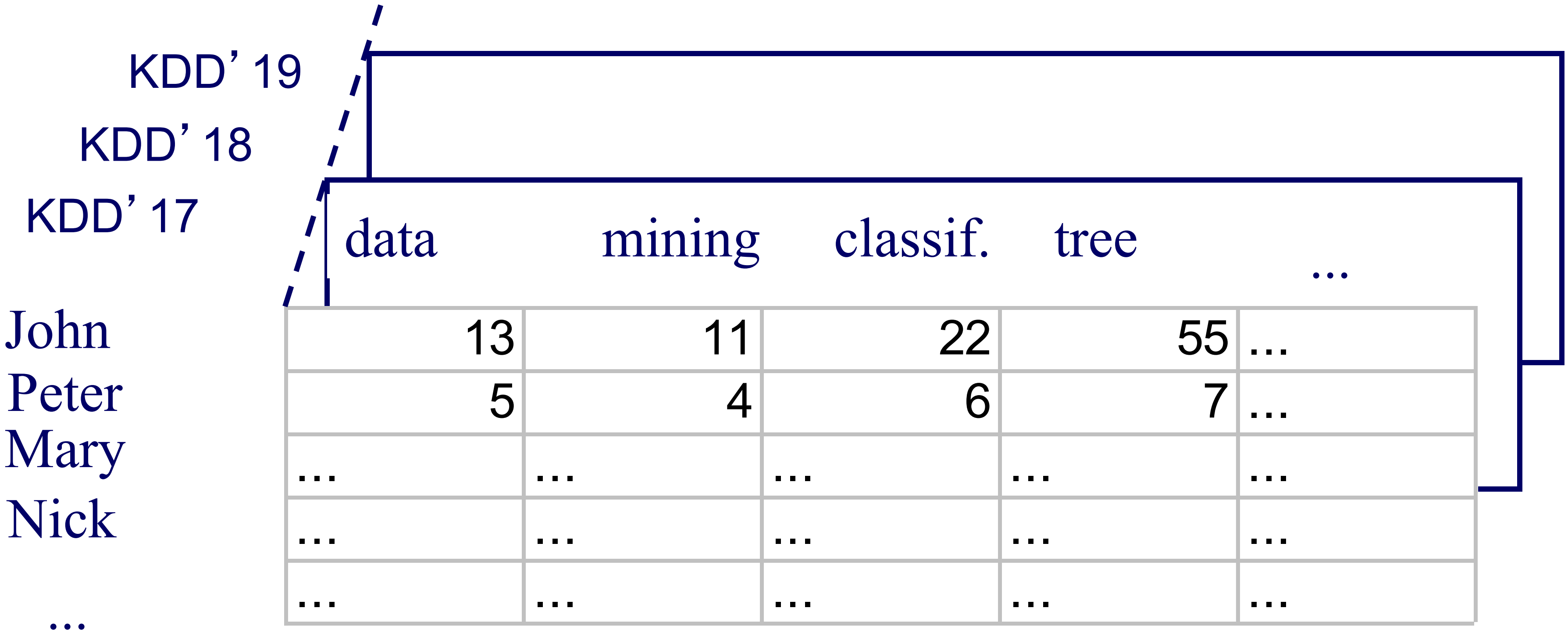
Tensor examples

- Q: What is a tensor?
- A: N-D generalization of matrix:

KDD' 17	data	mining	classif.	tree	…
John	13	11	22	55	…
Peter	5	4	6	7	…
Mary	…	…	…	…	…
Nick	…	…	…	…	…
…	…	…	…	…	…

Tensor examples

- Q: What is a tensor?
- A: N-D generalization of matrix:



KDD’ 19

KDD’ 18

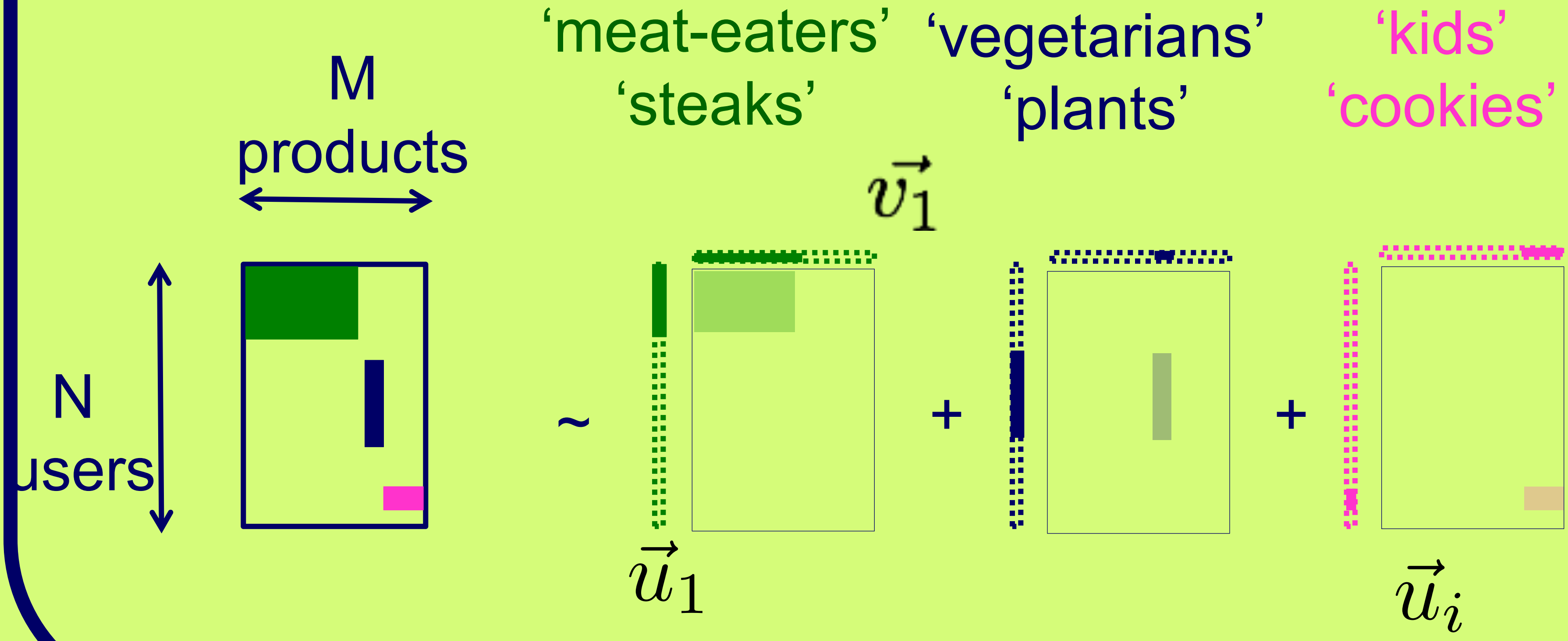
KDD’ 17

	data	mining	classif.	tree	...
John	13	11	22	55	...
Peter	5	4	6	7	...
Mary	...	...	...	...	...
Nick	...	...	...	...	...
...	...	...	...	...	...

Reminder (from SVD)

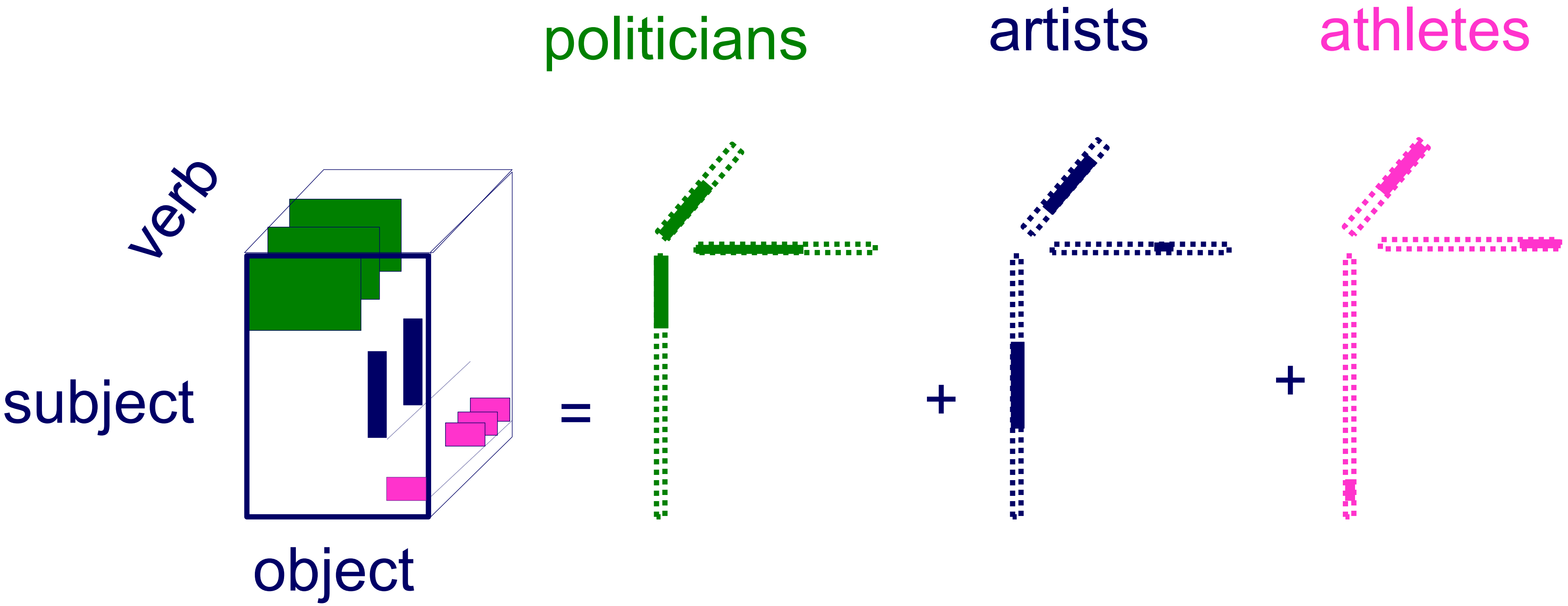
Tensor factorization

- Recall: (SVD) matrix factorization: finds blocks



Tensor factorization

One Approach: PARAFAC decomposition



Example Applications

➡ - TA1: Phonecall
- TA2: Network traffic

TA1: Anomaly detection in time-evolving graphs

- Anomalous communities in phone call data:
  - European country, 4M clients, data over 2 weeks

[PAKDD] “*Com2: Fast Automatic Discovery of Temporal (Comet) Communities”,* Miguel Araujo, Spiros Papadimitriou, Stephan Günnemann, Christos Faloutsos, Prithwish Basu, Ananthram Swami,Evangelos Papalexakis, Danai Koutra.

TA1: Anomaly detection in time-evolving graphs

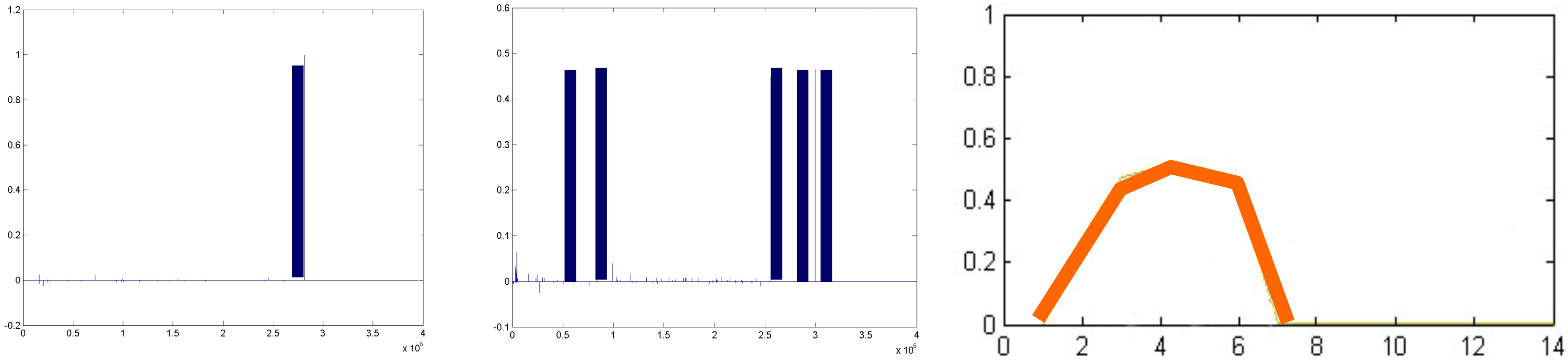
- Anomalous communities in phone call data:
  - European country, 4M clients, data over 2 weeks

PARAFAC

1 caller

5 receivers

4 days of activity



~200 calls to EACH receiver on EACH day!

TA1: Anomaly detection in time-evolving graphs

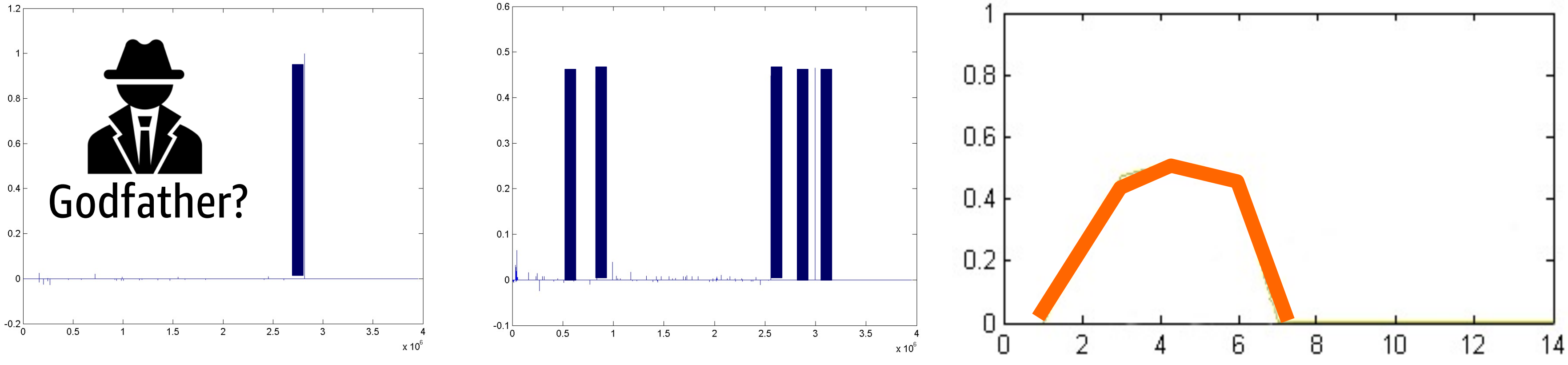
- Anomalous communities in phone call data:
  - European country, 4M clients, data over 2 weeks

PARAFAC

1 caller

5 receivers

4 days of activity



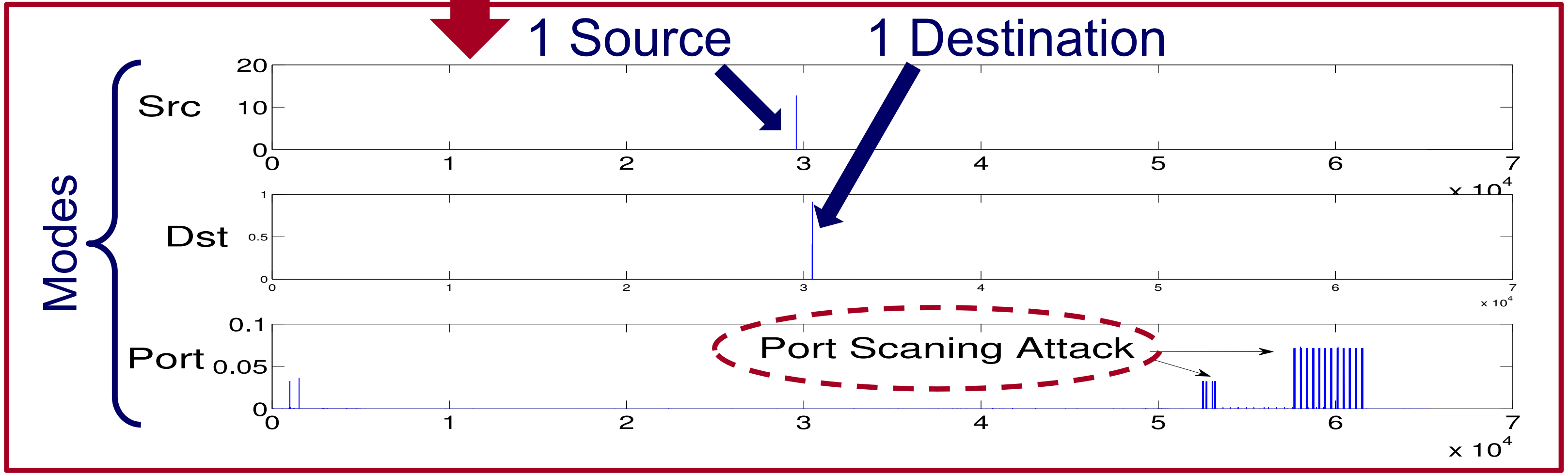
~200 calls to EACH receiver on EACH day!

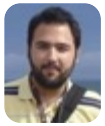
Example Applications

- TA1: Phonecall
- TA2: Network traffic

TA2: Anomaly detection in network traffic

PARAFAC

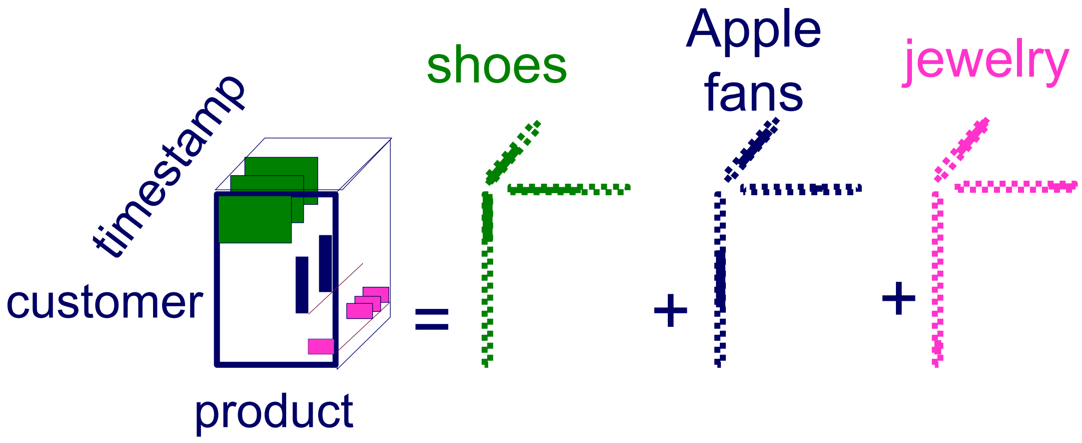




[ECML/PKDD] “ParCube: Sparse Parallelizable Tensor Decompositions”, Evangelos E. Papalexakis, Christos Faloutsos, Nikos Sidiropoulos

Take Away

- Tensor analysis finds latent variables (e.g., market-segments)
  - Deviations → Anomalies
  - Link Prediction
- Extends SVD/factorization, to higher-modes



Software Tools

- TensorLy: Tensor Learning in Python
  http://tensorly.org/stable/index.html

- Tensor Toolbox for MATLAB
  http://www.tensortoolbox.org/

References

- Tamara G. Kolda and Brett W. Bader
  Tensor Decompositions and Applications
  SIAM Rev., 51(3), pp 455–500, 2009

- Nicholas D. Sidiropoulos, Lieven De Lathauwer,, Xiao Fu,, Kejun Huang, Evangelos E. Papalexakis, and Christos Faloutsos
  Tensor Decomposition for Signal Processing and Machine Learning
  IEEE TSP, 65(13), July 1, 2017

Bird's eye view

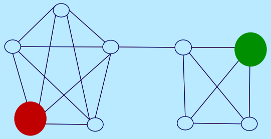
Tool Task	1.1 PR/HITS	1.1 PPR	1.2 METIS/ SVD	1.3 OddBall+	1.4 BP	2.1 FM	2.1 Tensor	2.2 HIN	2.3 SRL
1.1 Node Ranking	👍					(👍)			
1.1' Link Prediction		👍				👍	👍		
1.2 Comm. Detection			👍				👍		
1.3 Anomaly Detection				👍			👍		
1.4 Propagation					👍				

Part 1: Plain Graphs

Part 2: Complex Graphs

Bird’s eye view

- Part 2: Complex and Heterogeneous Graphs
  - – P 2.1: Factorization Methods
  - – P 2.2: Heterogeneous Information Networks
    - Metapaths
    - PathSim
  - – P 3.3: Statistical Relational Learning



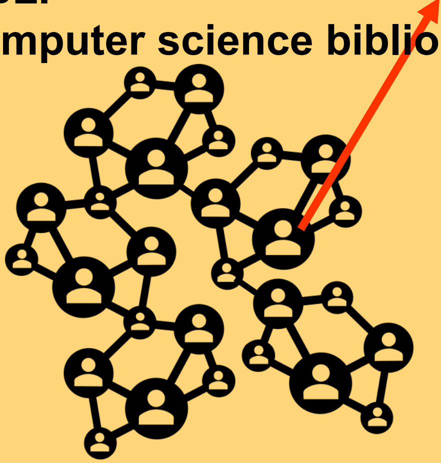
Question:

Q: How can we find node similarities in networks with extra information?

Question:

Q: In DBLP who are most similar to "Christos Faloutsos"?

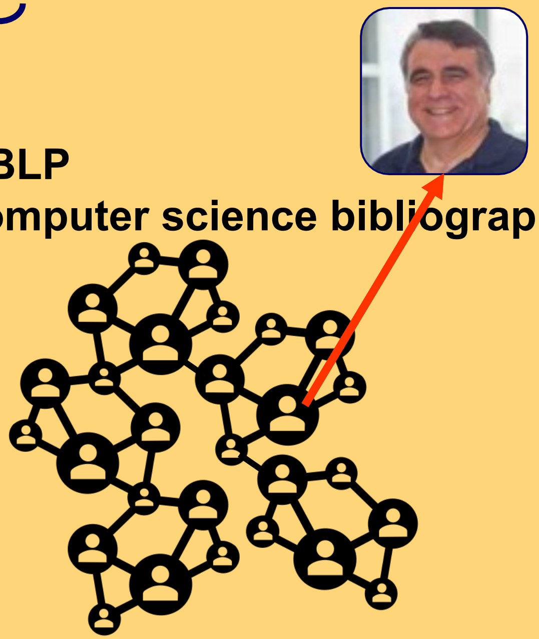
DBLP
computer science bibliography



Question:

Q: In DBLP who are most similar to “Christos Faloutsos”?

How to define?

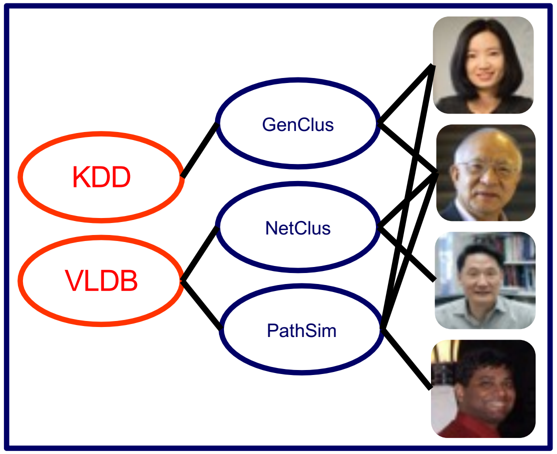


DBLP
computer science bibliography

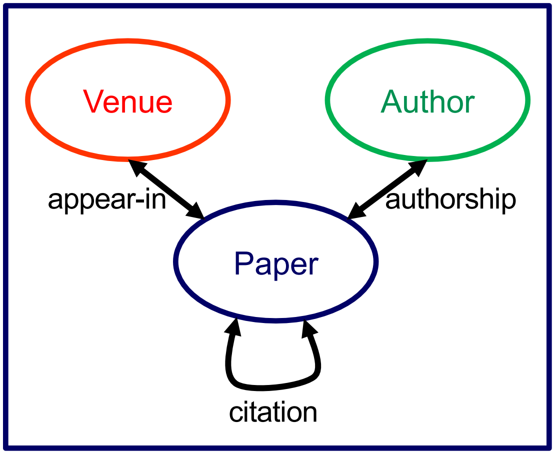
A: PathSim and Meta-path is one way!

Heterogeneous Information Networks (HIN)

HIN Instance

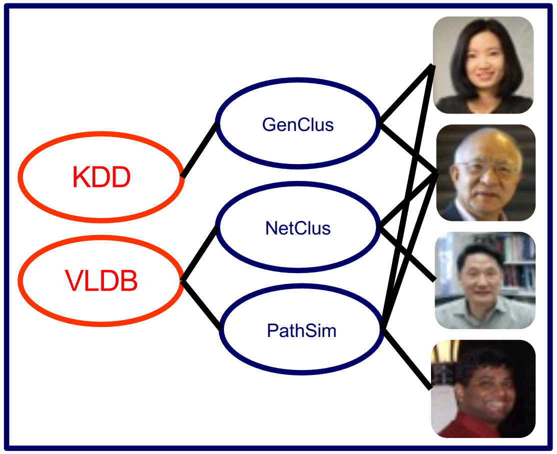


Network Schema
(Meta-level description of HIN)

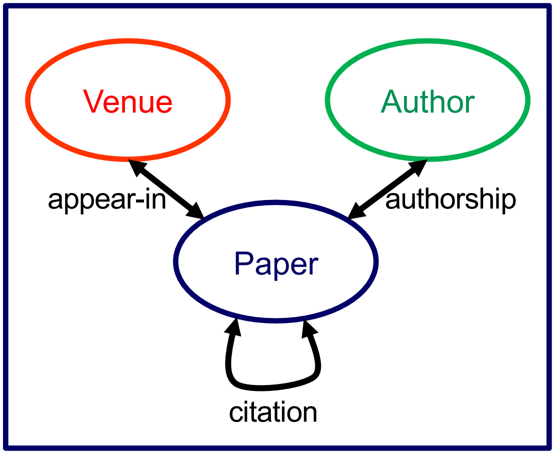


Heterogeneous Information Networks (HIN)

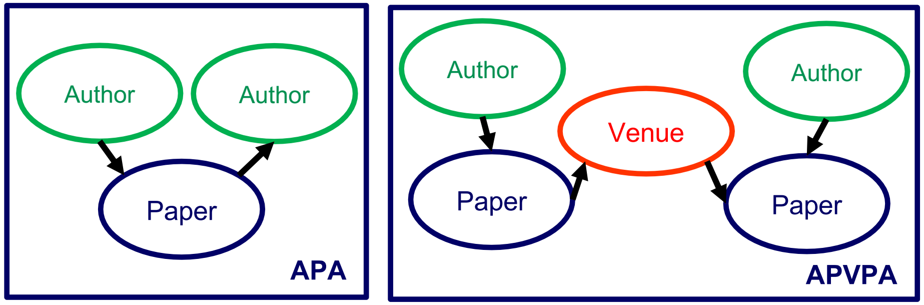
HIN Instance



Network Schema
(Meta-level description of HIN)

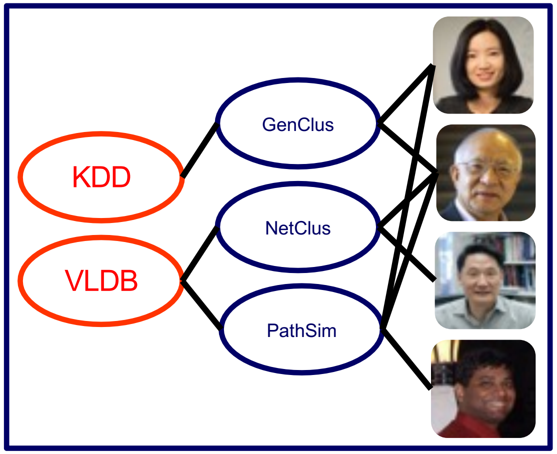


MetaPath (Meta-level description of paths)

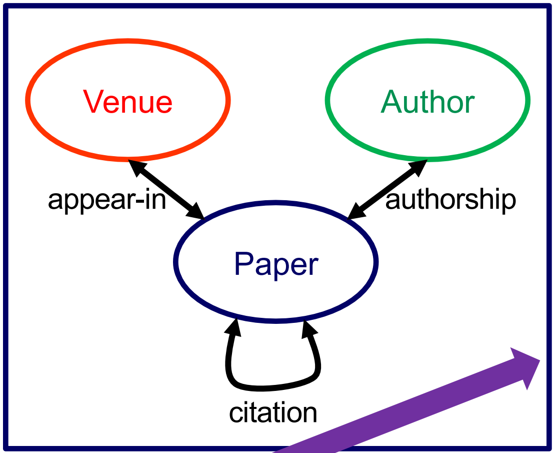


Heterogeneous Information Networks (HIN)

HIN Instance



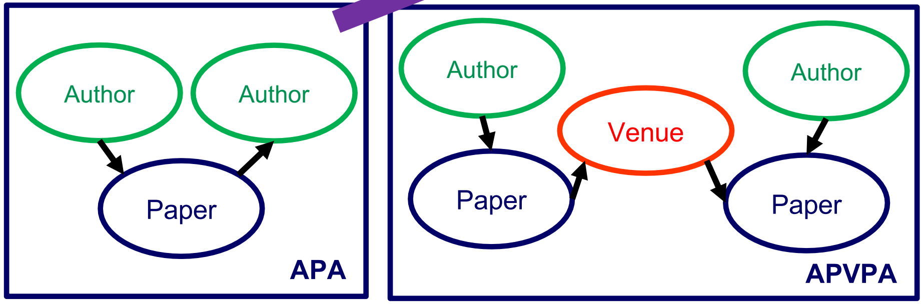
Network Schema
(Meta-level description of HIN)



Path Instance

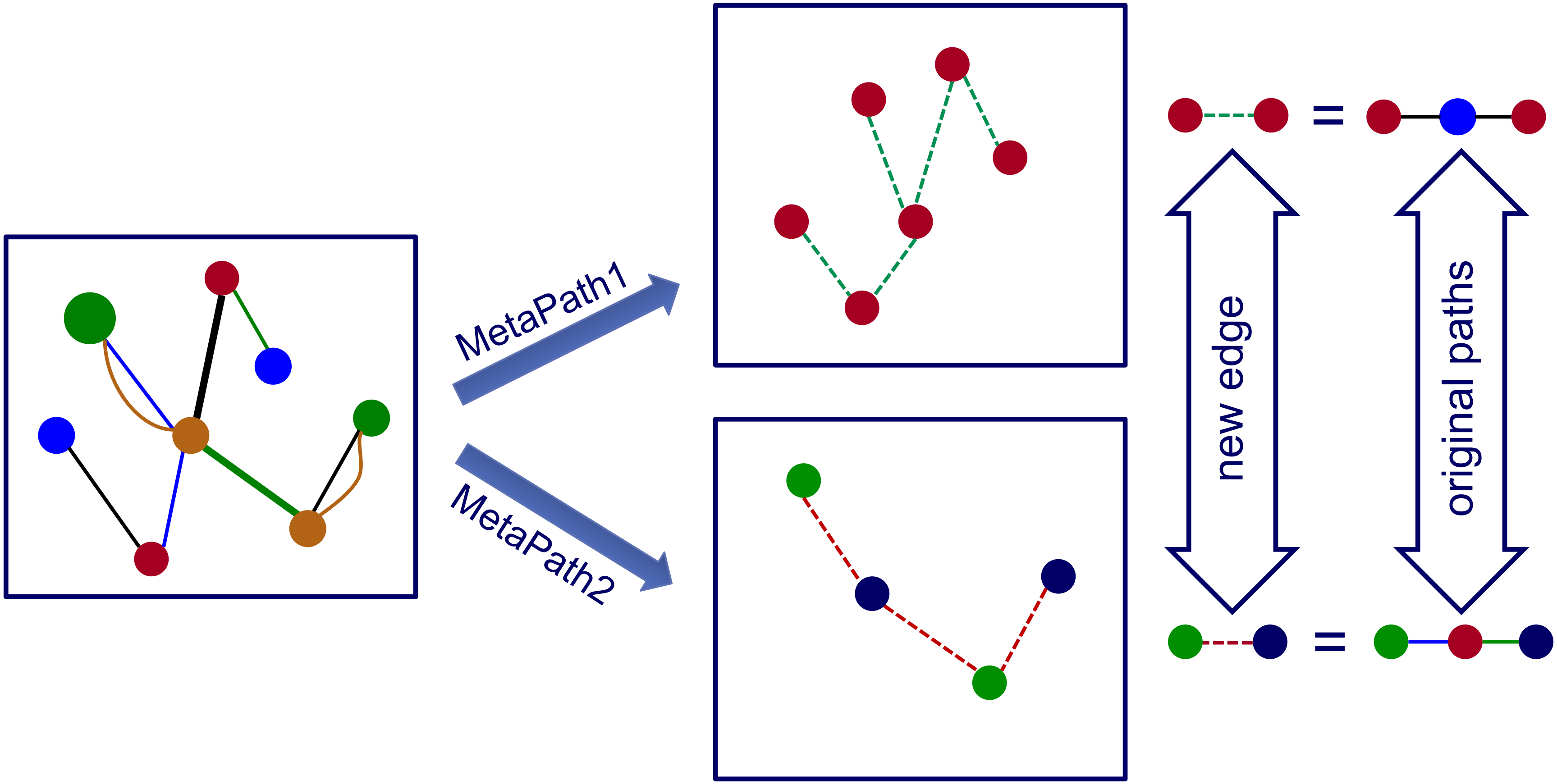
APA
Meaning:
Co-authors
Instances:
Sun-NetClus-Han Sun-PathSim-Yu

MetaPath (Meta-level description of paths)



APVPA
Meaning:
Similar interest colleagues
Instances:
Sun-PathSim-VLDB-PathSim-Han Sun-PathSim-VLDB-GenClus-Aggarwal

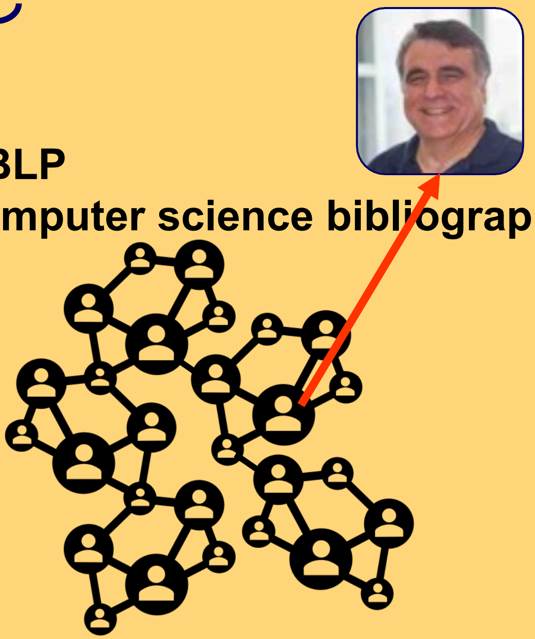
Implicit Meta-path Intuition



Question:

Q: In DBLP who are most similar to "Christos Faloutsos"?

How to define?



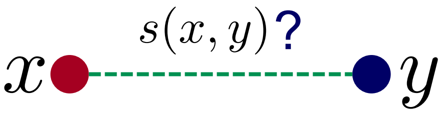
DBLP
computer science bibliography

A: PathSim and Meta-path
is one way!

Details

PathSim

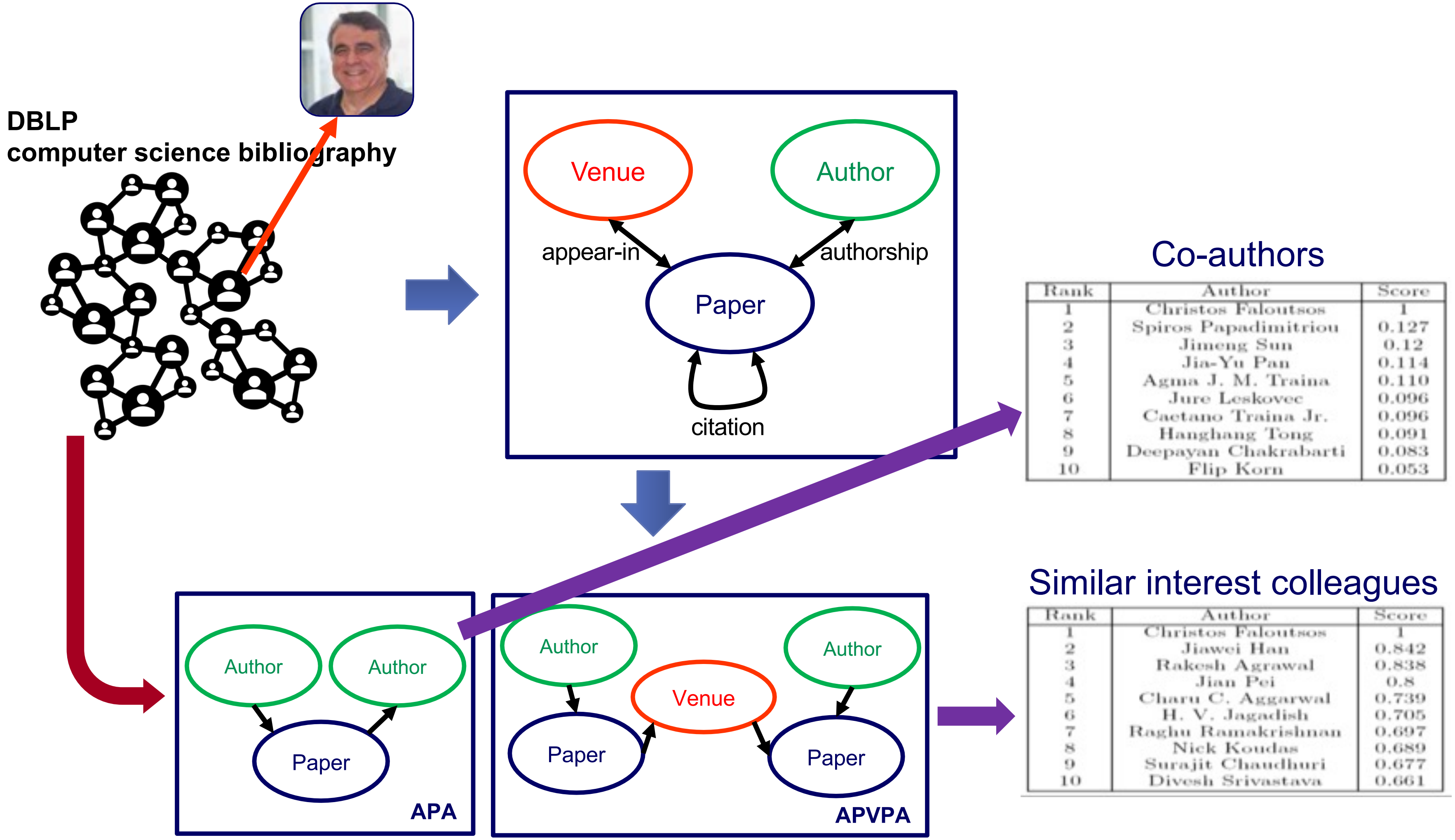
PathSim: Normalized path count between two nodes x, y following a meta-path P:



Number of paths between nodes following $\mathcal{P}$

$$s(x,y) = \frac{2 \times |\{p_{x \rightsquigarrow y} : p_{x \rightsquigarrow y} \in \mathcal{P}\}|}{|\{p_{x \rightsquigarrow x} : p_{x \rightsquigarrow x} \in \mathcal{P}\}| + |\{p_{y \rightsquigarrow y} : p_{y \rightsquigarrow y} \in \mathcal{P}\}|}$$

Different Meta-paths Give Different Semantics



Co-authors

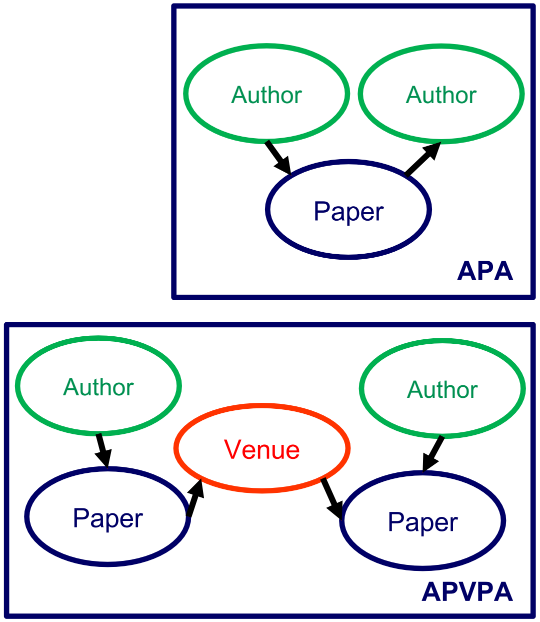
Rank	Author	Score
1	Christos Faloutsos	1
2	Spiros Papadimitriou	0.127
3	Jimeng Sun	0.12
4	Jia-Yu Pan	0.114
5	Agma J. M. Traina	0.110
6	Jure Leskovec	0.096
7	Caetano Traina Jr.	0.096
8	Hanghang Tong	0.091
9	Deepayan Chakrabarti	0.083
10	Flip Korn	0.053

Similar interest colleagues

Rank	Author	Score
1	Christos Faloutsos	1
2	Jiawei Han	0.842
3	Rakesh Agrawal	0.838
4	Jian Pei	0.8
5	Charu C. Aggarwal	0.739
6	H. V. Jagadish	0.705
7	Raghu Ramakrishnan	0.697
8	Nick Koudas	0.689
9	Surajit Chaudhuri	0.677
10	Divesh Srivastava	0.661

[VLDB] “Pathsim: Meta path-based top-k similarity search in heterogeneous information networks”, Sun, Y., Han, J., Yan, X., Yu, P. S., & Wu, T.

Meta-Path



- Similarity and Search: PathSim
- Link Prediction: PathPredict
- Clustering: PathSelClus

[Book] "Mining heterogeneous information networks: principles and methodologies"
Sun, Yizhou, and Jiawei Han

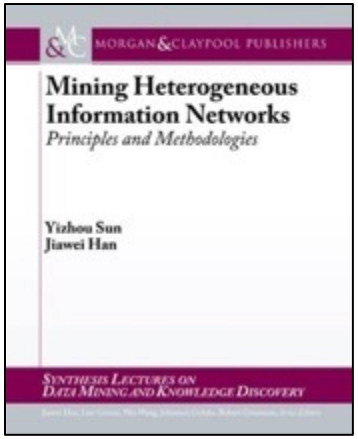
Software Tools

- Hetnetpy: https://het.io/software/#hetnetpy

References

- Shi, C., Li, Y., Zhang, J., Sun, Y., & Philip, S. Y. *A survey of heterogeneous information network analysis*
  IEEE Transactions on Knowledge and Data Engineering, 2016

- Sun, Yizhou, and Jiawei Han., *Mining heterogeneous information networks: principles and methodologies*
  Synthesis Lectures on Data Mining and Knowledge Discovery, 2012



MORGAN & CLAYPOOL PUBLISHERS

Mining Heterogeneous Information Networks

Principles and Methodologies

Yizhou Sun
Jiawei Han

SYNTHESIS LECTURES ON DATA MINING AND KNOWLEDGE DISCOVERY

Bird’s eye view

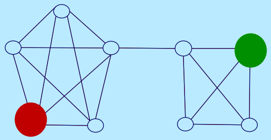
Tool Task	1.1 PR/HITS	1.1 PPR	1.2 METIS/ SVD	1.3 OddBall+	1.4 BP	2.1 FM	2.1 Tensor	2.2 HIN	2.3 SRL
1.1 Node Ranking	👍					(👍)		(👍)	
1.1’ Link Prediction		👍				👍	👍	👍	
1.2 Comm. Detection			👍				👍	(👍)	
1.3 Anomaly Detection				👍			👍		
1.4 Propagation					👍			(👍)	

Part 1:
Plain Graphs

Part 2:
Complex Graphs

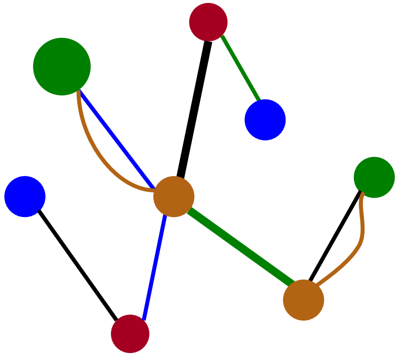
Bird’s eye view

- Part 2: Complex and Heterogeneous Graphs
  - P 2.1: Factorization Methods
  - P 2.2: Heterogeneous Information Networks
  - P 3.3: Statistical Relational Learning
    - P3.3.1: Node Labeling / Collective Classification
    - P3.3.2: Link Prediction / Recommender Systems
    - P3.3.3: Entity Resolution / Knowledge Graph Identification



Statistical Relational Learning

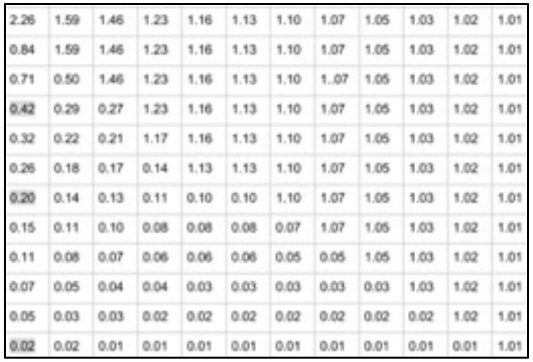
Real Data



Dependencies
& Structure

Flattening

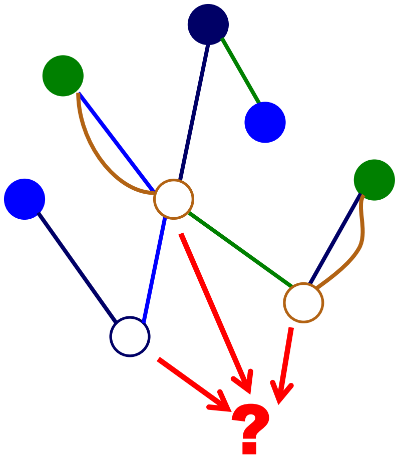
Transformed Data



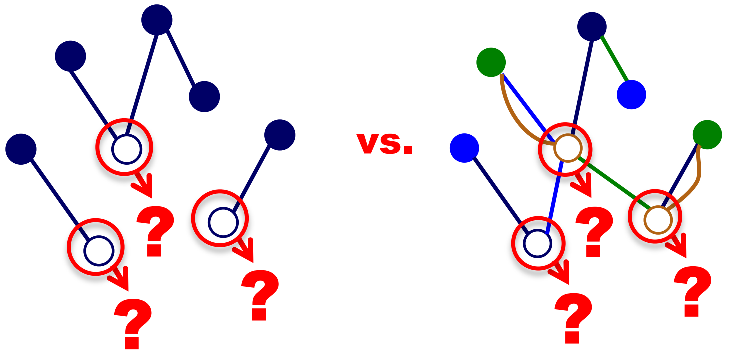
2.26	1.59	1.46	1.23	1.16	1.13	1.10	1.07	1.05	1.03	1.02	1.01
0.84	1.59	1.46	1.23	1.16	1.13	1.10	1.07	1.05	1.03	1.02	1.01
0.71	0.50	1.46	1.23	1.16	1.13	1.10	1..07	1.05	1.03	1.02	1.01
0.42	0.29	0.27	1.23	1.16	1.13	1.10	1.07	1.05	1.03	1.02	1.01
0.32	0.22	0.21	1.17	1.16	1.13	1.10	1.07	1.05	1.03	1.02	1.01
0.26	0.18	0.17	0.14	1.13	1.13	1.10	1.07	1.05	1.03	1.02	1.01
0.20	0.14	0.13	0.11	0.10	0.10	1.10	1.07	1.05	1.03	1.02	1.01
0.15	0.11	0.10	0.08	0.08	0.08	0.07	1.07	1.05	1.03	1.02	1.01
0.11	0.08	0.07	0.06	0.06	0.06	0.05	0.05	1.05	1.03	1.02	1.01
0.07	0.05	0.04	0.04	0.03	0.03	0.03	0.03	0.03	1.03	1.02	1.01
0.05	0.03	0.03	0.02	0.02	0.02	0.02	0.02	0.02	0.02	1.02	1.01
0.02	0.02	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	1.01

[Suitable for Most ML Algorithms]

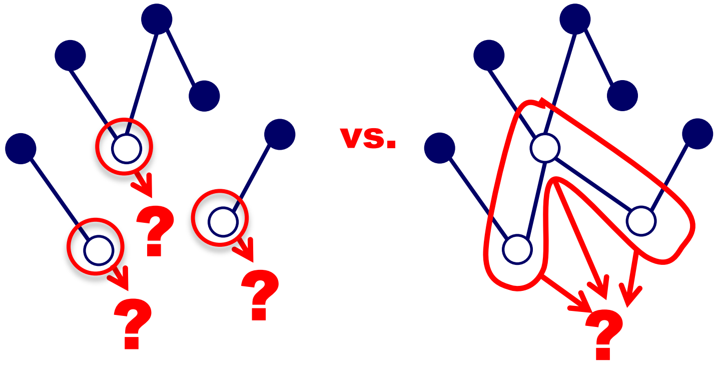
Complex Networks



1. Capture multi-relational nature

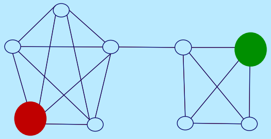


Joint Inference



Bird’s eye view

- Part 2: Complex and Heterogeneous Graphs
  - P 2.1: Factorization Methods
  - P 2.2: Heterogeneous Information Networks
  - P 3.3: Statistical Relational Learning
    - P3.3.1: Node Labeling / Collective Classification
    - P3.3.2: Link Prediction / Recommender Systems
    - P3.3.3: Entity Resolution / Knowledge Graph Identification

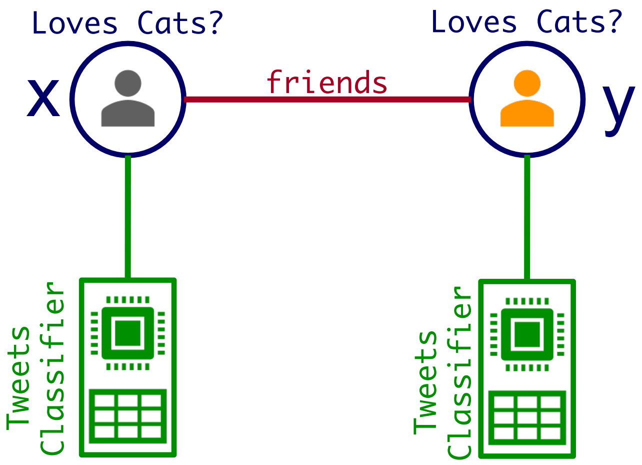


Question:

Q: How can we propagate labels in networks with extra information?

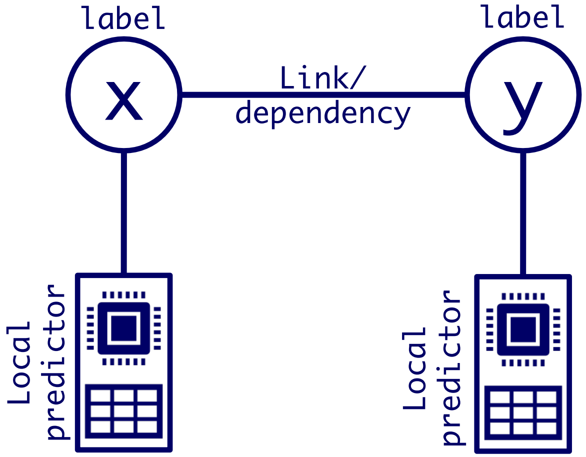
A: Statistical Relational Learning is one way.

SRL: Node Labeling [Collective Classification]

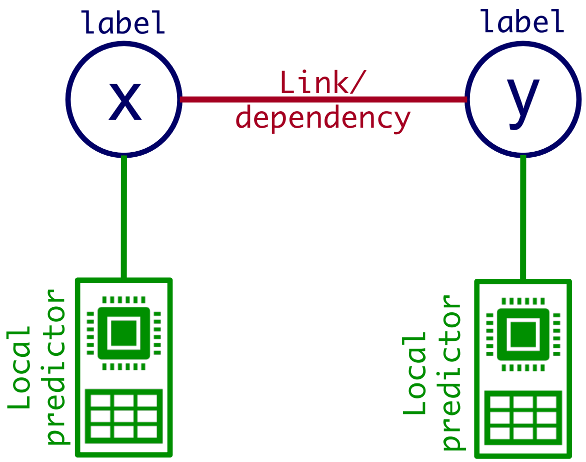


How can we use the friendship relation to improve the predictions?

SRL: Node Labeling [Collective Classification]



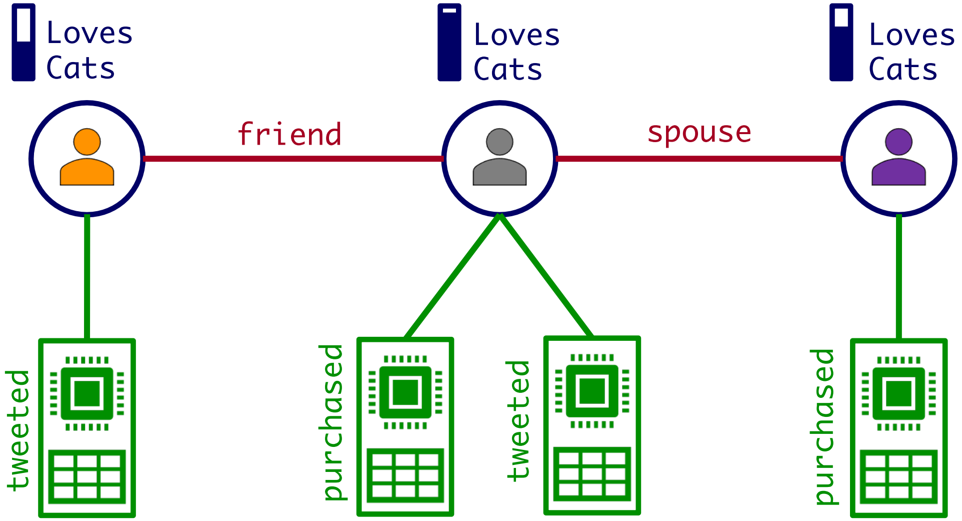
SRL: Node Labeling [Collective Classification]



SRL Answer:

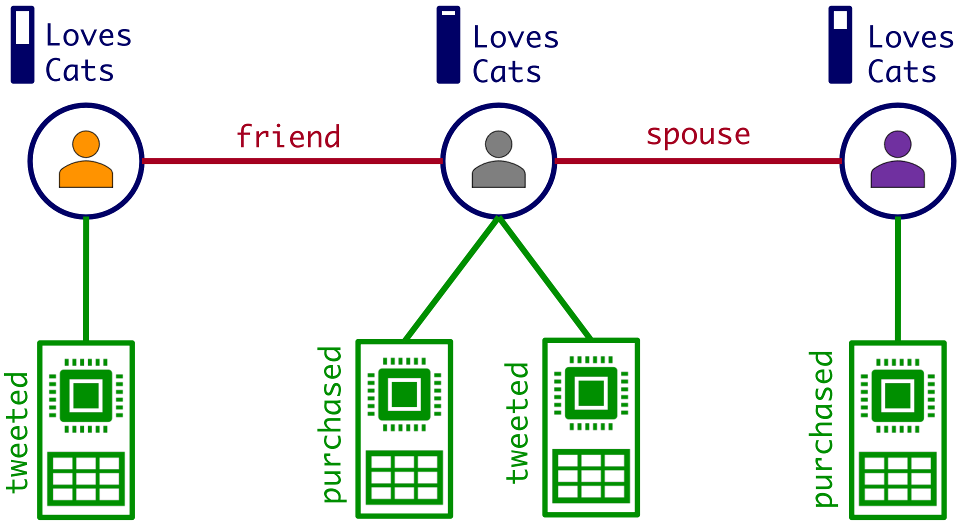
```
    local-predictor(x,l) -> label(x,l)
  label(x,l) & link(x,y) -> label(y,l)
```

SRL: Node Labeling [Collective Classification]



```
purchased(x, ”cat_food") -> loves(x, ”Cats")
tweeted(x, "#catslover") -> loves(x, ”Cats")

loves(x, ”Cats") & spouse(x,y) -> loves(y, ”Cats")
loves(x, ”Cats") & friend(x,y) -> loves(y, ”Cats")
```

SRL: Node Labeling [Collective Classification]

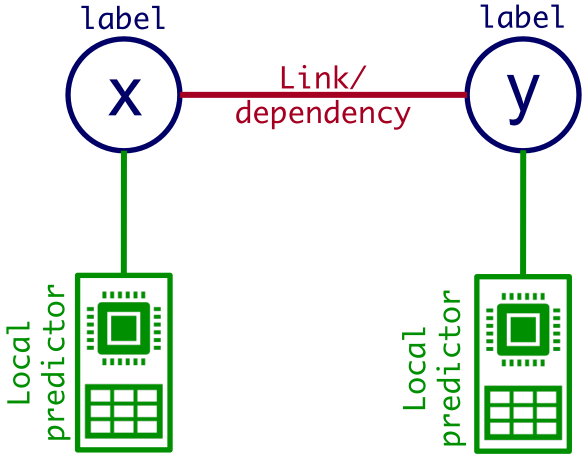


Weights:
- Given by user or
- Learned from data

Soft-values

```
0.9:  purchased(x, ”cat_food") -> loves(x, ”Cats")
0.8:  tweeted(x, "#catslover") -> loves(x, ”Cats")

0.85: loves(x, ”Cats") & spouse(x,y) -> loves(y, ”Cats")
0.7:  loves(x, ”Cats") & friend(x,y) -> loves(y, ”Cats")
```

SRL: Node Labeling [Collective Classification]

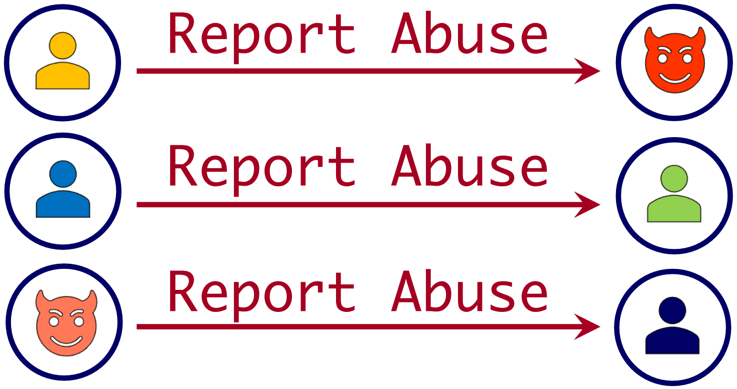


SRL Answer:

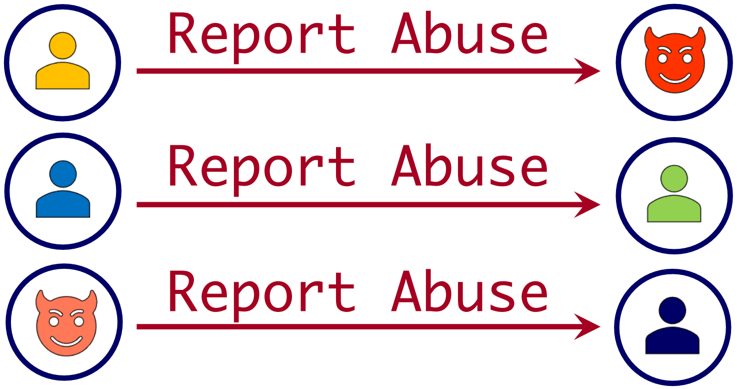
```
    local-predictor(x,l) -> label(x,l)
  label(x,l) & link(x,y) -> label(y,l)
```

Social Spammer Detection

Social Spammer Detection

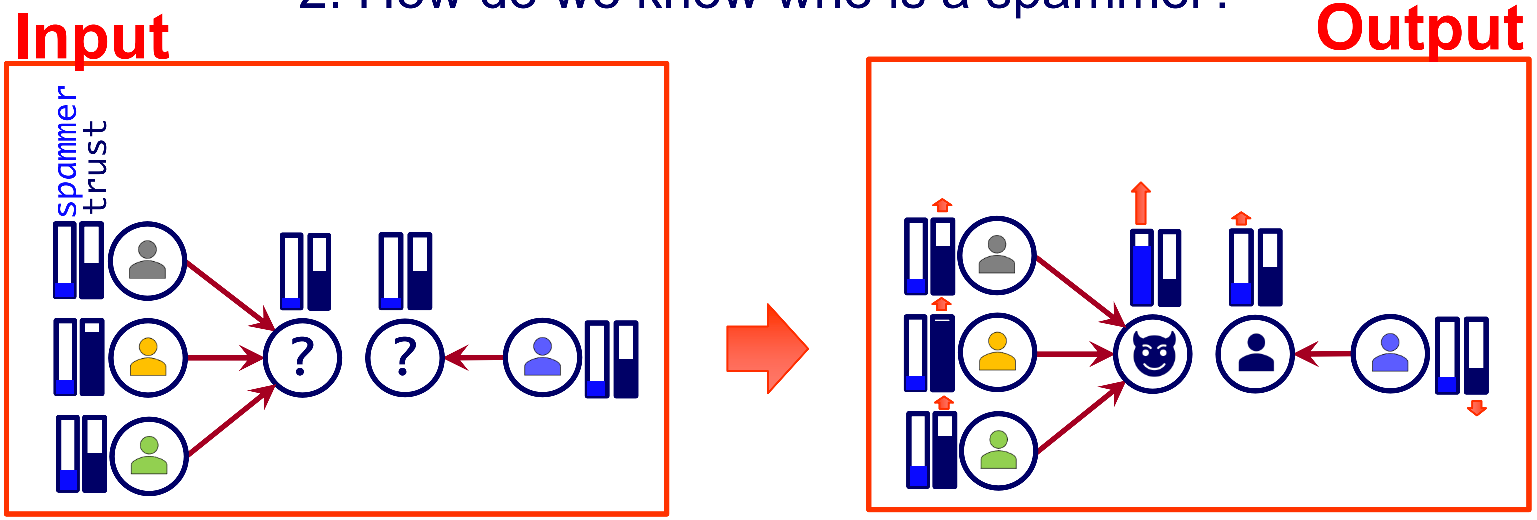


Social Spammer Detection



Task:

1. How do we know who is telling the truth?
2. How do we know who is a spammer?

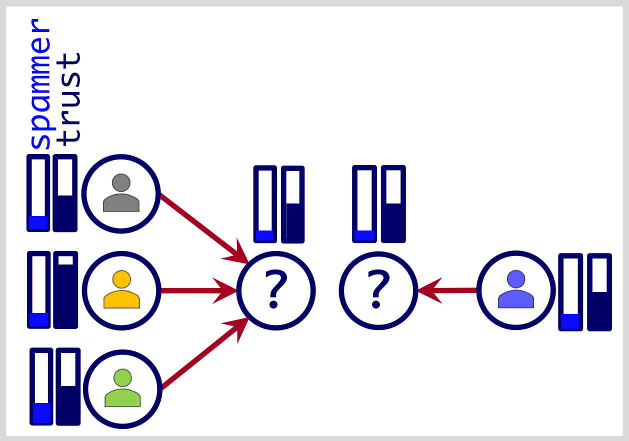


SRL Answer

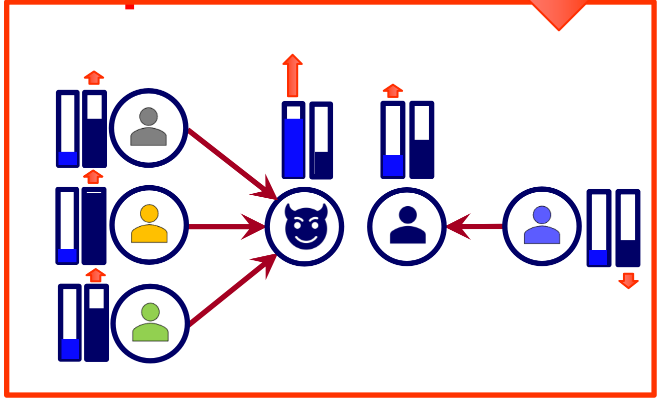
Input

```
              prior-trust(x) ->  trusted(x)

 trusted(x) & reported(x,y) ->  spammer(y)

 spammer(y) & reported(x,y) ->  trusted(x)
~spammer(y) & reported(x,y) -> ~trusted(x)

                                ~spammer(x)
```

+



Output



Statistical Relational Learning Frameworks

Alchemy (MLN)		https://alchemy.cs.washington.edu/
Probabilistic Soft Logic		https://psl.linqs.org/
Felix (Tuffy)		http://i.stanford.edu/hazy/felix/

How using PSL looks like:

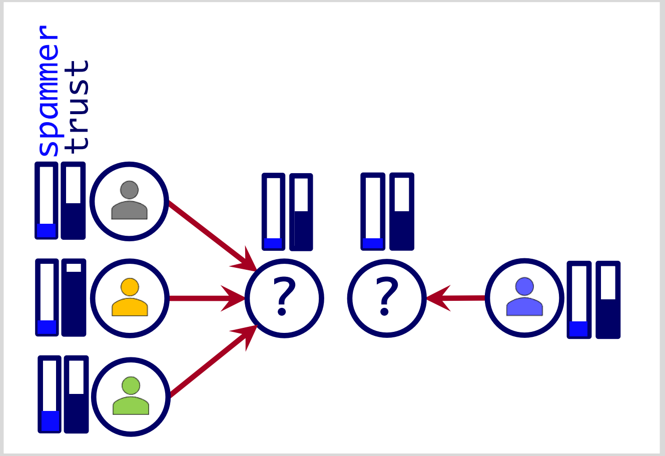
Input

Templates

```
               prior-trust(x) ->  trusted(x)

trusted(x) & reported(x,y) ->  spammer(y)

spammer(y) & reported(x,y) ->  trusted(x)
~spammer(y) & reported(x,y) -> ~trusted(x)

                              ~spammer(x)
```

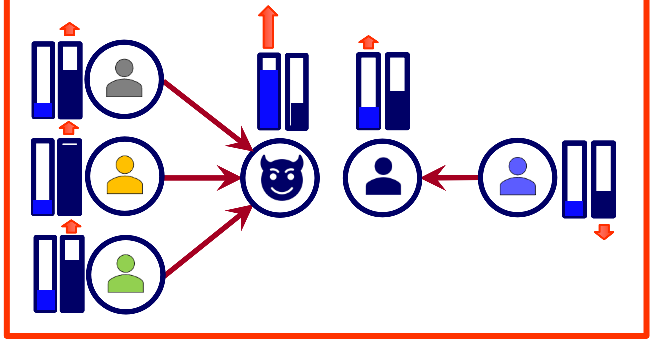
+

Data



PSL

Output



amazon

How using PSL looks like:

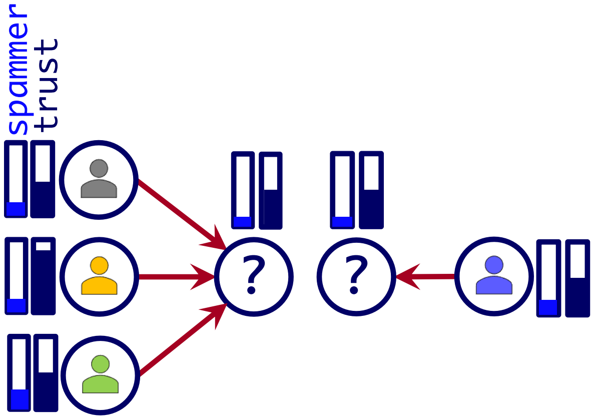
Input

Templates

```
             prior-trust(x) ->  trusted(x)

 trusted(x) & reported(x,y) ->  spammer(y)

 spammer(y) & reported(x,y) ->  trusted(x)
~spammer(y) & reported(x,y) -> ~trusted(x)

                               ~spammer(x)
```

+

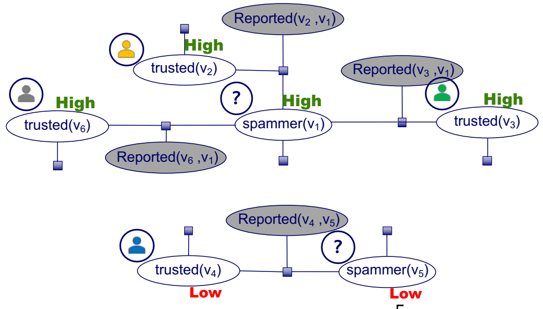
Data



PSL

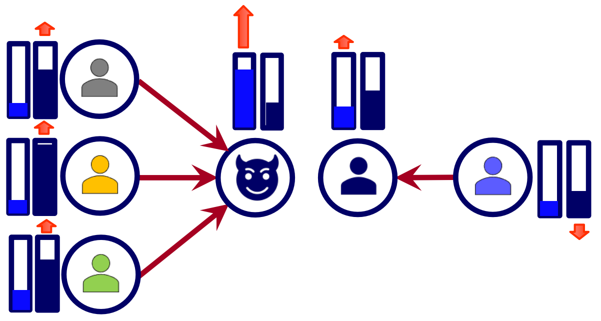
Grounding & Inference

(under the hood)



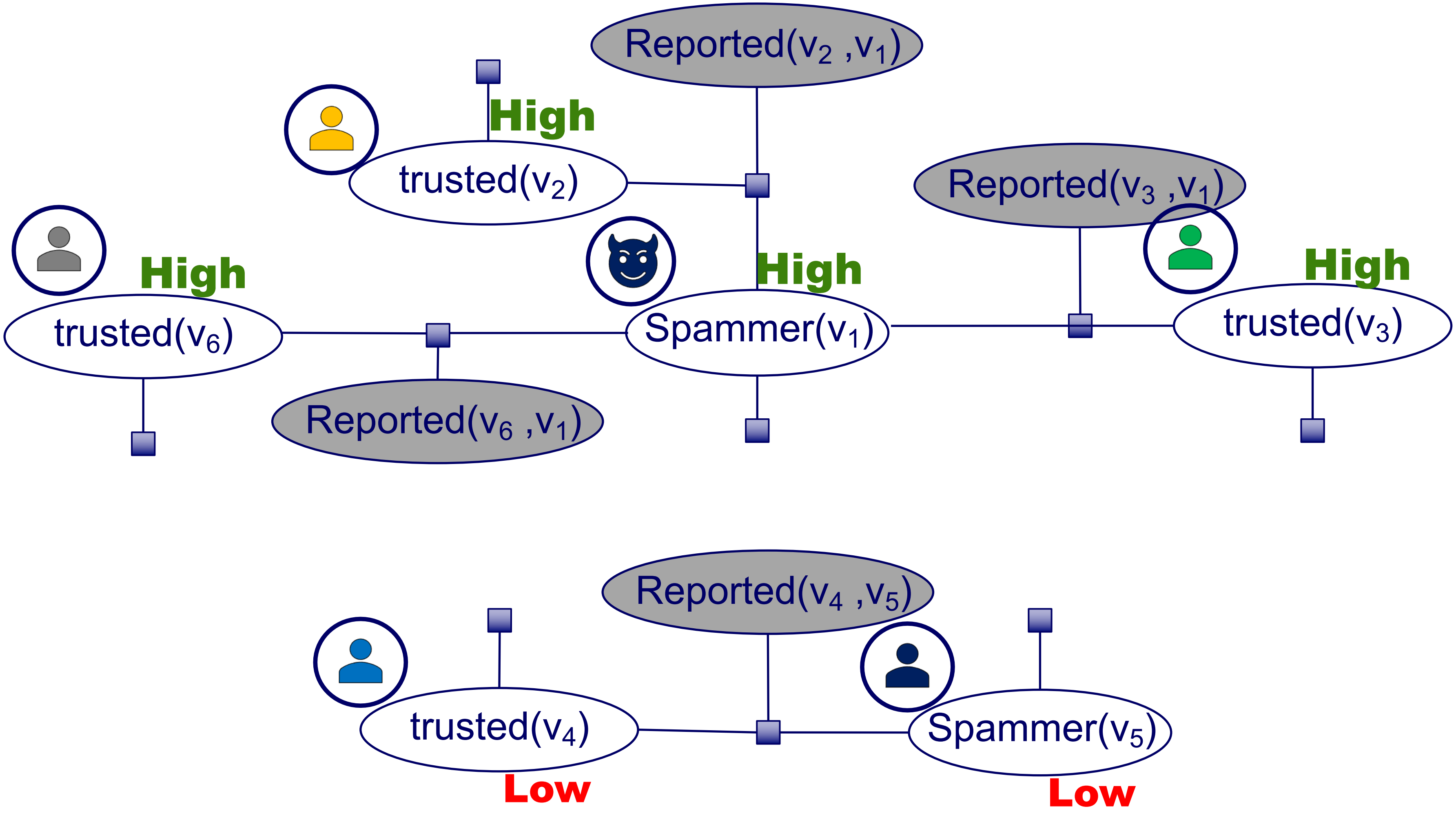
$$P\left(\mathbf{Y}|\mathbf{X}\right) = \frac{1}{Z(\lambda)} \exp\left[-\sum_{j=1}^{m} \lambda_j \phi_j(\mathbf{Y}, \mathbf{X})\right]$$

Output



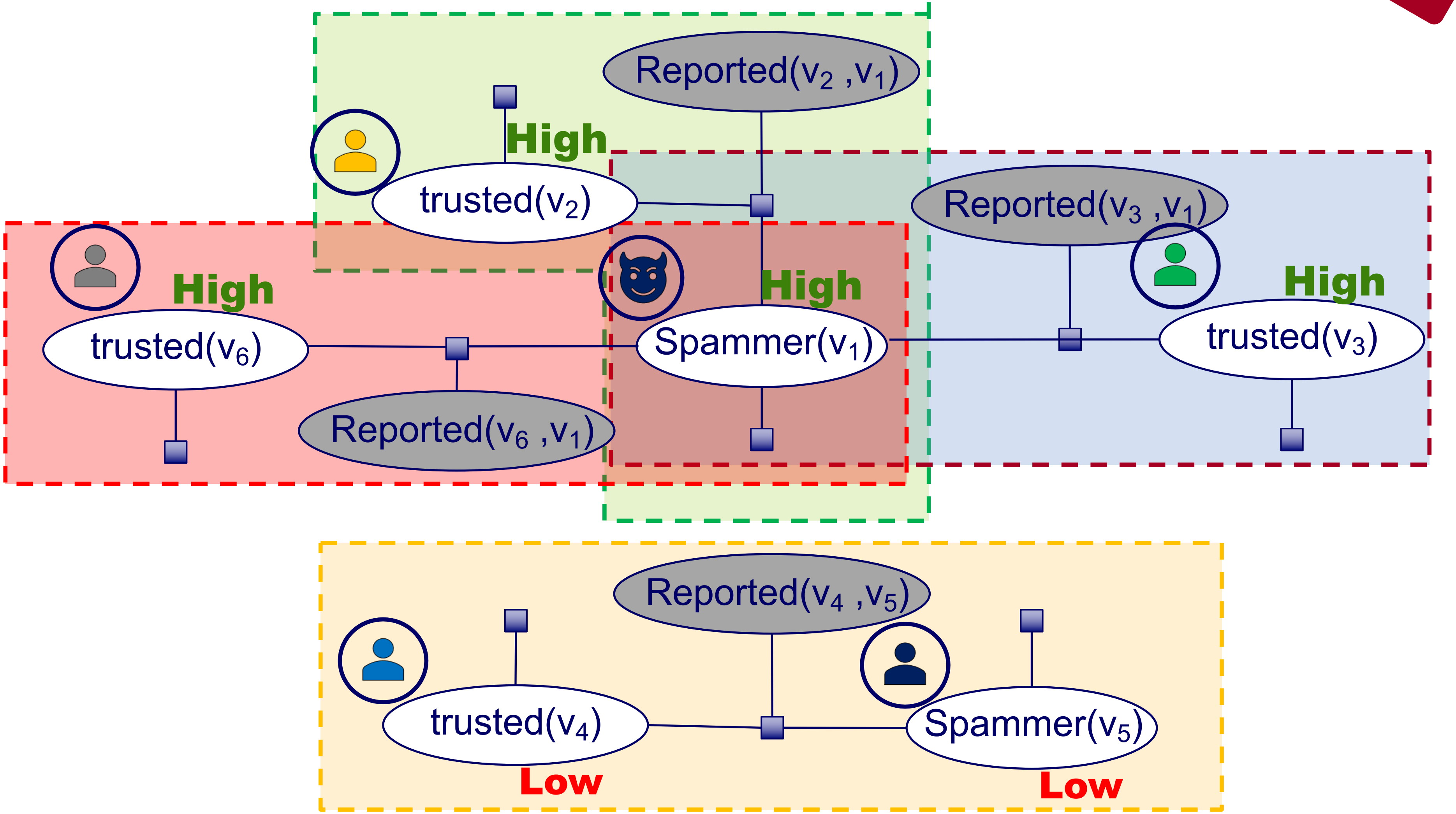
Desired PGM Model

Under the hood!



Under the hood!

Templates



Under the hood!

Probabilistic Soft Logic (PSL): A templating language with first-order logic syntax

Example PSL rule:

$$\texttt{w: }\overbrace{\texttt{trusted(x) \& reported(x,y)}}^{r_{body}}\texttt{ -> }\overbrace{\texttt{spammer(y)}}^{r_{head}}$$

Under the hood!

Probabilistic Soft Logic (PSL):
A templating language with first-order logic syntax

Example PSL rule:

$$\texttt{w: } \overbrace{\underbrace{\texttt{trusted(x)}}_{0 \le \text{Soft truth} \le 1} \;\texttt{\&}\; \texttt{reported(x,y)}}^{r_{\text{body}}} \;\texttt{->}\; \overbrace{\texttt{spammer(y)}}^{r_{\text{head}}}$$

$$\begin{cases} p \;\tilde{\wedge}\; q = \max(0,\; p+q-1) \\ p \;\tilde{\vee}\; q = \min(1,\; p+q) \\ \quad \neg p = 1-p \end{cases}$$

Under the hood!

Probabilistic Soft Logic (PSL): A templating language with first-order logic syntax

Example PSL rule:

$$\texttt{w: } \overbrace{\underbrace{\texttt{trusted(x)}}_{0 \le \text{Soft truth} \le 1} \ \texttt{\&} \ \texttt{reported(x,y)}}^{r_{body}} \ \texttt{->} \ \overbrace{\texttt{spammer(y)}}^{r_{head}}$$

$$\begin{cases} p \mathbin{\tilde{\wedge}} q = \max(0,\ p + q - 1) \\ p \mathbin{\tilde{\vee}} q = \min(1,\ p + q) \\ \neg p = 1 - p \end{cases}$$

Ground

```
w: trusted(“alice”) & reported(“alice”,”bob”) -> spammer(“bob”)
          0.7                 1                          ?
```

Under the hood!

Probabilistic Soft Logic (PSL):
A templating language with first-order logic syntax

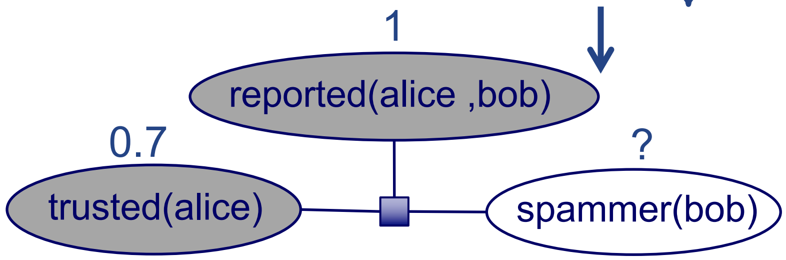
Example PSL rule:

$$\texttt{w: } \overbrace{\underbrace{\texttt{trusted(x)}}_{0 \le \text{Soft truth} \le 1} \ \texttt{\&}\ \texttt{reported(x,y)}}^{r_{\text{body}}} \ \texttt{->}\ \overbrace{\texttt{spammer(y)}}^{r_{\text{head}}}$$

$$\begin{cases} p \mathbin{\tilde{\wedge}} q = \max(0,\ p+q-1) \\ p \mathbin{\tilde{\vee}} q = \min(1,\ p+q) \\ \neg p = 1-p \end{cases}$$

Ground

$$\underbrace{\texttt{w: } \underset{0.7}{\texttt{trusted("alice")}} \ \texttt{\&}\ \underset{1}{\texttt{reported("alice","bob")}} \ \texttt{->}\ \underset{?}{\texttt{spammer("bob")}}}$$



Probabilistic Soft Logic (PSL): A templating language with first-order logic syntax

Under the hood!

Example PSL rule:

r_{body} r_{head}

```
w: trusted(x) & reported(x,y) -> spammer(y)
```

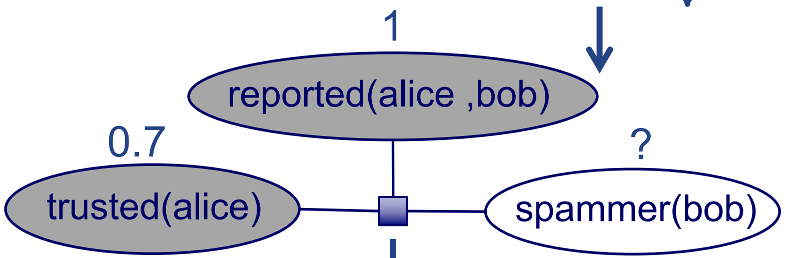
0 ≤ Soft truth ≤ 1

$$\begin{cases} p \,\tilde{\wedge}\, q = \max(0,\ p + q - 1) \\ p \,\tilde{\vee}\, q = \min(1,\ p + q) \\ \neg p = 1 - p \end{cases}$$

Ground

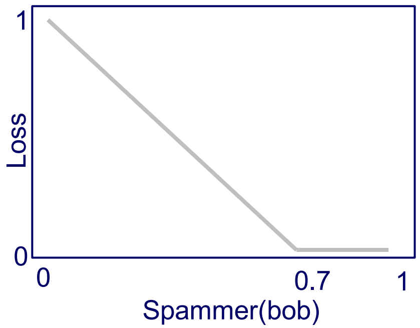
```
w: trusted(“alice”) & reported(“alice”,”bob”) -> spammer(“bob”)
```

0.7 1 ?



distance to satisfaction

$$\ell = \max\left\{\text{value}(r_{\text{body}}) - \text{value}(r_{\text{head}}), 0\right\}$$



Probabilistic Soft Logic (PSL): A templating language with first-order logic syntax

Under the hood!

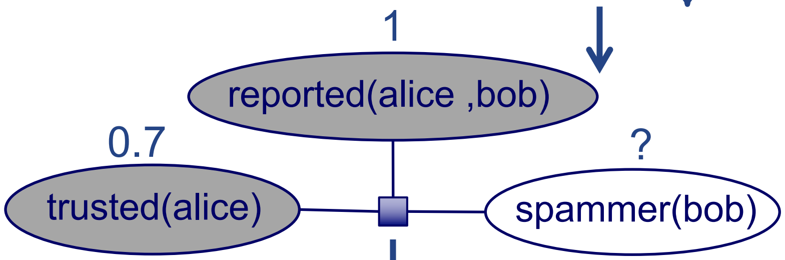
Example PSL rule:

$$\texttt{w: }\overbrace{\underbrace{\texttt{trusted(x)}}_{0 \le \text{Soft truth} \le 1}\texttt{ \& reported(x,y)}}^{r_{\text{body}}}\texttt{ -> }\overbrace{\texttt{spammer(y)}}^{r_{\text{head}}}$$

$$\begin{cases} p \ \tilde{\wedge}\ q = \max(0,\ p+q-1) \\ p \ \tilde{\vee}\ q = \min(1,\ p+q) \\ \neg p = 1-p \end{cases}$$

Ground

$$\underbrace{\texttt{w: }\overset{0.7}{\texttt{trusted(“alice”)}}\texttt{ \& }\overset{1}{\texttt{reported(“alice”,”bob”)}}\texttt{ -> }\overset{?}{\texttt{spammer(“bob”)}}}$$



distance to satisfaction

$$\ell = \max\left\{\text{value}(r_{\text{body}}) - \text{value}(r_{\text{head}}), 0\right\} \longrightarrow \overbrace{\phi_j(\mathbf{Y},\mathbf{X})} = \left[\ell_j(\mathbf{Y},\mathbf{X})\right]$$

$$P(\mathbf{Y}|\mathbf{X}) = \frac{1}{Z(\lambda)} \exp\left[-\sum_{j=1}^{m} \lambda_j \underbrace{\phi_j(\mathbf{Y},\mathbf{X})}\right]$$

Unknown variables

Evidence

How using PSL looks like:

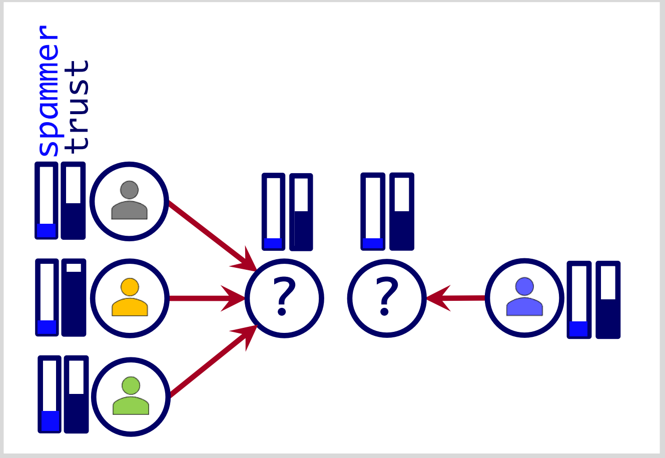
Input

Templates

```
             prior-trust(x) ->  trusted(x)

trusted(x) & reported(x,y) ->  spammer(y)

spammer(y) & reported(x,y) ->  trusted(x)
~spammer(y) & reported(x,y) -> ~trusted(x)

                              ~spammer(x)
```

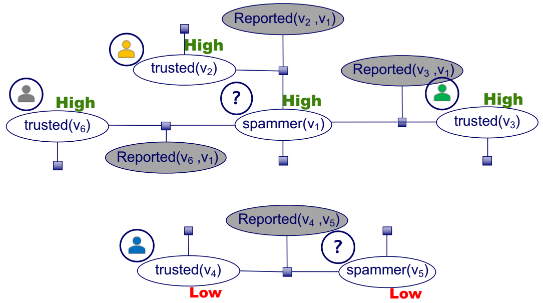
+

Data



PSL

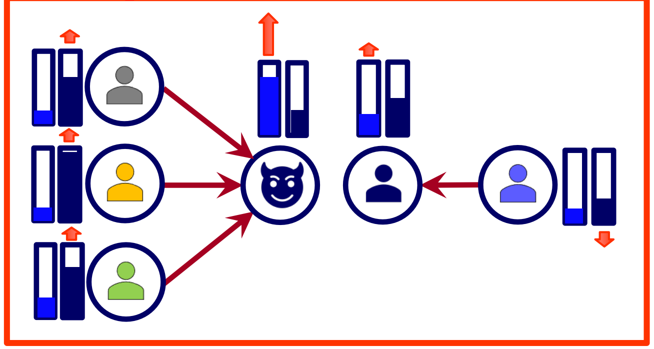
Grounding & Inference



$$P(\mathbf{Y}|\mathbf{X}) = \frac{1}{Z(\lambda)} \exp\left[-\sum_{j=1}^{m} \lambda_j \phi_j(\mathbf{Y},\mathbf{X})\right]$$

(under the hood)

Output



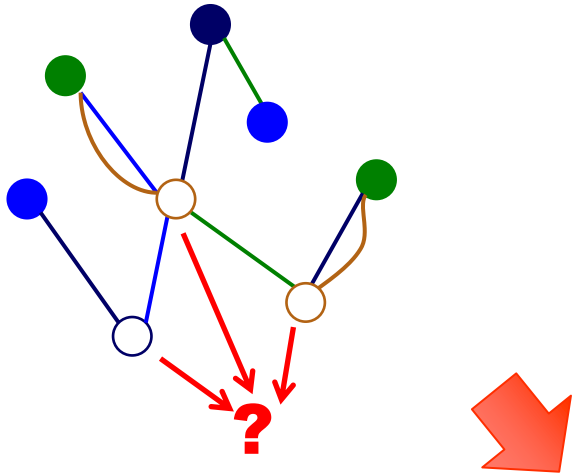
Social Spammer Detection

- Collective model:

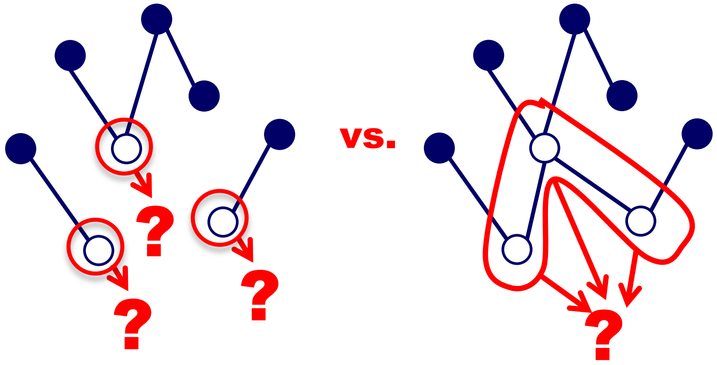
```
             prior-trust(x) ->  trusted(x)

 trusted(x) & reported(x,y) ->  spammer(y)

 spammer(y) & reported(x,y) ->  trusted(x)
~spammer(y) & reported(x,y) -> ~trusted(x)

                               ~spammer(x)
```

Experiments	**AU-PR**	**AU-ROC**
Collective Classification	**0.790 ± 0.005**	**0.788 ± 0.003**

Node Classification



Joint Inference



Report Model

- Collective model:

```
             prior-trust(x) ->  trusted(x)

 trusted(x) & reported(x,y) ->  spammer(y)

 spammer(y) & reported(x,y) ->  trusted(x)
~spammer(y) & reported(x,y) -> ~trusted(x)

                               ~spammer(x)
```

- Non-collective model (≃ weighted sum of the reports):

```
prior-trust(x) & reported(x,y) ->  spammer(y)

                                  ~spammer(x)
```

Classification Using Reports

Experiments	AU-PR	AU-ROC
Non-collective model	0.690 ± 0.003	0.624 ± 0.001
Collective model	**0.790 ± 0.005**	**0.788 ± 0.003**

[KDD] "Collective Spammer Detection in Evolving Multi-Relational Social Networks", Fakhraei, S., Foulds, J., Shashanka, M., & Getoor, L.

Bird’s eye view

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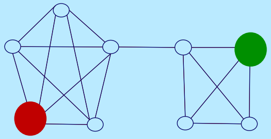
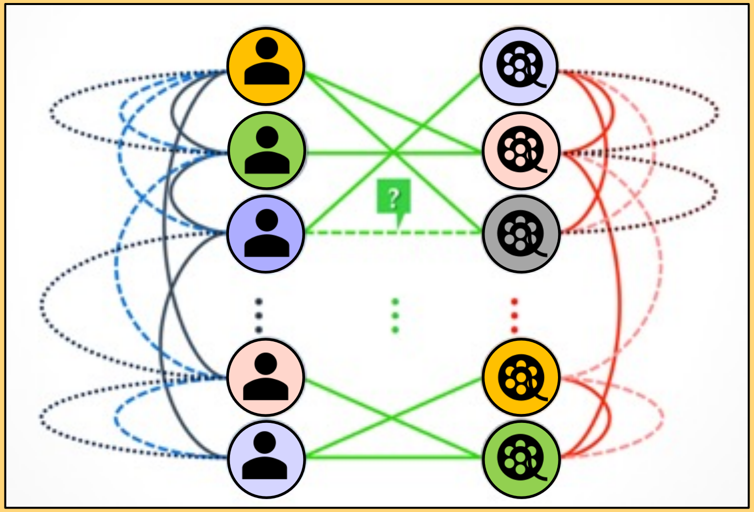
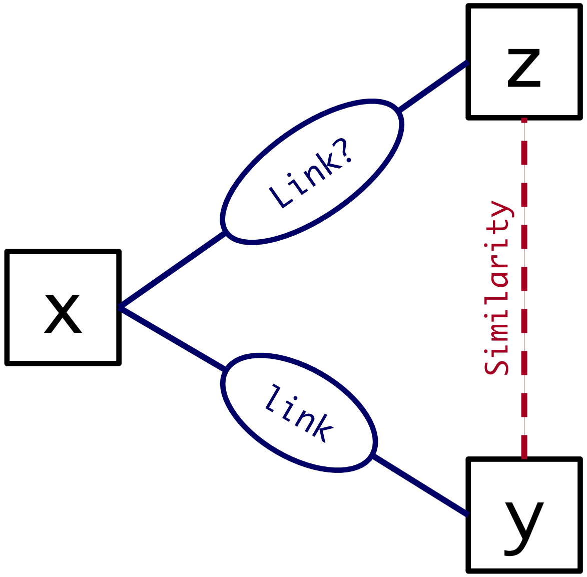


Question:

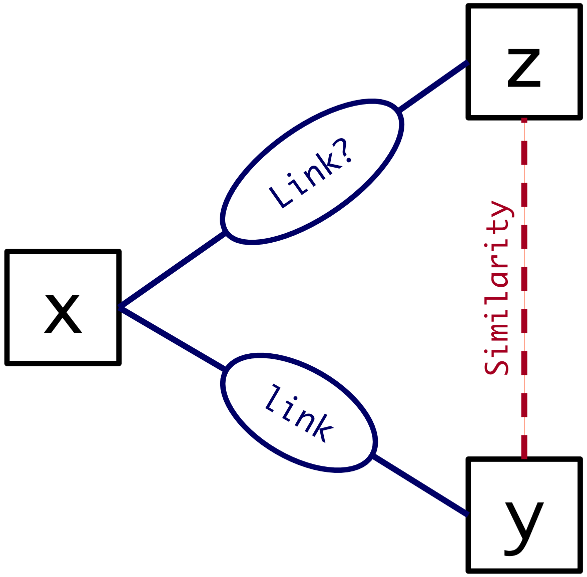


1. How can we use multiple similarities between nodes to infer link values?
2. How can we propagate link information?
3. How can we add additional model signals?

Link Inference Pattern

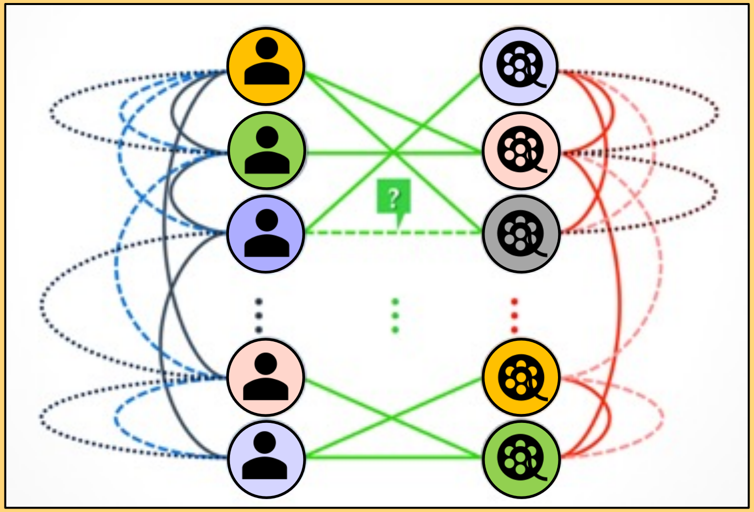


Link Inference Template



```
w: link(x,y) & similar(y,z) -> link(x,z)
```

Question:



? 1. How can we use multiple similarities between nodes to infer link values?

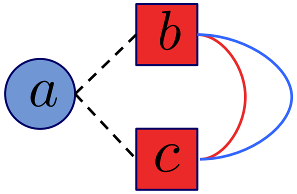
? 2. How can we propagate link information?

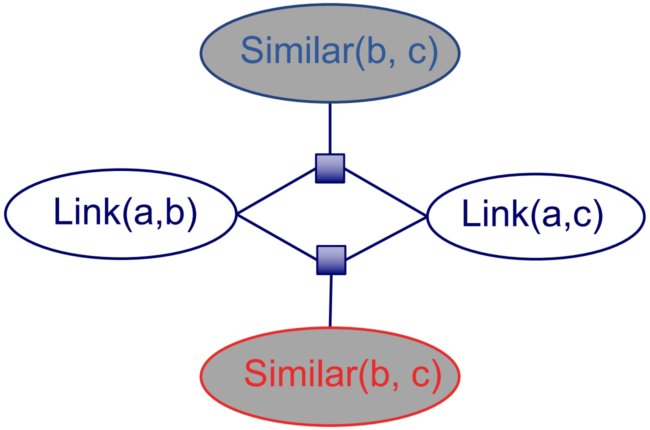
3. How can we add additional model signals?

Details

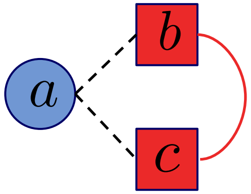
Link Inference Model Characteristics

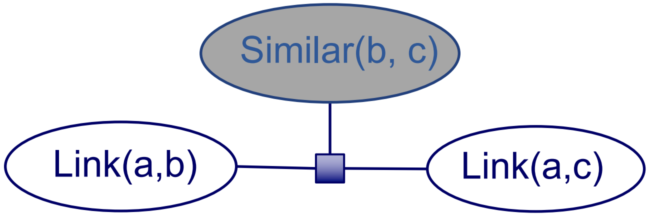
- Support multiple relations



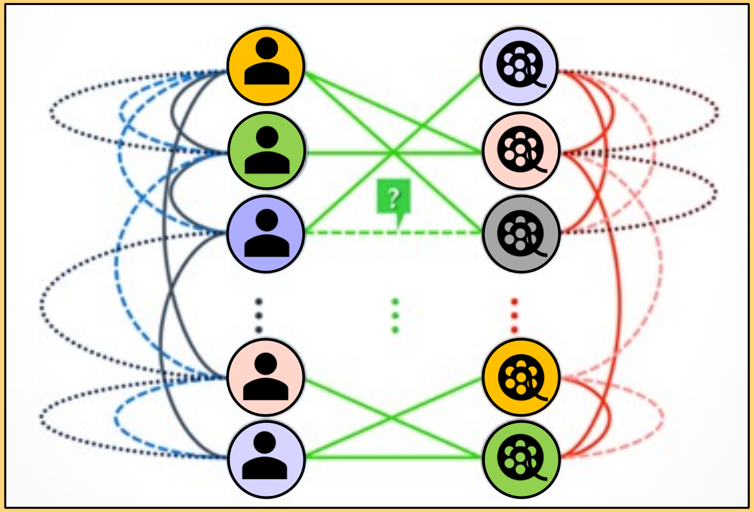


- Joint inference of link values





Question:

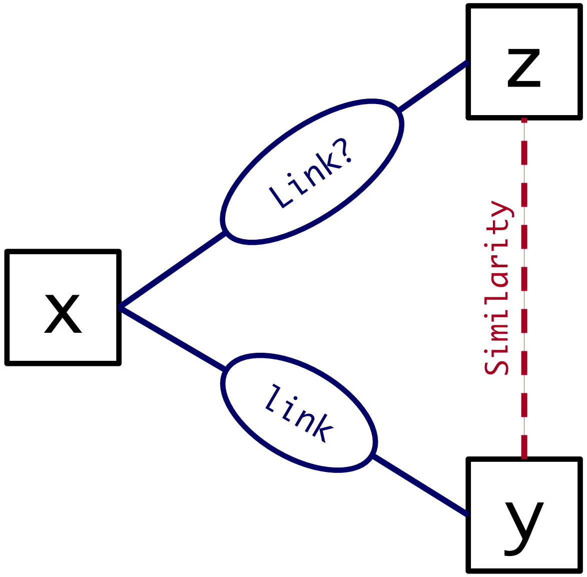


👍 1. How can we use multiple similarities between nodes to infer link values?

👍 2. How can we propagate link information?

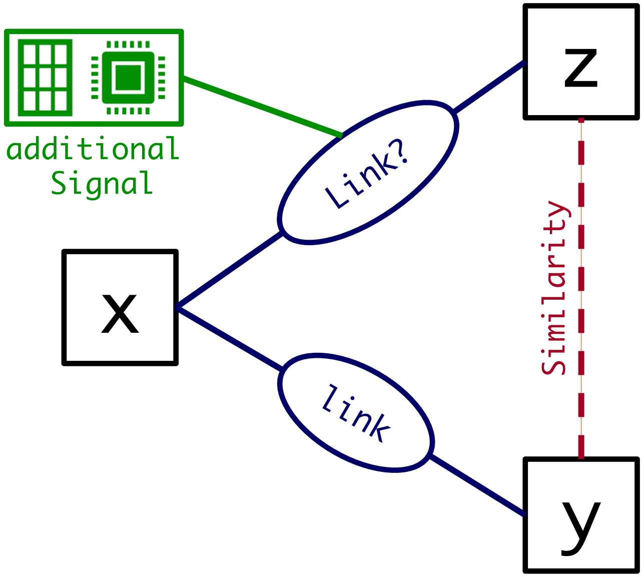
? 3. How can we add additional model signals?

Can we add additional signals?



```
link(x,y) & similar(y,z) -> link(x,z)
```

Can we add additional signals?

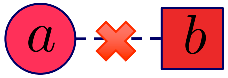


```
link(x,y) & similar(y,z) -> link(x,z)
   additional-signal(x,y) -> link(x,y)
```

Details

Typical Additional Signals

- Enforce sparsity

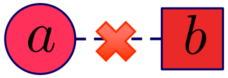


`~rating(u,i)`

Details

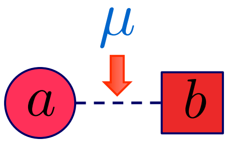
Typical Additional Signals

- Enforce sparsity



```
~rating(u,i)
```

- Distribution statistics

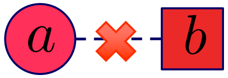


```
mean-rating-user(u) -> rating(u,i)
```

Details

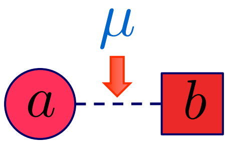
Typical Additional Signals

- Enforce sparsity



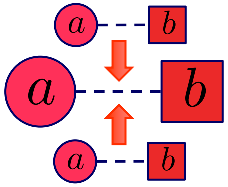
```
~rating(u,i)
```

- Distribution statistics



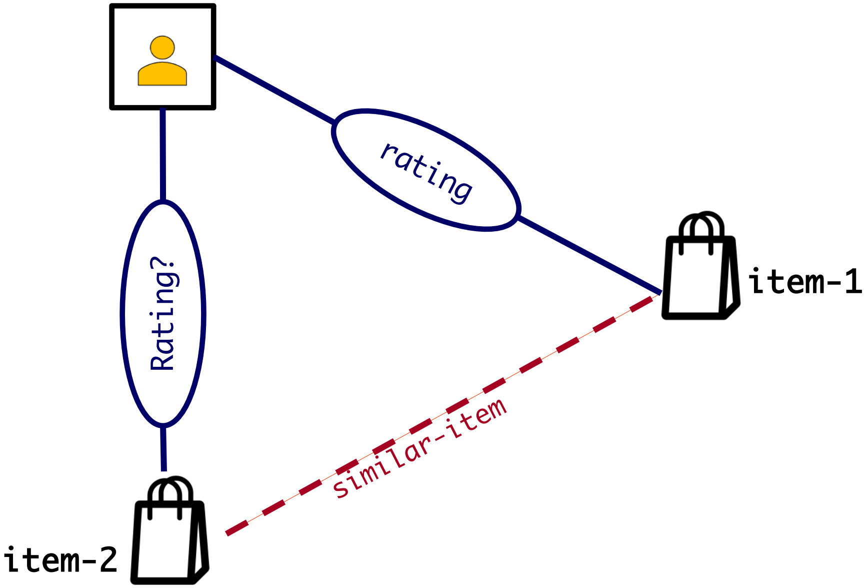
```
mean-rating-user(u) -> rating(u,i)
```

- Predictions from other models



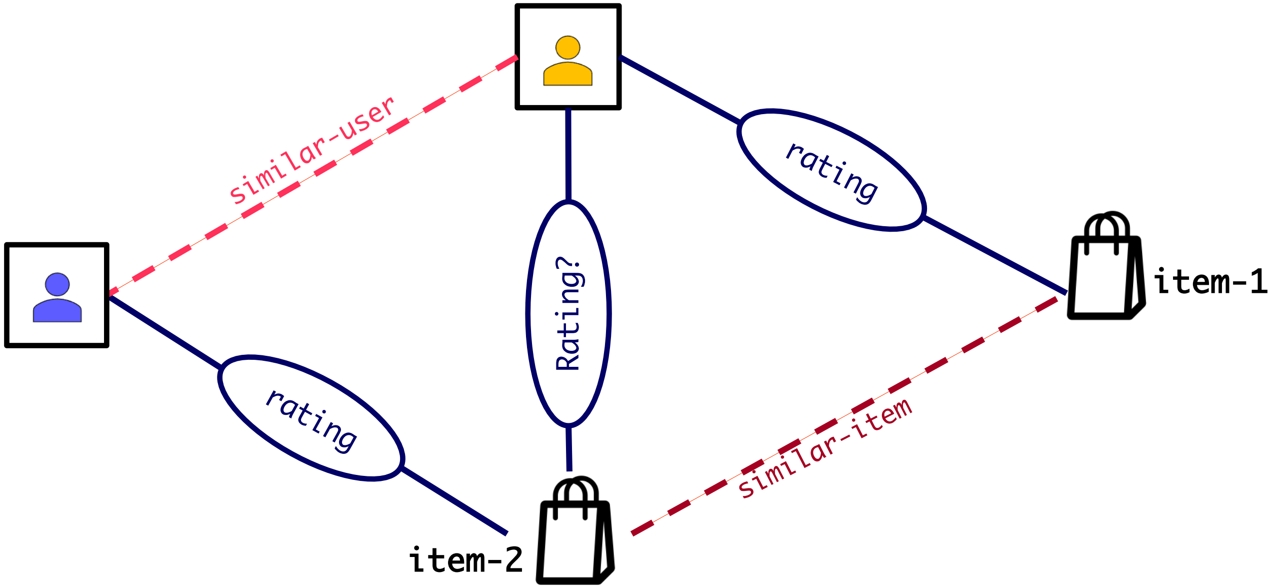
```
FM-rating(u,i) -> rating(u,i)
```

Template for Recommender Systems



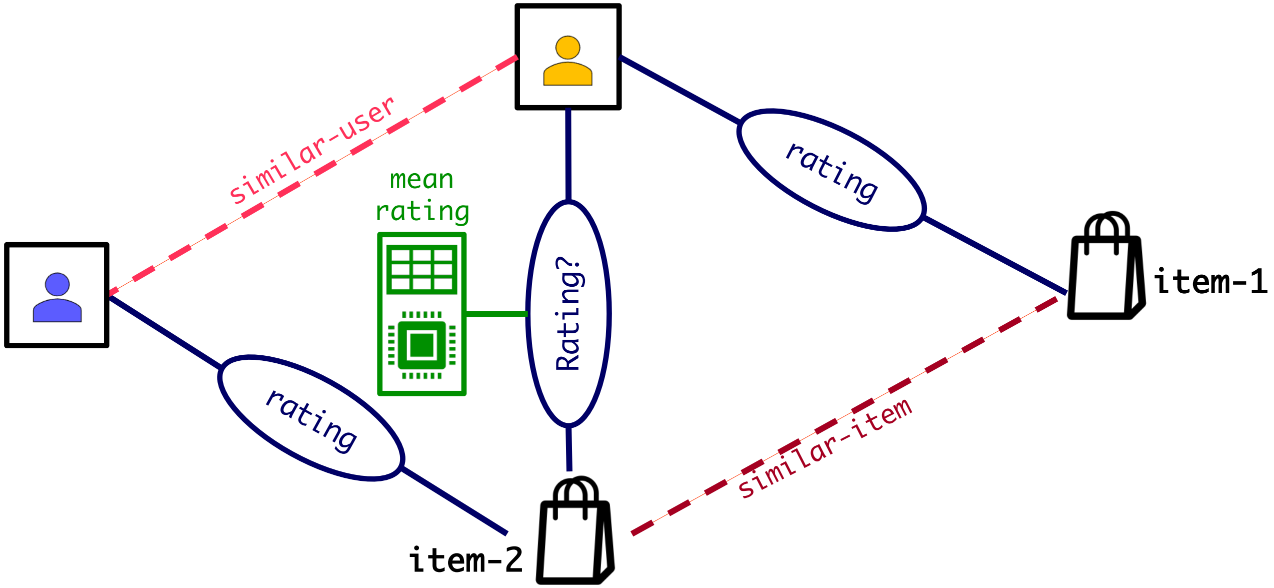
rating(u,i1) & similar-item(i1,i2) -> rating(u,i2)

Template for Recommender Systems



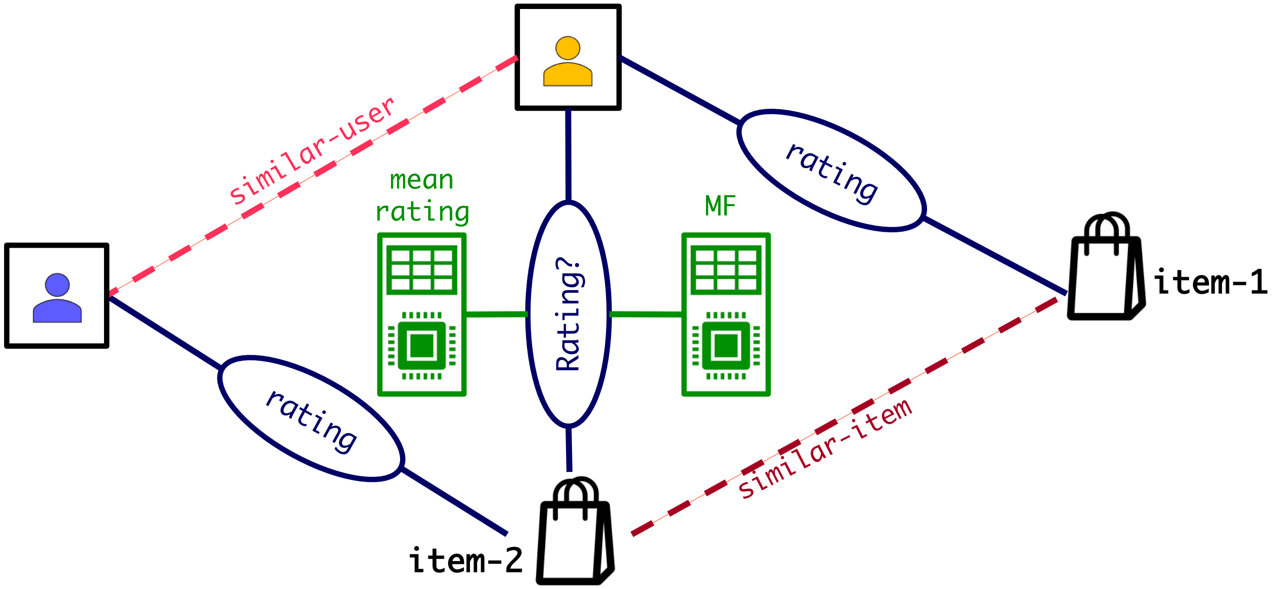
```
rating(u,i1) & similar-item(i1,i2) -> rating(u,i2)
rating(u1,i) & similar-user(u1,u2) -> rating(u2,i)
```

Template for Recommender Systems



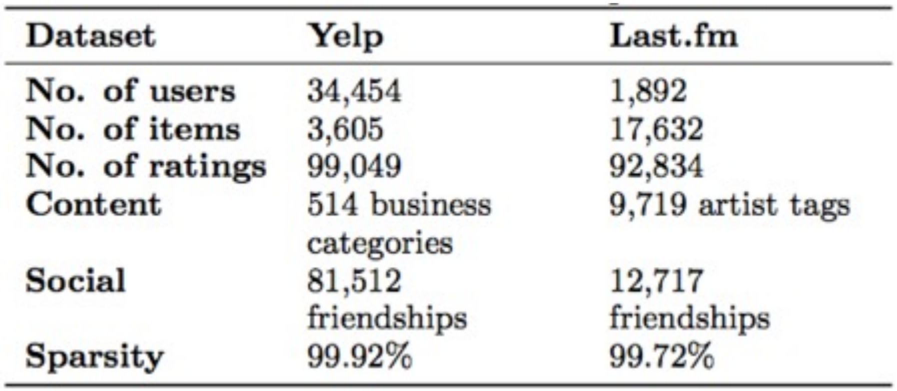
```
rating(u,i1) & similar-item(i1,i2) -> rating(u,i2)
rating(u1,i) & similar-user(u1,u2) -> rating(u2,i)

                mean-rating-user(u) -> rating(u,i)
```

Template for Recommender Systems

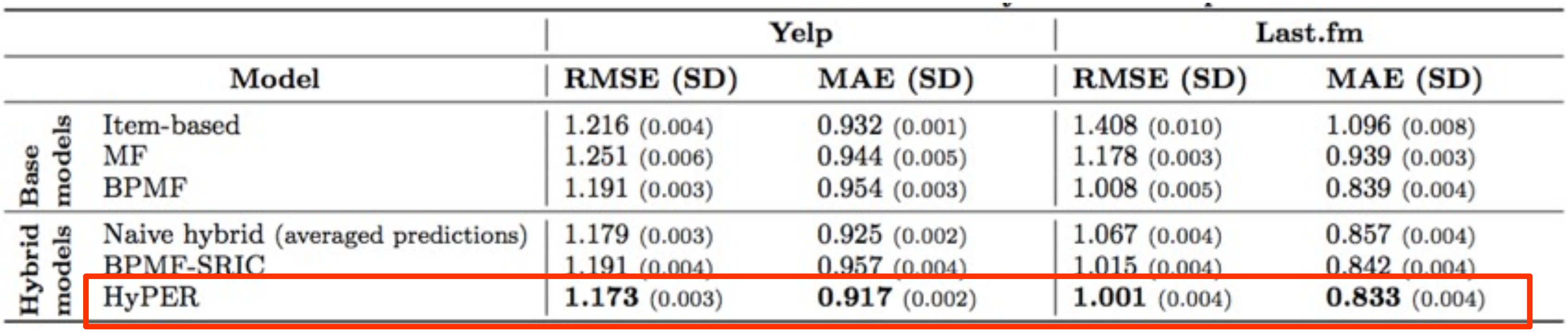


```
rating(u,i1) & similar-item(i1,i2) -> rating(u,i2)
rating(u1,i) & similar-user(u1,u2) -> rating(u2,i)

                 mean-rating-user(u) -> rating(u,i)
                 mean-rating-item(i) -> rating(u,i)

                      MF-rating(u,i) -> rating(u,i)
```

Experimental Validation



Dataset	Yelp	Last.fm
No. of users	34,454	1,892
No. of items	3,605	17,632
No. of ratings	99,049	92,834
Content	514 business categories	9,719 artist tags
Social	81,512 friendships	12,717 friendships
Sparsity	99.92%	99.72%

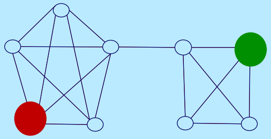


		Yelp		Last.fm	
	Model	RMSE (SD)	MAE (SD)	RMSE (SD)	MAE (SD)
Base models	Item-based	1.216 (0.004)	0.932 (0.001)	1.408 (0.010)	1.096 (0.008)
	MF	1.251 (0.006)	0.944 (0.005)	1.178 (0.003)	0.939 (0.003)
	BPMF	1.191 (0.003)	0.954 (0.003)	1.008 (0.005)	0.839 (0.004)
Hybrid models	Naive hybrid (averaged predictions)	1.179 (0.003)	0.925 (0.002)	1.067 (0.004)	0.857 (0.004)
	BPMF-SRIC	1.191 (0.004)	0.957 (0.004)	1.015 (0.004)	0.842 (0.004)
	HyPER	**1.173** (0.003)	**0.917** (0.002)	**1.001** (0.004)	**0.833** (0.004)

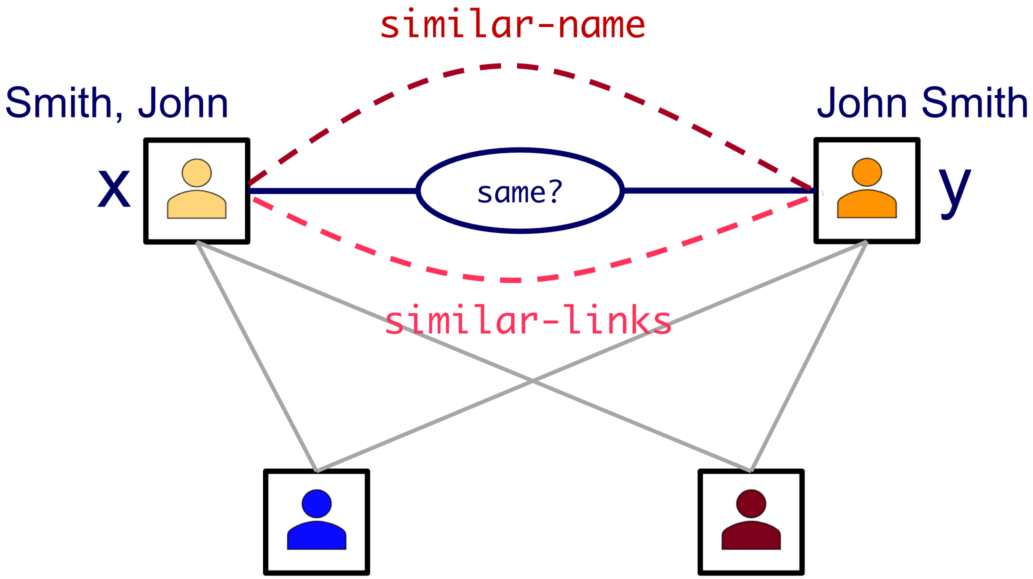
[RecSys] "HyPER: A Flexible and Extensible Probabilistic Framework for Hybrid Recommender Systems", Kouki, P., Fakhraei, S., Foulds, J., Eirinaki, M., & Getoor, L

Bird's eye view

- Part 2: Complex and Heterogeneous Graphs
  - P 2.1: Factorization Methods
  - P 2.2: Heterogeneous Information Networks
  - P 3.3: Statistical Relational Learning
    - P3.3.1: Node Labeling / Collective Classification
    - P3.3.2: Link Prediction / Recommender Systems
    - P3.3.3: Entity Resolution / Knowledge Graph Identification



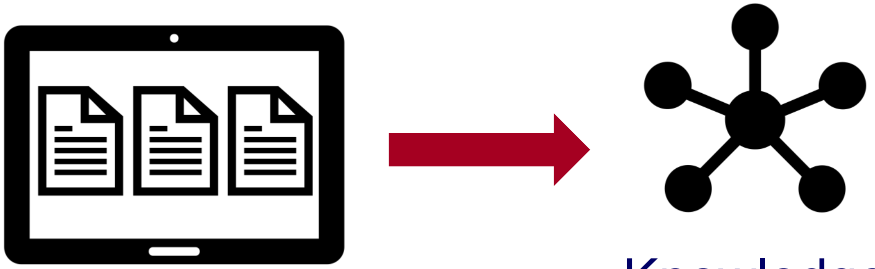
Entity Resolution



```
  similar-name(x,y) ->   same(x,y)
 similar-links(x,y) ->   same(x,y)

same(x,y) &  same(y,z) ->   same(x,z)
```

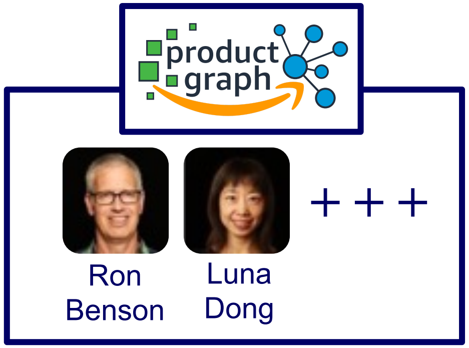
Knowledge Graph Identification

How can we integrate noisy extracted facts into a knowledge graph?



Documents collection

Knowledge graph



Ron Benson

Luna Dong

We can:

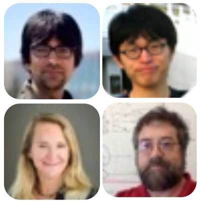
- Perform collective classification, entity resolution, link prediction
- Enforce ontological constraints
- Integrate different knowledge source information
- Combine them all!

Knowledge Graph Identification

```
// Ontological relations
             subsumes(l1,l2) &      label(e,l1) ->      label(e,l2)
            exclusive(l1,l2) &      label(e,l1) ->     ~label(e,l2)
              inverse(r1,r2) & relation(r1,e,o) -> relation(r2,o,e)
                 domain(r,l) &  relation(r,e,o) ->       label(e,l)
                  range(r,l) &  relation(r,e,o) ->       label(o,l)


// Entity resolution
          same-entity(e1,e2) &      label(e1,l) ->      label(e2,l)
          same-entity(e1,e2) & relation(r,e1,o) -> relation(r,e1,o)

// Integrating additional sources
                                 label-nyt(e,l) ->       label(e,l)
                             label-youtube(e,l) ->       label(e,l)
                      relation-wikipedia(r,e,o) ->  relation(r,e,o)

// Sparsity
                                                   ~relation(r,e,o)
                                                        ~label(e,l)
```

Experimental Validation

	NELL		MusicBrainz		FreeBase	
	AUC	F1	AUC	F1	AUC	F1
MLN Ontology (Jiang, ICDM)	0.899	0.836				
Additional sources	0.888	0.843	0.672	0.788	0.416	0.734
Entity resolution	0.809	0.804	0.797	0.831		
Ontological relations	0.899	0.832	0.753	0.832	0.569	0.805
All of the above	**0.904**	**0.854**	**0.901**	**0.919**	**0.724**	**0.840**



[ISWC] "Knowledge graph identification",
Pujara, J., Miao, H., Getoor, L., & Cohen, W.

[AI Magazine] "Using semantics and statistics to turn data into knowledge",
Pujara, J., Miao, H., Getoor, L., & Cohen, W.

Software Tools

– PSL: Probabilistic soft logic
  https://psl.linqs.org/

– Alchemy: Markov Logic Networks
  https://alchemy.cs.washington.edu/

References

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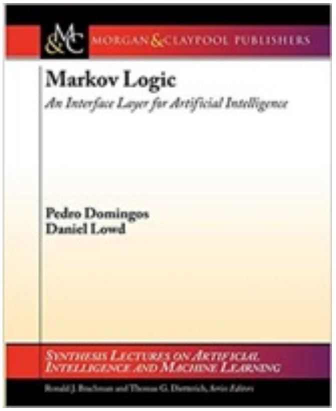
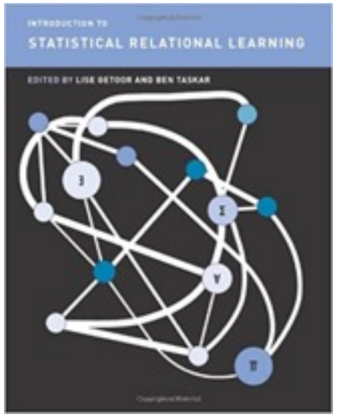
  Hinge-loss markov random fields and probabilistic soft logic
  The Journal of Machine Learning Research, 2017

- Domingos, Pedro, and Daniel Lowd
  Markov logic: An interface layer for artificial intelligence
  Synthesis lectures on artificial intelligence and machine learning, 2009

- Lise Getoor, Ben Taskar (editors)
  Introduction to Statistical Relational Learning
  MIT Press, 2007


MORGAN & CLAYPOOL PUBLISHERS
Markov Logic
An Interface Layer for Artificial Intelligence
Pedro Domingos
Daniel Lowd
SYNTHESIS LECTURES ON ARTIFICIAL INTELLIGENCE AND MACHINE LEARNING
Ronald J. Brachman and Thomas G. Dietterich, Series Editors


INTRODUCTION TO
STATISTICAL RELATIONAL LEARNING
EDITED BY LISE GETOOR AND BEN TASKAR

Bird’s eye view

Tool Task	1.1 PR/HITS	1.1 PPR	1.2 METIS/ SVD	1.3 OddBall+	1.4 BP	2.1 FM	2.1 Tensor	2.2 HIN	2.3 SRL
1.1 Node Ranking	👍					(👍)		(👍)	👍
1.1’ Link Prediction		👍				👍	(👍)	👍	👍
1.2 Comm. Detection			👍				👍	(👍)	(👍)
1.3 Anomaly Detection				👍			👍		
1.4 Propagation					👍			(👍)	👍

Part 1: Plain Graphs

Part 2: Complex Graphs