

#### Network Alignment: Recent Advances and Future Directions





# **Mining on Multiple Networks**







## **Multiple Networks Are Prevalent**





# **Multiple Networks: Examples**

Multiple social networks are inter-linked





# **Multiple Networks: Examples**

• Multiple transaction networks are inter-linked





# What Is Network Alignment?

• Find node correspondence across multiple networks





# Network Alignment: Prob. Def.

- Given:
  - a set of networks  $\{\mathcal{G}_l\}$   $(l \ge 2)$  where  $\mathcal{G}_l = \{\mathcal{V}_l, \mathcal{E}_l, \mathcal{A}_l\}$ ;
    - $\mathcal{V}_l, \mathcal{E}_l, \mathbf{A}_l$  are the nodes, edges and adjacency matrix of  $\mathcal{G}_l$ ;
  - prior alignment matrices  $\{H_{l_1,l_2}\}$  between  $\mathcal{G}_{l_1}$  and  $\mathcal{G}_{l_2}$ .
- Find: the alignment matrices  $\{S_{l_1,l_2}\}$  between  $\mathcal{G}_{l_1}$  and  $\mathcal{G}_{l_2}$ .







## Why Do We Care?





# **Related Setting: Graph Matching**

• It solves for the permutation matrix  ${\it P}$  that minimizes

$$\|\boldsymbol{A}_2 - \boldsymbol{P}^T \boldsymbol{A}_1 \boldsymbol{P}\|_F^2 + \operatorname{Tr}(\boldsymbol{H}^T \boldsymbol{P})$$

- Can be interpreted as a quadratic assignment problem
- $P \in \{0,1\}^{n \times n}$ , P1 = 1,  $1^T P = 1^T$
- Need relaxations on the constraints
  - Doubly stochastic relaxation
  - Spectral relaxation
- Optional external information H





# **Related Setting: Entity Alignment**

• To align entities across knowledge graphs





Xu, Kun, et al. "Cross-lingual knowledge graph alignment via graph matching neural network." *arXiv preprint arXiv:1905.11605* (2019).



# **Traditional Methods**

• Graph matching-based methods [Koutra'13, Zhang'15]

$$\min_{\mathbf{S}} \|\mathbf{A}_2 - \mathbf{S}^T \mathbf{A}_1 \mathbf{S}\|_F^2$$

- Assumption: networks are noisy permutations of each other
- Sparse probabilistic relaxation, i.e.,  $0 \le S_{ij} \le 1$ ,  $\|S\|_0 \le t$
- For bipartite graphs,  $\min_{P,Q} \|B_2 PB_1Q\|_F^2$  [Koutra'13]

Koutra, Danai, Hanghang Tong, and David Lubensky. "Big-align: Fast bipartite graph alignment." 2013 IEEE 13th International Conference on Data Mining. IEEE, 2013. Zhang, Jiawei, and S. Yu Philip. "Multiple anonymized social networks alignment." 2015 IEEE International Conference 11 on Data Mining. IEEE, 2015.



# **Traditional Methods**

- Random walk-based methods (e.g., IsoRank) [Singh'08, Liao'09]
  - Intuition: random walks on Kronecker product graph

 $\boldsymbol{s} = \alpha (\boldsymbol{A}_1 \otimes \boldsymbol{A}_2) \boldsymbol{s} + (1 - \alpha) \boldsymbol{h}$ 





Singh, Rohit, Jinbo Xu, and Bonnie Berger. "Pairwise global alignment of protein interaction networks by matching neighborhood topology." *Annual International Conference on Research in Computational Molecular Biology*. Springer, Berlin, Heidelberg, 2007. Liao, Chung-Shou, et al. "IsoRankN: spectral methods for global alignment of multiple protein networks." *Bioinformatics* 25.12 (2009): i253-i258.



# **Key Challenge #1: Complexity**

- Time complexity:
  - Most of existing works have an at least  $O(n^2)$  time complexity
  - Inefficient computations for large-scale networks
- Space complexity:
  - At least  $O(n^2)$  to store the alignment matrix
  - Costly memory consumptions
- **Q:** How to efficiently solve network alignment?





## **Key Challenge #2: Variety**

- Networks have rich contextual information
  - Node attributes, e.g., gender, age, etc.
  - Edge attributes, e.g., relation types, etc.



• **Q:** How to encode contextual information to enhance the alignment performance?





# **Key Challenge #3: Heterogeneity**

- Networks appear in various sources
  - Networks may capture distinct information
    - Facebook: to connect friend, family, etc.
    - LinkedIn: to connect professionals
  - Same nodes have different behavior patterns
    - E.g., a user is very active in Facebook but quiet in Twitter
- **Q:** How to handle the heterogeneity behind multisourced networks?



## RoadMap



- Motivations and Background
- Part I: Recent Network Alignment Algorithms
- Part II: Network Alignment Applications
- Part III: Future Research Directions

## **Overview of Part I**







# **Pairwise Network Alignment**

- Given: two networks  $\mathcal{G}_1$ ,  $\mathcal{G}_2$  with/without attributes
- Find: the node correspondence across networks





Illustrative example of pairwise network alignment w/o attributes



## **Consistency-Based Methods**

- Intuition:
  - If two nodes are aligned, e.g., node-a in  $\mathcal{G}_1$  and node-x in  $\mathcal{G}_2$
  - Then their neighbors are likely to be aligned





# **NetAlign: A Message Passing Method**

• Key idea: to maximize the number of overlaps





# **NetAlign – Formulation #1**

- To maximize the # of overlaps
  - Equivalent to maximizing the # of nonzeros in A
  - $\frac{\beta}{2} s^T A s$



- A(ii', jj') = 1 if
  A<sub>1</sub>(i, j) = 1
  - $A_2(i',j') = 1$
  - H(i,i') > 0, H(j,j') > 0
- $s_{ii'}A(ii',jj')s_{jj'}$  is high if
  - *i*, *i*' are likely to be aligned
  - j, j' are likely to be aligned



# **NetAlign – Formulation #2**

- Encode the prior knowledge
  - $s^T \operatorname{vec}(H) = \sum_{ii'} S(i, i') H(i, i') \rightarrow \text{score from prior knowledge}$
- Valid matching constraints
  - $\sum_{i', s.t. H(i,i')>0} S(i,i') \leq 1$
  - $\sum_{i,s.t. H(i,i')>0} \mathbf{S}(i,i') \le 1$
  - $S(i, i') \in \{0, 1\}$







# NetAlign – Factor Graph



 Edges: connecting each function node to the variable nodes it acts on





# NetAlign – Algorithm

- Belief propagation
  - Iteratively makes local and greedy decisions
  - Updated by passing messages between nodes in factor graph
- Messages  $m_{ii' \rightarrow f_i}^t, m_{ii' \rightarrow g_{i'}}^t$ 
  - Control matching constraints
  - Also contain info about term  $\alpha s^T \operatorname{vec}(H)$
- Messages  $m_{ii' \rightarrow h_{ii'jj'}}^t$ 
  - Agents in a square should communicate
  - Term  $\frac{\beta}{2} s^T A s$







## **Experimental Results**

Alg.	Data		Overlap	Sol. Time	Total Time
MWM	musm-homo	393	36.2%	_	_
	dmela-scere	135	35.4%		_
	lcsh-small	119	36.8%		_
	lcsh2wiki	2346	13.3%	—	_
Iso	musm-homo	1027	94.5%	0.0	0.4
	dmela-scere	301	79.0%	3.7	10.7
	lcsh-small	257	79.6%	0.0	0.7
	lcsh2wiki	11732	66.6%	11.7	587.3
MP	musm-homo	1076	99.0%	2.6	13.2
	dmela-scere	369	96.9%	26.7	34.9
	lcsh-small	316	97.8%	7.6	12.6
	lcsh2wiki	15974	90.7%	3795.3	4198.4
MP++	musm-homo	1062	97.7%	14.4	17.3
	dmela-scere	376	98.7%	28.7	33.3
	lcsh-small	318	98.5%	11.8	15.2
	lcsh2wiki	15771	89.6%	4103.8	4990.2
MR	musm-homo	1070	98.4%	12.5	12.6
	dmela-scere	375	98.4%	22.7	79.4
	lcsh-small	318	98.5%	4.1	16.8
	lcsh2wiki	16836	95.6%	4878.2	4988.0

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# Final: Attributed Network Alignment

#### • Given:

- two networks  $\{G_l\}$  (l = 1, 2) where  $G_l = \{V_l, \mathcal{E}_l, A_l, N_l, E_l\}$ and  $N_l, E_l$  denote the node attributes and edge attributes;
- prior alignment matrices H between  $\mathcal{G}_1$  and  $\mathcal{G}_2$ .
- Find: the alignment matrix S between  $G_1$  and  $G_2$ .





# **Final – Formulation #1**

- Topological consistency
  - Intuition: similar node-pairs tend to have similar neighboring node-pairs



- Example:
  - Large S(a, x)
  - Large  $A_1(a, b)$  and  $A_2(x, y)$

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Zhang, Si, and Hanghang Tong. "Final: Fast attributed network alignment." *Proceedings of the 22nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*. 2016.

large S(b, y)



## **Final – Formulation #2**

- Node attribute consistency
  - Intuition: similar node-pairs share similar node attributes



• Large  $S(a, x) \longrightarrow$  node-*a* and node-*x* share similar attributes

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# **Final – Formulation #3**

- Edge attribute consistency
  - Intuition: similar node-pairs connect to their neighbor-pairs via similar edge attributes



- Example:
  - Large S(a, x)
  - Large  $\boldsymbol{S}(b, y)$







# **Final – Overall Formulation**

Objective function

$$\min_{\mathbf{S}} J(\mathbf{S}) = \sum_{a,b,x,y} \left[ \frac{\mathbf{S}(x,a)}{\sqrt{f(x,a)}} - \frac{\mathbf{S}(y,b)}{\sqrt{f(y,b)}} \right]^2 \frac{\text{#1. Topology Consistency}}{A_1(a,b)A_2(x,y)} \\
\times \Phi(x,a)\Phi(y,b) \times \Psi((x,y),(a,b))$$
#2. Node Attribute Consistency #3. Edge Attribute Consistency

• Matrix-form objective function

$$\min_{S} J(S) = \min_{S} \sum_{v,w} \left[ \frac{s(v)}{\sqrt{D(v,v)}} - \frac{s(w)}{\sqrt{D(w,w)}} \right]^2 W(v,w)$$
  
$$s = \operatorname{vec}(S) = \min_{S} s^T (I - \widetilde{W})s$$
 attributed Kronecker product

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# **Final – Algorithm**

- Fixed-point solution: by setting derivative to 0
  - Converges to the global optimal solution

$$\boldsymbol{s} = a\widetilde{\boldsymbol{W}}\boldsymbol{s} + (1-\alpha)\boldsymbol{h} \Rightarrow \boldsymbol{s} = (1-\alpha)(\boldsymbol{I} - \alpha\widetilde{\boldsymbol{W}})^{-1}\boldsymbol{h}$$

- Intuition: a similarity propagation to neighboring node-pairs, which is additionally calibrated by node/edge attributes
- Speed-up variants:
  - Low-rank approximation for full alignment
  - Low-rank approximation for on-query alignment



#### Final – Low-Rank Approximation Algorithm

• If we only consider node attributes

$$\boldsymbol{s} = (1-\alpha) \left( \boldsymbol{I} - \alpha \boldsymbol{D}_N^{-\frac{1}{2}} \boldsymbol{N} (\boldsymbol{A}_1 \otimes \boldsymbol{A}_2) \boldsymbol{N} \boldsymbol{D}_N^{-\frac{1}{2}} \right)^{-1} \boldsymbol{h}$$

• Key Idea: Low rank approximation of  $A_1$  and  $A_2$ 



• **Complexity**:  $O(n^6)$  or  $O(mnt_{max}) \rightarrow O(n^2r^4)$ 



#### **Final – Experimental Results**



**Observation**: attributes help improve network alignment.





#### **Final – Experimental Results**



**Observation**: FINAL gains a better quality-speed balance.





#### **Final – Experimental Results**



**Observation**: FINAL On-Query gains around 90% accuracy relative to exact FINAL-N, but more than 100 times faster.

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## **Final – More on Computations**

- Further speed-up: from  $O(n^2)$  to O(m)
  - Key idea: indirect representation of  $\boldsymbol{S}$  [1]
  - Theorem: Low-rank of  $A_1$  and  $A_2 \rightarrow$  low-rank of S

- Alignment quality: linear complexity w/o approximation
  - Multilevel alignment (perfect interpolation theorem) [2]
  - Implicit Krylov subspace methods [3]

[1] Zhang, Si, et al. "ineat: Incomplete network alignment." 2017 IEEE International Conference on Data Mining (ICDM). IEEE, 2017.
 [2] Zhang, Si, et al. "Multilevel network alignment." The World Wide Web Conference. 2019.
 [3] Du, Boxin, and Hanghang Tong. "Fasten: Fast sylvester equation solver for graph mining." Proceedings of the 24th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining. 2018.

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#### **Overview of Part I**







### **Embedding-Based Methods**

- Intuition: to learn node representations that
  - Preserve structural/attribute proximity within networks
  - Preserve proximity across aligned nodes



# IONE: Aligning Users by Network Embedding

- Background: network embedding by LINE (2<sup>nd</sup> order)
  - Compute two distributions:

Empirical distribution of neighborhood structure:

Model distribution of neighborhood structure:

$$\hat{p}_{2}(v_{j} \mid v_{i}) = \frac{W_{ij}}{\overset{\circ}{a} W_{ik}}$$

$$p_{2}(v_{j} \mid v_{i}) = \frac{\exp(\vec{u}_{i}^{T} \vec{u}_{j})}{\sum_{k \in V} \exp(\vec{u}_{k}^{T} \vec{u}_{i})}$$

• Minimize the KL divergence by omitting constant terms  $O_2 = \bigotimes_{i}^{\circ} KL(\hat{p}_2(|v_i|), p_2(|v_i|)) = -\bigotimes_{(i,j)\hat{i} E}^{\circ} W_{ij} \log p_2(v_j | v_i)$ 



Tang, Jian, et al. "Line: Large-scale information network embedding." Proceedings of the 24th international conference on world wide web. 2015. Liu, Li, et al. "Aligning Users across Social Networks Using Network Embedding." *Ijcai*. 2016.



# **IONE – Within-Network Embedding**

- Intuition: to preserve structure proximity
- Embedding vectors for node-*i* 
  - A node vector  $oldsymbol{u}_i$
  - Context vectors: (1) input context  $oldsymbol{u}_i^\prime$ , (2) output context  $oldsymbol{u}_i^{\prime\prime}$

Input context model distribution:

$$p_1(v_j|v_i) = \frac{\exp\left(\overrightarrow{u_j'}^T, \overrightarrow{u_i}\right)}{\sum_{k=1}^{|V|} \exp\left(\overrightarrow{u_k'}^T, \overrightarrow{u_i}\right)}$$

Output context model distribution:

$$p_2(v_i|v_j) = \frac{\exp\left(\overrightarrow{u_i''}^T \cdot \overrightarrow{u_j}\right)}{\sum_{k=1}^{|V|} \exp\left(\overrightarrow{u_k''}^T \cdot \overrightarrow{u_j}\right)}$$

Empirical distributions:  $\hat{p}_1(i,j) = w_{ij}/d_i^{out}$   $\hat{p}_2(i,j) = w_{ij}/d_j^{in}$ 

• Objective: minimize KL divergences

### **IONE – Cross-Network Embedding**

• Intuition: aligned nodes coincide in embedding space

Model distribution:

$$p_1(v_j^Y | v_k^X) = \frac{\exp(\boldsymbol{u}_j^{Y^T} \boldsymbol{u}_k^X)}{\sum_{k \in V_X} \exp(\boldsymbol{u}_j^{Y^T} \boldsymbol{u}_k^X)}$$

**Empirical distribution:**  $\hat{p}_1(v_j^Y | v_k^X) = \sum_{v_i \in V_Y} p_a(v_i^Y | v_k^X) \times \frac{w_{ij}}{d_i^{out}}$ 

- $p_a(v_i^Y | v_k^X)$ : probability that  $v_k^X$  and  $v_i^Y$  are aligned
- Objective: minimize KL divergences
  - e.g.,  $p_1(v_j^Y | v_i^X)$  vs.  $\hat{p}_1(v_j^Y | v_i^X)$



#### **IONE – Model Inference**

• SGD with negative sampling

$$\log p_1(v_j^X | v_i^X) \propto \log \sigma(\overrightarrow{u_j}'^{X^T} \cdot \overrightarrow{u_i}^X) + \Sigma_{m=1}^K E_{v_n \sim p_n(v)} \log \sigma(-\overrightarrow{u_n}'^{X^T} \cdot \overrightarrow{u_i}^X)$$

$$\log p_1(v_j^Y | v_k^X) \propto \log \sigma(\overrightarrow{u_j}'^{Y^T} \cdot \overrightarrow{u_k}^X) + \sum_{m=1}^K E_{v_n \sim p_n(v)} \log \sigma(-\overrightarrow{u_n}'^{Y^T} \cdot \overrightarrow{u_k}^X)$$





#### **IONE – Experimental Results**

• Dataset: Foursquare-Twitter



Liu, Li, et al. "Aligning Users across Social Networks Using Network Embedding." Ijcai. 2016.



#### **IONE – Case Study**



Liu, Li, et al. "Aligning Users across Social Networks Using Network Embedding." Ijcai. 2016.

# **DeepLink: Deep Learning for User Identity Linkage**

- Motivations:
  - Heterogeneity across networks  $\rightarrow$  Complex alignment
  - Scarcity of labeled alignment → Supervised training is not easy
- Key questions:
  - How to learn non-linear transformation for alignment?
  - How to boost supervised training algorithm?
- Key idea: use deep neural network with dual-learning



# **DeepLink – Network Embedding**

- Key idea: pre-trained Skip-gram based embedding
  - To predict the context of a center node



- Context sampling:
  - Random walks from center nodes
- Objective function:
  - Original: to maximize

$$p(u_{t+j} \mid u_t) = \frac{\exp(\mathbf{v}_{u_{t+j}}^{\mathrm{T}} \mathbf{v}_{u_t}')}{\sum_{i=1}^{m} \exp(\mathbf{v}_{u_i}^{\mathrm{T}} \mathbf{v}_{u_t}')}$$

• With negative sampling:

 $\log[\sigma(\mathbf{v}_{u_{t+j}}^{\mathrm{T}}\mathbf{v}_{u_{t}}')] + \sum_{i=1}^{K} \mathbb{E}_{u_{i} \sim p_{n}(u)}[\log(1 - \sigma(\mathbf{v}_{u_{i}}^{\mathrm{T}}\mathbf{v}_{u_{t}}'))]$ 

# **DeepLink – Neural Mapping Learning**

- Goal: to learn non-linear alignment across networks
- Intuition: neural networks capture complex nonlinearity
- Key idea: use two multilayer perceptrons as mappings
  - One MLP (denoted by  $\Phi$ ) to map from network  $\mathcal{G}^s$  to  $\mathcal{G}^t$
  - Another MLP (denoted by  $\Phi^{-1}$ ) for  $\mathcal{G}^t$  to  $\mathcal{G}^s$



# **DeepLink – Dual Learning**

- Goal: to address the lack of labeled alignment
- Components:
  - Unsupervised alignment pre-training uses node embedding to learning two weak mapping functions  $\Phi$  and  $\Phi^{-1}$
  - Supervised alignment learning uses labeled alignment to improve weak mapping functions



# **DeepLink – Unsupervised Pre-training**

- Goal: to learn self-consistent mappings
- Method: autoencoder type of architecture
  - Encoder: mapping function  $\Phi$
  - Decoder: mapping function  $\Phi^{-1}$
- Objective function:
  - Minimize difference between  $\Phi^{-1}(\Phi(v_u))$  and  $v_u$



# **DeepLink – Supervised Learning**

- Key idea: align according to some reward functions
- Method:
  - Find k-similar embeddings  $v'(u_i)$  in  $\mathcal{G}^t$  for mapped embeddings of node-a in  $\mathcal{G}^s$ , i.e.,  $u_i \in \text{Top}(\Phi(v(u_a)))$



# **DeepLink – Experimental Results**

• Dataset: Foursquare-Twitter

	Precision						
	P@1	P@5	P@9	P@13	P@21	P@30	
CRW	0.0000	0.0219	0.0476	0.0538	0.0909	0.1603	
MAG	0.0638	0.1362	0.1705	0.2081	0.2708	0.3229	
MAH	0.0500	0.1219	0.1886	0.2148	0.2513	0.0003	
ONE	0.1229	0.2533	0.3038	0.3510	0.4071	0.4270	
IONE	0.2238	0.4033	0.4638	0.5010	0.5571	0.5970	
DeepLink	0.3447	0.5942	0.6609	0.6866	0.7000	0.7048	

#### Comparisons of alignment precision.

**Observation:** DeepLink achieves highest accuracy in top-k identity matching.



# **DeepLink – Experimental Results**

• Visualization of cosine similarities of randomly sampled anchor nodes (the more diagonalized, the better).





(a) IONE Anchor Nodes







#### **Observations:**

- IONE disrupts the embedding similarities of labeled alignment pairs after training.
- In contrast, DeepLink still preserves the anchor linkage.
- Similarly for testing anchor nodes.

(c) IONE Testing Nodes

(d) DeepLink Testing Nodes



#### **Regal: Representation Learning-Based Graph Alignment**



	Regal	IONE
Key idea	matrix factorization	skip-gram w/ negative sampling
Attributes	w/ node attributes	w/o attributes
Supervision	unsupervised	semi-supervised
Complexity	sub-quadratic	sub-quadratic





#### **Regal – Overview**

- Node feature extraction
- Node embedding learning by matrix factorization
- Network alignment





# **Regal – Node Feature Extraction**

- Structural identity
  - $\mathcal{R}_{u}^{k}$ : the set of nodes exactly k steps away from u
  - $d_u^k(i)$ : the number of nodes in  $\mathcal{R}_u^k$  with degree of i
  - $d_u = \sum_{i=1}^{K} \delta^{k-1} d_u^k$  ( $\delta$  is the discount factor)
  - Logarithmic binning:  $d_u^k(i)$  is the number of nodes  $u \in \mathcal{R}_u^k$  such that  $\lfloor \log_2 \deg(u) \rfloor = i$
- Attribute-based identity
  - Node input feature vector  $f_u$





# **Regal – Cross-Network Node Similarity**

Direct computation

 $sim(u, v) = \exp[-\gamma_s \|\boldsymbol{d}_u - \boldsymbol{d}_v\|_2^2 - \gamma_a \times dist(\boldsymbol{f}_u, \boldsymbol{f}_v)]$ 

- Limitation: costly computation  $O(n^2)$  where  $n = n_1 + n_2$
- Efficient computation
  - Reduce to node-landmark similarity
  - $\mathcal{L}$ : a set of p landmark nodes chosen randomly
  - Node-landmark similarity matrix: C(u, v),  $v \in \mathcal{L}$
  - Landmark-landmark similarity

$$\boldsymbol{W}(v_1, v_2) = \boldsymbol{C}(v_1, v_2), v_1 \in \mathcal{L}$$







# **Regal – Node Embedding Learning**

Nystrom-based approximation

$$\boldsymbol{S} \approx \boldsymbol{\tilde{S}} = \boldsymbol{C} \boldsymbol{W}^{+} \boldsymbol{C}^{T}$$

- W<sup>+</sup>: pseudo-inverse of W
- Embedding:  $Y = CU\Sigma^{\frac{1}{2}}$  where  $[U, \Sigma, V] = SVD(W^+)$





# **Regal – Alignment Inference**

- K-D tree for fast similarity search
- Similarity scores:

$$sim(u,v) = e^{-\|\widetilde{Y}_1[u] - \widetilde{Y}_2[v]\|_2^2}$$

- Complexity:
  - Feature extraction:  $O(nKd_{avg}^2)$
  - Node similarity: O(npb)
  - Node embedding:  $O(np^2)$
  - Alignment:  $O(n \log n)$









#### **Regal – Experimental Results**

• Data constructions: (1) noisy permutations of one network, (2) synthetic node attributes



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### **Regal – Experimental Results**

• Running time:

Dataset	Arxiv	PPI	Arenas
FINAL	4182 (180)	62.88 (32.20)	3.82 (1.41)
NetAlign	149.62 (282.03)	22.44 (0.61)	1.89 (0.07)
IsoRank	17.04 (6.22)	6.14 (1.33)	0.73 (0.05)
Klau	1291.00 (373)	476.54 (8.98)	43.04 (0.80)
REGAL-node2vec	709.04 (20.98)	139.56 (1.54)	15.05 (0.23)
REGAL-struc2vec	1975.37 (223.22)	441.35 (13.21)	74.07 (0.95)
REGAL	86.80 (11.23)	18.27 (2.12)	2.32 (0.31)

Faster computations due to landmark strategy and K-D tree search.



#### **Overview of Part I**





#### **Gromov-Wasserstein Learning for Graph Matching and Node Embedding**

- Backgrounds:
  - Networks are often noisy.
  - Many methods learn specific transformations across embeddings of different networks.
- Key question:
  - How to jointly learn node embeddings and infer alignment?
- Benefits of joint problem:
  - Distance between learned node embeddings as auxiliary information of edges → help reduce noise
  - Learn in same manifold  $\rightarrow$  lower risk of model misspecification



Xu, Hongteng, et al. "Gromov-wasserstein learning for graph matching and node embedding." arXiv preprint arXiv:1901.06003 (2019).

### **GWL - Preliminaries**

- Gromov-Wasserstein distance
  - An optimal transport-like distance for metric spaces
  - Calculates distances between pairs of samples of each domain
  - Measures how these distances compare to those in other domains
- Gromov-Wasserstein discrepancy
  - A relaxation by using dissimilarity measurement instead of strict distance metrics
- Metric-measure space of a graph
  - Corresponds to a pair  $(C, \mu) \in R^{|V| \times |V|} \times \Sigma^{|V|}$  of a graph G.
  - $C = [c_{ij}]$  represents a node distance/dissimilarity matrix.
  - $\boldsymbol{\mu} = [\mu_i]$  is the empirical distribution of nodes.



#### **GWL - Gromov-Wasserstein Learning Framework**

- Gromov-Wasserstein discrepancy between graphs
  - Given  $G_s$  and  $G_t$ , the discrepancy between  $(C_s, \mu_s)$  and  $(C_t, \mu_t)$

$$d_{GW}(\boldsymbol{\mu}_{s}, \boldsymbol{\mu}_{t}) := \min_{\boldsymbol{T} \in \Pi(\boldsymbol{\mu}_{s}, \boldsymbol{\mu}_{t})} \sum_{i, j, i', j'} L(c_{ij}^{s}, c_{i'j'}^{t}) T_{ii'} T_{jj'}$$
$$= \min_{\boldsymbol{T} \in \Pi(\boldsymbol{\mu}_{s}, \boldsymbol{\mu}_{t})} \langle L(\boldsymbol{C}_{s}, \boldsymbol{C}_{t}, \boldsymbol{T}), \boldsymbol{T} \rangle.$$

- $L(\cdot, \cdot)$ : element-wise loss, e.g., mean square or KL-divergence
- **T**: optimal transport between nodes of two networks, indicating probabilities of alignment

• 
$$\boldsymbol{L}_{jj'} = \sum_{i,i'} L\left(c_{ij}^{s}, c_{i'j'}^{t}\right) \boldsymbol{T}_{ii'}$$

• 
$$L(C_s, C_t, T) = [L_{jj'}] \in R^{|V_s| \times |V_t|}$$

#### **GWL - Gromov-Wasserstein Learning** Framework

- Proposed model
  - Use node embeddings  $X_s$ ,  $X_t$  for dissimilarity matrices

$$\min_{\mathbf{X}_{s}, \mathbf{X}_{t}} \min_{\mathbf{T} \in \Pi(\boldsymbol{\mu}_{s}, \boldsymbol{\mu}_{t})} \underbrace{\langle \boldsymbol{L}(\boldsymbol{C}_{s}(\boldsymbol{X}_{s}), \boldsymbol{C}_{t}(\boldsymbol{X}_{t}), \boldsymbol{T}), \boldsymbol{T} \rangle}_{\text{Gromov-Wasserstein discrepancy}} \\ + \underbrace{\alpha \langle \boldsymbol{K}(\boldsymbol{X}_{s}, \boldsymbol{X}_{t}), \boldsymbol{T} \rangle}_{\text{Wasserstein discrepancy}} + \underbrace{\beta R(\boldsymbol{X}_{s}, \boldsymbol{X}_{t})}_{\text{prior information}}.$$

•  $C_s(X_s) = (1 - \alpha)C_s + \alpha K(X_s, X_s)$  where  $C_s$  is computed by edge weights and  $K(X_s, X_s)$  measures distance within same network based on node embedding.

• 
$$R(X_s, X_t) = \sum_{k=s,t} L(K(X_k, X_k), C_k) + L(K(X_s, X_t), C_{st})$$

#### Optional when given labeled alignment

# **GWL – Learning Algorithm**

- Alternatively learn optimal transport and embedding
- Learning optimal transport
  - Proximal point method

 $\min_{\boldsymbol{T} \in \Pi(\boldsymbol{\mu}_s, \boldsymbol{\mu}_t)} \langle \boldsymbol{L}(\boldsymbol{C}_s(\boldsymbol{X}_s^{(m)}), \boldsymbol{C}_t(\boldsymbol{X}_t^{(m)}), \boldsymbol{T}), \boldsymbol{T} \rangle \\ + \alpha \langle \boldsymbol{K}(\boldsymbol{X}_s^{(m)}, \boldsymbol{X}_t^{(m)}), \boldsymbol{T} \rangle + \gamma \mathrm{KL}(\boldsymbol{T} \| \boldsymbol{T}^{(n)})$ 

A proximal term based on KL-divergence

Updating embeddings



Relational matching between graphs Cost = |d(A, D) - d(1, 2)|

topology

• Given optimal transport  $\widehat{m{T}}^{(m)}$ , solve by gradient descent

 $\min_{\boldsymbol{X}_s, \boldsymbol{X}_t} \alpha_m \langle \boldsymbol{K}(\boldsymbol{X}_s, \boldsymbol{X}_t), \ \widehat{\boldsymbol{T}}^{(m)} \rangle + \beta R(\boldsymbol{X}_s, \boldsymbol{X}_t)$ 



Xu, Hongteng, et al. "Gromov-wasserstein learning for graph matching and node embedding." arXiv preprint arXiv:1901.06003 (2019).

Embedding space of nodes

Update optimal transport based

### **GWL – Experimental Results**

- Communication network alignment
  - Dataset: MC3 used in the Mini-Challenge 3 of VAST Challenge 2018
- Model Variants:
  - GWL-C and GWL-R: use cosine and RBF distance on embeddings
  - GWD: no embedding
     -based distance

Method	Call→Email (Sparse)	Call→Email (Dense)		
Method	Node Correctness (%)	Node Correctness (%)		
GAA	34.22	0.53		
LRSA	38.20	2.93		
TAME	37.39	2.67		
GRAAL	39.67	0.48		
MI-GRAAL	35.53	0.64		
MAGNA++	7.88	0.09		
HugAlign	36.21	3.86		
NETAL	36.87	1.77		
GWD	23.16±0.46	$1.77 \pm 0.22$		
GWL-R	$39.64 \pm 0.57$	$3.80 \pm 0.23$		
GWL-C	<b>40.45</b> ±0.53	<b>4.23</b> ±0.27		



#### **GWL – Experimental Results**

- Procedure recommendation
  - Dataset: MIMIC-III dataset
  - Goal: recommend suitable procedures for patients, according to their disease characteristics.

Method	Top-1 (%)			Top-5 (%)		
Wiethou	Р	R	F1	Р	R	F1
Word2Vec	39.95	13.27	18.25	28.89	46.98	32.59
GloVe	32.66	13.01	17.22	27.93	44.79	31.47
DWL (Scratch)	37.89	12.42	17.16	27.39	43.81	30.81
DWL (Finetune)	40.00	13.76	18.71	30.59	48.56	34.28
GWD-R	46.29	17.01	22.32	31.82	43.81	33.77
GWD-C	43.16	15.79	20.77	31.42	42.99	33.25
GWL-R	46.20	16.93	22.22	32.03	44.75	34.18
GWL-C	47.46	17.25	22.71	32.09	45.64	34.31



Xu, Hongteng, et al. "Gromov-wasserstein learning for graph matching and node embedding." arXiv preprint arXiv:1901.06003 (2019).

#### **Overview of Part I**







# **Collective Network Alignment**

- Goal: to find alignment across multiple networks
- Possible solution
  - Find pairwise alignment
  - Then combine
  - Transitivity constraint may be violated



 $G^1$ 

Username:

Ortiz Brandy

- Problem setting:
  - Given: more than two networks  $\mathcal{G} = \{\mathcal{G}_1, \cdots, \mathcal{G}_m\}$
  - Find: alignment across  $G_i$ ,  $G_j$   $(i, j = 1, \dots, m)$  jointly

#### Multiple Anonymized Social Networks Alignment

- Goal: to find anchor links/alignment across multiple networks without attributes
- Key challenge: how to preserve transitivity property





Zhang, Jiawei, and S. Yu Philip. "Multiple anonymized social networks alignment." 2015 IEEE International Conference on Data Mining. IEEE, 2015.

#### UMA – Unsupervised Pairwise Alignment

- Key idea: to minimize the alignment inconsistency
  - I.e., the number of non-shared edges between those mapped from  $\mathcal{G}^{(i)}$  and those in  $\mathcal{G}^{(j)}$
- Mathematical formulation

$$\begin{split} \bar{\mathbf{T}}^{(i,j)} &= \arg\min_{\mathbf{T}^{(i,j)}} \left\| (\mathbf{T}^{(i,j)})^{\top} \mathbf{S}^{(i)} \mathbf{T}^{(i,j)} - \mathbf{S}^{(j)} \right\|_{F}^{2} \\ s.t. \quad \mathbf{T}^{(i,j)} \in \{0,1\}^{|\mathcal{U}^{(i)}| \times |\mathcal{U}^{(j)}|}, \\ & \mathbf{T}^{(i,j)} \mathbf{1}^{|\mathcal{U}^{(j)}| \times 1} \preccurlyeq \mathbf{1}^{|\mathcal{U}^{(i)}| \times 1}, \\ & (\mathbf{T}^{(i,j)})^{\top} \mathbf{1}^{|\mathcal{U}^{(i)}| \times 1} \preccurlyeq \mathbf{1}^{|\mathcal{U}^{(j)}| \times 1}, \\ & \text{one-to-one mapping constraints} \end{split}$$

- $\mathbf{S}^{(i)}$ ,  $\mathbf{S}^{(j)}$ : adjacency matrices of networks  $\mathcal{G}^{(i)}$  and  $\mathcal{G}^{(j)}$
- $T^{(i,j)}$ : alignment matrix from  $\mathcal{G}^{(i)}$  to  $\mathcal{G}^{(j)}$

Zhang, Jiawei, and S. Yu Philip. "Multiple anonymized social networks alignment." 2015 IEEE International Conference on Data Mining. IEEE, 2015.
#### **UMA – Transitivity Penalties**

- Measure the number of inconsistent edges between the mapped from  $\mathcal{G}^{(i)} \to \mathcal{G}^{(j)} \to \mathcal{G}^{(k)}$  and  $\mathcal{G}^{(i)} \to \mathcal{G}^{(k)}$
- Mathematical formulation

$$C(\{G^{(i)}, G^{(j)}, G^{(k)}\}) = \left\| (\mathbf{T}^{(j,k)})^{\top} (\mathbf{T}^{(i,j)})^{\top} \mathbf{S}^{(i)} \mathbf{T}^{(i,j)} \mathbf{T}^{(j,k)} - (\mathbf{T}^{(i,k)})^{\top} \mathbf{S}^{(i)} \mathbf{T}^{(i,k)} \right\|_{F}^{2}$$

• Extension to  $n \ (n \ge 3)$  networks

$$C(\{G^{(1)}, G^{(2)}, \cdots, G^{(n)}\}) = \sum_{\forall \{G^{(i)}, G^{(j)}, G^{(k)}\} \subset \{G^{(1)}, G^{(2)}, \cdots, G^{(n)}\}} C(\{G^{(i)}, G^{(j)}, G^{(k)}\})$$



#### **UMA – Optimization Problem**

- **Objective:** to minimize the alignment inconsistency and transitivity penalties simultaneously
- Mathematical formulation

 $\bar{\mathbf{T}}^{(i,j)},\bar{\mathbf{T}}^{(j,k)},\bar{\mathbf{T}}^{(k,i)}$ 

$$= \arg \min_{\mathbf{T}^{(i,j)},\mathbf{T}^{(j,k)},\mathbf{T}^{(k,i)}} \left\| (\mathbf{T}^{(i,j)})^{\top} \mathbf{S}^{(i)} \mathbf{T}^{(i,j)} - \mathbf{S}^{(j)} \right\|_{F}^{2}$$

$$+ \left\| (\mathbf{T}^{(j,k)})^{\top} \mathbf{S}^{(j)} \mathbf{T}^{(j,k)} - \mathbf{S}^{(k)} \right\|_{F}^{2} + \left\| (\mathbf{T}^{(k,i)})^{\top} \mathbf{S}^{(k)} \mathbf{T}^{(k,i)} - \mathbf{S}^{(i)} \right\|_{F}^{2}$$

$$+ \alpha \cdot \left\| (\mathbf{T}^{(j,k)})^{\top} (\mathbf{T}^{(i,j)})^{\top} \mathbf{S}^{(i)} \mathbf{T}^{(i,j)} \mathbf{T}^{(j,k)} - \mathbf{T}^{(k,i)} \mathbf{S}^{(i)} (\mathbf{T}^{(k,i)})^{\top} \right\|_{F}^{2}$$

$$T \text{ ansitivity penalties }$$

$$s.t \quad \mathbf{T}^{(i,j)} \in \{0,1\}^{|\mathcal{U}^{(i)}| \times |\mathcal{U}^{(j)}|}, \mathbf{T}^{(j,k)} \in \{0,1\}^{|\mathcal{U}^{(j)}| \times |\mathcal{U}^{(k)}|}$$

$$\mathbf{T}^{(k,i)} \in \{0,1\}^{|\mathcal{U}^{(k)}| \times |\mathcal{U}^{(i)}|}$$

$$\mathbf{T}^{(i,j)} \mathbf{1}^{|\mathcal{U}^{(j)}| \times 1} \preccurlyeq \mathbf{1}^{|\mathcal{U}^{(j)}| \times 1}, (\mathbf{T}^{(j,k)})^{\top} \mathbf{1}^{|\mathcal{U}^{(j)}| \times 1} \preccurlyeq \mathbf{1}^{|\mathcal{U}^{(j)}| \times 1}$$

$$\mathbf{T}^{(i,j)} \mathbf{1}^{|\mathcal{U}^{(k)}| \times 1} \preccurlyeq \mathbf{1}^{|\mathcal{U}^{(j)}| \times 1}, (\mathbf{T}^{(j,k)})^{\top} \mathbf{1}^{|\mathcal{U}^{(j)}| \times 1} \preccurlyeq \mathbf{1}^{|\mathcal{U}^{(k)}| \times 1}$$

$$\mathbf{T}^{(k,i)} \mathbf{1}^{|\mathcal{U}^{(i)}| \times 1} \preccurlyeq \mathbf{1}^{|\mathcal{U}^{(k)}| \times 1}, (\mathbf{T}^{(k,i)})^{\top} \mathbf{1}^{|\mathcal{U}^{(k)}| \times 1} \preccurlyeq \mathbf{1}^{|\mathcal{U}^{(k)}| \times 1}$$

$$\mathbf{T}^{(k,i)} \mathbf{1}^{|\mathcal{U}^{(i)}| \times 1} \preccurlyeq \mathbf{1}^{|\mathcal{U}^{(k)}| \times 1}, (\mathbf{T}^{(k,i)})^{\top} \mathbf{1}^{|\mathcal{U}^{(k)}| \times 1} \preccurlyeq \mathbf{1}^{|\mathcal{U}^{(i)}| \times 1}$$

$$\mathbf{T}^{(k,i)} \mathbf{1}^{|\mathcal{U}^{(k)}| \times 1} \preccurlyeq \mathbf{1}^{|\mathcal{U}^{(k)}| \times 1}, (\mathbf{T}^{(k,i)})^{\top} \mathbf{1}^{|\mathcal{U}^{(k)}| \times 1} \preccurlyeq \mathbf{1}^{|\mathcal{U}^{(i)}| \times 1}$$

$$\mathbf{T}^{(k,i)} \mathbf{1}^{|\mathcal{U}^{(k)}| \times 1} \preccurlyeq \mathbf{1}^{|\mathcal{U}^{(k)}| \times 1}, (\mathbf{T}^{(k,i)})^{\top} \mathbf{1}^{|\mathcal{U}^{(k)}| \times 1} \preccurlyeq \mathbf{1}^{|\mathcal{U}^{(i)}| \times 1}$$

#### **UMA – Transitive Network Matching**

- Goal: to solve for binary variable  $x_{l,m}^{(i,j)}$  indicating whether node  $u_l$  in  $\mathcal{G}^{(i)}$  is aligned with node  $u_m$  in  $\mathcal{G}^{(j)}$
- $\max_{\mathbf{x}^{(i,j)},\mathbf{x}^{(j,k)},\mathbf{x}^{(k,i)}} \sum_{l,m} x_{l,m}^{(i,j)} \mathbf{T}^{(i,j)}(l,m) + \sum_{l,m} x_{l,m}^{(i,j)} \mathbf{T}^{(i,j)}(l,m)$  Optimization problem  $+\sum x_{l,m}^{(i,j)}\mathbf{T}^{(i,j)}(l,m),$ • Select high scores in alignment  $\sum_{l,m} x_{l,m}^{(i,j)} \le 1, \sum_{l,m} x_{l,o}^{(i,k)} \le 1, \forall u_l^{(i)} \in \mathcal{U}^{(i)}$  $u_m^{(j)} \in \mathcal{U}^{(j)}$  $\sum_{i \in \mathcal{U}^{(i)}} x_{m,l}^{(j,i)} \le 1, \sum_{u_o^{(k)} \in \mathcal{U}^{(k)}} x_{m,o}^{(j,k)} \le 1, \forall u_m^{(j)} \in \mathcal{U}^{(j)},$ One-to-one constraint  $u_i^{(i)} \in \mathcal{U}^{(i)}$  $\sum \quad x_{o,l}^{(k,i)} \leq 1, \quad \sum \quad x_{o,m}^{(k,j)} \leq 1, \forall u_o^{(k)} \in \mathcal{U}^{(k)}$  Transitivity constraint  $x_{l,m}^{(i,j)} + x_{m,o}^{(j,k)} + x_{o,l}^{(k,i)} \neq 2, \forall l \in \{1, 2, \cdots, |\mathcal{U}^{(i)}|\},\$  $\forall m \in \{1, 2, \cdots, |\mathcal{U}^{(j)}|\}, \forall o \in \{1, 2, \cdots, \mathcal{U}^{(k)}|,$  $x_{l,m}^{(i,j)} \in \{0,1\}, \forall u_l^{(i)} \in \mathcal{U}^{(i)}, u_m^{(j)} \in \mathcal{U}^{(j)}.$  $x_{m,o}^{(j,k)} \in \{0,1\}, \forall u_m^{(j)} \in \mathcal{U}^{(j)}, u_o^{(k)} \in \mathcal{U}^{(k)}.$  $x_{a,l}^{(k,i)} \in \{0,1\}, \forall u_a^{(k)} \in \mathcal{U}^{(k)}, u_l^{(i)} \in \mathcal{U}^{(i)}.$



#### **UMA – Experimental Results**

- Dataset: Stack Overflow, Super User and Programmers
- Alignment performance



#### **COSNET: Connecting Social Networks** with Local and Global Consistency



- Intuitions: binary classification over node pairs
  - Instances: node pairs  $X = \{x_i\}$
  - Labels:  $Y = \{y_i\}, y_i = 1$  if  $x_i$  refers to same node, otherwise 0
- Factors considered:
  - Node feature consistency (e.g., user profiles)
  - Structural consistency
  - Global consistency (i.e., transitivity constraints)





#### **COSNET – Node Feature Consistency**

- Intuition: to encode the feature similarity for  $x_i$
- Formulation:

$$E_l(Y,X) = \sum_i \mathbf{w}_l^{\mathsf{T}} \mathbf{g}_l(\mathbf{x}_i, y_i)$$

- $\boldsymbol{g}_l(\boldsymbol{x}_i, y_i)$  is a vector-valued feature function
  - Encodes the user profile similarity for node pair  $x_i$
- w<sub>l</sub> is the model parameter





#### **COSNET – Structural Consistency**

- Intuition:
  - If two nodes are aligned, their neighbors are likely to be aligned
- Matching graph  $MG = (V_{MG}, E_{MG})$ 
  - Same as Kronecker product graph
- Pairwise formulation:

$$E_{e}(Y,X) = \sum_{\langle \mathbf{x}_{i},\mathbf{x}_{j} \rangle \in E_{MG}} \mathbf{w}_{e}^{\mathsf{T}} \mathbf{f}_{e}(y_{i},y_{j})$$
$$\mathbf{f}_{e}(y_{i},y_{j}) = \begin{cases} (1,0,0)^{\mathsf{T}} & \text{if } y_{i} = y_{j} = 0\\ (0,1,0)^{\mathsf{T}} & \text{if } y_{i} + y_{j} = 1\\ (0,0,1)^{\mathsf{T}} & \text{if } y_{i} = y_{j} = 1 \end{cases}$$





#### 80

**COSNET – Global Consistency Violation** 

DEFINITION 2 (GLOBAL INCONSISTENCY). Given a set of social networks **G**, a set of user pairs X and the corresponding labels Y, if there exists a sequence of user pairs  $\langle \mathbf{x}_{i_1}, \mathbf{x}_{i_2}, \cdots, \mathbf{x}_{i_n} \rangle$ , such that

$$\forall i = i_1, i_2, \cdots, i_n, y_i = 1$$

and

$$\forall k = 1, 2, \cdots, n-1, \mathcal{V}_{i_k}^2 = \mathcal{V}_{i_{k+1}}^1$$

and

For the pair 
$$\langle \mathcal{V}_{i_n}^2, \mathcal{V}_1^1 \rangle$$
, the corresponding label  $y_j = 0$ 

then we say that the assigned labels Y causes global inconsistency given  $\mathbf{G}$  and X.







#### **COSNET – Global Consistency**

• Triadic closure in the matching graph







#### **COSNET – Model Learning**

• Objective function:

$$E(Y, X) = \sum_{\mathbf{x}_i \in V_{MG}} \mathbf{w}_l^{\mathsf{T}} \mathbf{g}_l(\mathbf{x}_i, y_i) + \sum_{\langle \mathbf{x}_i, \mathbf{x}_j \rangle \in E_{MG}} \mathbf{w}_e^{\mathsf{T}} \mathbf{f}_e(y_i, y_j)$$
$$+ \sum_{c \in T_{MG}} \mathbf{w}_t^{\mathsf{T}} \mathbf{f}_t(Y_c)$$

• Define distance of two matching configurations Y and Y'

$$\Delta(Y,Y') = \sum_{\mathbf{x}_i \in V_{MG}} \delta_l(y_i, y'_i) + \sum_{c \in T_{MG}} \delta_c(Y_c, Y'_c) + \sum_{\langle \mathbf{x}_i, \mathbf{x}_j \rangle \in E_{MG}} \delta_e(\langle y_i, y_j \rangle, \langle y'_i, y'_j \rangle)$$
  
Hamming distance





#### **COSNET – Model Learning**

• By max-margin theory:

$$\begin{split} \min_{W} \frac{1}{2} ||W||^2 + \mu\xi \\ \text{s.t.} \quad E(\hat{Y}, X; W) \leq E(Y, X; W) - \Delta(Y, \hat{Y}) + \xi \end{split}$$

- $\hat{Y}$ , Y: input labeled configuration and learned configuration
- $W = (w_l, w_e, w_t)$ : model parameters
- $\xi$ : slack variable to handle non-separable data
- $\mu$ : trade-off between the maximum margin & error penalty
- Constraint: distance between the energy of  $\hat{Y}$ , Y at least  $\Delta(\hat{Y}, Y)$





#### **COSNET – Model Learning**

- The original problem is intractable.
- Use Lagrangian relaxation for dual decomposition

$$\min_{W,\lambda} \frac{1}{2} ||W||^2 + \mu(E(\hat{Y}, X; W) - \max_{\lambda} L(Y, X, \lambda; W))$$
  
s.t. 
$$\sum_{y_i \in Y_i} \lambda_i^f = 0, \ \forall f \in \mathcal{F}$$

- $f \in \mathcal{F}$ : factor functions
- $\lambda$ : Lagrange multipliers
- Convex and non-differentiable
- Solution: projected sub-gradient method



#### **COSNET – Public Dataset**



Data statistics

Dataset	Network	#Users	#Relationships		
	Twitter	40,171,624	1,468,365,182		
SNS	LiveJournal	3,017,286	87,037,567		
	Flickr	215,495	9,114,557		
	Last.fm	136,420	1,685,524		
	MySpace	854,498	6,489,736		
Academia	LinkedIn	2,985,414	25,965,384		
	ArnetMiner	1,053,188	3,916,907		
	VideoLectures	11,178	786,353		

• Link: <u>https://www.aminer.cn/cosnet</u>



#### **COSNET – Experimental Results**



- Connecting social media sites
  - Twitter, LiveJournal, Last.fm, Flickr, MySpace







#### **COSNET – Experimental Results**

Connecting Aminer with LinkedIn and VideoLectures





#### **Overview of Part I**





#### **Embedding-Based Collective Network Alignment**

 Goal: to learn node embeddings that can infer alignment in the embedding space





#### **Cross-Network Embedding for Multi-Network Alignment**

- Motivations: networks heterogeneity
  - Different networks may own different semantic meanings;
  - Same node may have distinct embeddings in different networks
- Goal: to learn node embeddings for multiple network alignment
- Key question: how to capture the commonness among anchor node counterparts and specific semantics in different networks?



#### **CrossMNA – Cross Network Embedding**

• Key idea: split node embedding into two components

$$\boldsymbol{v}_i^k = \boldsymbol{W}\boldsymbol{u}_i + \boldsymbol{r}^k$$

- Intra-vector  $\boldsymbol{v}_i^k$ : captures structural information in a network
- Inter-vector  $\boldsymbol{u}_i$ : captures the commonness of anchor node
- Network vector  $r^k$ : captures network-specific semantics



Chu, Xiaokai, et al. "Cross-network embedding for multi-network alignment." The World Wide Web Conference. 2019.

#### **CrossMNA – Experimental Results**

• Multiple network alignment



Chu, Xiaokai, et al. "Cross-network embedding for multi-network alignment." The World Wide Web Conference. 2019.

#### **CrossMNA – Experimental Results**

Multiple network link prediction

Dataset	arXiv			SacchCere			Twitter		
	30%	50%	80%	30%	50%	80%	30%	50%	80%
DeepWalk	87.86	94.41	98.12	69.20	73.96	78.29	57.09	59.96	63.74
LINE	75.05	85.73	94.75	60.54	65.05	68.87	53.12	52.97	53.22
node2vec	88.06	94.57	97.11	71.15	76.33	80.16	56.84	61.22	65.93
PMNE	90.12	94.47	95.24	77.61	79.85	81.35	61.12	70.72	75.91
MELL	93.51	96.30	98.84	76.18	79.92	81.21	70.64	75.89	79.84
CrossMNA	96.46	97.53	99.19	76.88	81.12	82.59	75.85	80.48	85.29
							-		

**Observation:** CrossMNA performs better due to transmitting complementary information across networks.



#### **CrossMNA – Experimental Results**

• Scalability: memory usage



**Observation:** CrossMNA has less memory usage than other baseline methods.



Chu, Xiaokai, et al. "Cross-network embedding for multi-network alignment." The World Wide Web Conference. 2019.

#### **Overview of Part I**





#### **Higher-order Network Alignment**

- Higher-order network mining:
  - Involves higher-order structures, instead of edges
- Motivations:
  - Traditional approaches (e.g., NetAlign) aim to maximize # of conserved edges (overlaps/squares).
  - Leverage higher-order structures exist in networks (e.g., motifs, clusters, etc.).
- Single-level: use higher-order structures to align nodes
- Multilevel: to align both nodes and clusters at multi-level



#### **Triangular Alignment (TAME)**

- Network motifs: connected subgraphs that occurs with significantly higher frequency
  - 3<sup>rd</sup>-order: 3-node line, triangle



• *k*<sup>th</sup>-order: k-node star, etc.



• Objective: to maximize # of aligned substructures



#### **TAME – Formulation #1**

Binary quadratic program in NetAlign





#### **TAME – Formulation #2**

- Relaxed formulation
  - Remove one-to-one constraint and relax x to be any reals
  - Add a 2-norm constraint on x to make it bounded

 $\begin{array}{ll} \underset{\boldsymbol{x}}{\text{maximize}} & (\triangle_{H \times G}) \boldsymbol{x}^3 \\ \text{subject to} & \|\boldsymbol{x}\| = 1. \end{array} \longrightarrow \text{Tensor eigenvector problem} \end{array}$ 

- The classic SS-HOPM is costly to solve it.
- Implicit kernel for computing tensor-vector products

$$(\triangle_{H \times G} \boldsymbol{x}^{2})_{ii'} = \sum_{jj',kk'} \triangle_{H \times G}(ii',jj',kk')\boldsymbol{x}(jj')\boldsymbol{x}(kk') \qquad \qquad \triangle_{H \times G} \boldsymbol{x}^{2}(ii') = \sum_{j,j',k,k'} \triangle_{G}(i,j,k) \triangle_{H}(i',j',k')\mathbf{X}(j,j')\mathbf{X}(k,k') \qquad \qquad \triangle_{H \times G} \boldsymbol{x}^{2}(ii') = \sum_{j,j',k,k'} \sum_{j,j',k,k'} \sum_{j'} \mathbf{X}(j,j') \sum_{k'} \triangle_{H}(i',j',k')\mathbf{X}(k,k') \qquad \qquad (j,k) \in \mathcal{N}_{\triangle_{G}}(i)$$



#### **TAME – Algorithm**

- Key ideas:
  - To use implicit tensor-kernel product  $\widetilde{x} = \Delta_{H imes G} x^2$  for

 $\Delta_{H\times G} \boldsymbol{x}^3 = \boldsymbol{x}^T \widetilde{\boldsymbol{x}}$ 

- SS-HOPM main loop computes topological similarity matrices
- A score function to solve a bipartite max-weight matching

To encode integer constraint of X and one-to-one mapping constraint

Algorithm 2 The Triangular AlignMEnt (TAME) algorithm **nput:** Triangle tensors  $\triangle_G, \triangle_H$ ; Sequence similarities w; Shift parameter  $\beta$ **Cutput:** The best topological scores **X** from any iteration k = 0 {Iteration number}  $w \leftarrow w / \|w\|$  $x_0 = w$  $t_0 = 0$ 4: 5: repeat  $\tilde{x}_{k+1} = \operatorname{imp} \overline{\operatorname{TTV}}(\triangle_{C}, \triangle_{H}, x_{k})$  $\lambda_{k+1} = x_k^T \tilde{x}_{k+1}$  $\hat{x}_{k+1} = \tilde{x}_{k+1} + \beta x_k$  $\mathbf{X}_{k+1} = \operatorname{unvec}(x_{k+1})$  $t_{k+1} = \mathbf{score}(\mathbf{X}_{k+1})$ 11: Update  $(\mathbf{X}, t)_{\text{best}}$  to  $(\mathbf{X}, t)_{k+1}$  if  $t_{k+1} > t_{\text{best}}$ 12: k = k + 113: 14: **until**  $\lambda_k - \lambda_{k-1}$  is small or the max iteration is hit 15: return X<sub>best</sub>



#### **TAME – Experimental Results**

• Alignment quality on yeast vs. human dataset





#### **TAME – Experimental Results**

• Metric: # of conserved triangles



**Observation:** TAME ranks the highest in terms of the number of conserved triangles





### Multilevel Network Alignment

- **Goals:** to find node correspondence as well as the correspondence among clusters at different levels
- Motivation:
  - Networks exhibit hierarchical cluster-within-clusters structure



Zhang, Si, et al. "Multilevel network alignment." The World Wide Web Conference. 2019.



#### Moana – Challenges

• C1: Alignment accuracy



- Errors propagate through levels
- C2: Scalability Better than quadratic?

Zhang, Si, et al. "Multilevel network alignment." The World Wide Web Conference. 2019.



#### **Moana – Problem Definition**

- Given:
  - (1) adjacency matrices  $\overline{A}_1$ ,  $\overline{B}_1$  of two undirected networks;
  - (2) a sparse prior alignment preference **H**<sub>1</sub>;
  - (3) the number of levels  $L \ge 2$  of interests.
- Find: a set of alignment matrices  $\boldsymbol{S}_l$  at level-l,  $l = 1, \cdots, L$ 
  - where  $S_1$  indicates the alignment at the node level



Zhang, Si, et al. "Multilevel network alignment." The World Wide Web Conference. 2019.

## Moana Formulation: Multilevel Optimization

- Generic strategy
  - coarsening  $\rightarrow$  alignment  $\rightarrow$  interpolation
- Alignment interpolations
  - Bilinear interpolations by  $\pmb{P}_l\in R^{p_l\times n_1}, \pmb{Q}_l\in R^{q_l\times n_2}$   $(p_l\le n_1,q_l\le n_2)$
  - w.l.o.g.,  $\boldsymbol{S}_1 = \boldsymbol{Q}_1^T \boldsymbol{S}_2 \boldsymbol{P}_1$  between level-1 & level-2

### Moana Formulation: Multilevel Optimization

• Multilevel alignment formulation

Level-1: 
$$\min_{\boldsymbol{s}_1} \alpha \boldsymbol{s}_1^T (\boldsymbol{I} - \boldsymbol{A}_1 \otimes \boldsymbol{B}_1) \boldsymbol{s}_1 + (1 - \alpha) \|\boldsymbol{s}_1 - \boldsymbol{h}_1\|_2^2$$
  
If  $\boldsymbol{P}_1 \boldsymbol{P}_1^T = \boldsymbol{I}$  and  $\boldsymbol{Q}_1 \boldsymbol{Q}_1^T = \boldsymbol{I}$ 

Level-2:  $\min_{s_2} \alpha s_2^T (I - A_2 \otimes B_2) s_2 + (1 - \alpha) \|s_2 - h_2\|_2^2$ 

- $\boldsymbol{A}_2 = \boldsymbol{P}_1 \boldsymbol{A}_1 \boldsymbol{P}_1^T$ ,  $\boldsymbol{B}_2 = \boldsymbol{Q}_1 \boldsymbol{B}_1 \boldsymbol{Q}_1^T$  and  $\boldsymbol{H}_2 = \boldsymbol{Q}_1 \boldsymbol{H}_1 \boldsymbol{P}_1^T$
- same properties (e.g., convexity) and algorithm as FINAL-P
- 'good' (semi-) orthogonal  $P_1$ ,  $Q_1$  make  $A_2$ ,  $B_2$  well-represented

FINAL-P

at node level

# Moana Formulation: Perfect Interpolation

- Denote  $S_l^*$ ,  $S_{l+1}^*$  are optimal solutions at level-l and level-(l+1)
- Perfect interpolation (to address error propagation):

Interpolation from the optimal alignment matrix at level-(l + 1) is equal to that at level-l

- If  $\boldsymbol{P}_l, \boldsymbol{Q}_l \; (l = 1, \cdots, L 1)$  are orthogonal
- Then  $\boldsymbol{S}_l^* = \boldsymbol{Q}_l^T \boldsymbol{S}_{l+1}^* \boldsymbol{P}_l$


#### Moana – Coarsening Algorithm

- Generic strategy
  - Coarsening  $\rightarrow$  alignment  $\rightarrow$  interpolation
- Network coarsening by  $\boldsymbol{P}_l$ ,  $\boldsymbol{Q}_l$ 
  - $\boldsymbol{A}_{l+1} = \boldsymbol{P}_l \boldsymbol{A}_l \boldsymbol{P}_l^T$ ,  $\boldsymbol{B}_{l+1} = \boldsymbol{Q}_l \boldsymbol{B}_l \boldsymbol{Q}_l^T$
- Requirements on  $oldsymbol{P}_l$ ,  $oldsymbol{Q}_l$ 
  - **Perfect interpolation:** they are **orthogonal** matrix
  - Efficient computation: they are sparse matrix
  - Informative coarsening: they can uncover hierarchical cluster-within-clusters structures



#### Moana – Coarsening Algorithm

• Multiresolution matrix factorization



- Coarsening procedure
  - $\boldsymbol{P}_{L-1} \cdots \boldsymbol{P}_2 \boldsymbol{P}_1 \boldsymbol{A}_1 \boldsymbol{P}_1^T \boldsymbol{P}_2^T \cdots \boldsymbol{P}_{L-1}^T = \boldsymbol{A}_L \rightarrow \widetilde{\boldsymbol{A}}_L$
  - $\boldsymbol{Q}_{L-1} \cdots \boldsymbol{Q}_2 \boldsymbol{Q}_1 \boldsymbol{B}_1 \boldsymbol{Q}_1^T \boldsymbol{Q}_2^T \cdots \boldsymbol{Q}_{L-1}^T = \boldsymbol{B}_L \to \widetilde{\boldsymbol{B}}_L$
- $S(S_{B_l}, S_{A_l})$  indicates the alignment among clusters at the *l*-th granularity



Kondor, Risi, Nedelina Teneva, and Vikas Garg. "Multiresolution matrix factorization." *International Conference on Machine Learning*. 2014.

# Moana – Alignment Algorithm

- Generic strategy
  - coarsening  $\rightarrow$  alignment  $\rightarrow$  interpolation
- Alignment across the coarsest networks

$$\widetilde{\boldsymbol{S}}_{L} = \alpha \begin{bmatrix} \widetilde{\boldsymbol{B}}_{L_{1}} & \boldsymbol{0} \\ \boldsymbol{0} & \widetilde{\boldsymbol{B}}_{L_{2}} \end{bmatrix} \begin{bmatrix} \widetilde{\boldsymbol{S}}_{L_{1}} & \widetilde{\boldsymbol{S}}_{L_{2}} \\ \widetilde{\boldsymbol{S}}_{L_{3}} & \widetilde{\boldsymbol{S}}_{L_{4}} \end{bmatrix} \begin{bmatrix} \widetilde{\boldsymbol{A}}_{L_{1}} & \boldsymbol{0} \\ \boldsymbol{0} & \widetilde{\boldsymbol{A}}_{L_{2}} \end{bmatrix} + (1-\alpha) \begin{bmatrix} \widetilde{\boldsymbol{H}}_{L_{1}} & \widetilde{\boldsymbol{H}}_{L_{2}} \\ \widetilde{\boldsymbol{H}}_{L_{3}} & \widetilde{\boldsymbol{H}}_{L_{4}} \end{bmatrix}$$

block-wise computation

$$\widetilde{\boldsymbol{S}}_{L_1} = \alpha \widetilde{\boldsymbol{B}}_{L_1} \widetilde{\boldsymbol{S}}_{L_1} \widetilde{\boldsymbol{A}}_{L_1} + (1-\alpha) \widetilde{\boldsymbol{H}}_{L_1} \\ \widetilde{\boldsymbol{S}}_{L_2} = \alpha \widetilde{\boldsymbol{B}}_{L_1} \widetilde{\boldsymbol{S}}_{L_2} \widetilde{\boldsymbol{A}}_{L_2} + (1-\alpha) \widetilde{\boldsymbol{H}}_{L_2}$$

$$\widetilde{\boldsymbol{S}}_{L_3} = \alpha \widetilde{\boldsymbol{B}}_{L_2} \widetilde{\boldsymbol{S}}_{L_3} \widetilde{\boldsymbol{A}}_{L_1} + (1-\alpha) \widetilde{\boldsymbol{H}}_{L_3}$$
  
$$\widetilde{\boldsymbol{s}}_{L_4} = (1-\alpha) \big( \boldsymbol{I} - \alpha \widetilde{\boldsymbol{A}}_{L_2} \otimes \widetilde{\boldsymbol{B}}_{L_3} \big)^{-1} \widetilde{\boldsymbol{h}}_{L_4}$$

- Alignment at finer levels
  - perfect interpolations:  $\boldsymbol{S}_{l} = \boldsymbol{Q}_{l}^{T} \boldsymbol{S}_{l+1} \boldsymbol{P}_{l}$



 $\tilde{\mathbf{A}}_{L} = \boldsymbol{\Pi}_{A} \begin{bmatrix} \tilde{\mathbf{A}}_{L_{1}} & \mathbf{0} \\ \mathbf{0} & \tilde{\mathbf{A}}_{L_{2}} \end{bmatrix} \boldsymbol{\Pi}_{A}^{T}$  $\tilde{\mathbf{B}}_{L} = \boldsymbol{\Pi}_{B} \begin{bmatrix} \tilde{\mathbf{B}}_{L_{1}} & \mathbf{0} \\ \mathbf{0} & \tilde{\mathbf{B}}_{L_{2}} \end{bmatrix} \boldsymbol{\Pi}_{B}^{T}$ 



#### Moana – Experimental Setups

- Datasets
  - Gr-Qc network vs. its permutation (nodes: 5,241 vs. 5,241)
  - Google+ vs. its permutation (nodes: 23,628 vs. 23,628)
  - Amazon co-purchasing networks (nodes: 74,596 vs. 66,951)
  - ACM vs DBLP coauthor networks (nodes: 9,872 vs. 9,916)







**Observations:** (1) the performance of Moana is close to FINAL-P; (2) Moana outperforms all other methods.

Zhang, Si, et al. "Multilevel network alignment." The World Wide Web Conference. 2019.





**Observation:** Moana achieves a good performance in cluster alignment at different levels.

Zhang, Si, et al. "Multilevel network alignment." The World Wide Web Conference. 2019.







# **Observation:** Moana can unveil meaningful alignment of clusters at different granularities.

Zhang, Si, et al. "Multilevel network alignment." The World Wide Web Conference. 2019.







**Observation:** (1)Moana scales linearly w.r.t. the number of edges; (2)Moana scales linearly w.r.t. the number of nonzero elements in  $H_1$ .

#### **Overview of Part I**





# **Entity Alignment**

- Goal: to link entities among multiple knowledge graphs
- Problem Definition:
  - Given KGs { $KG_i | KG_i = (E_i, R_i, T_i)$ } and seed alignment  $\mathcal{L}$ ;
  - Find all the aligned entities



#### Iterative Entity Alignment via Joint Knowledge Embeddings

- Key components:
  - Knowledge embedding: TransE, PTransE
  - Joint embedding: translation-based, linear transformation
  - Iterative alignment: adding newly aligned entities



Zhu, Hao, et al. "Iterative Entity Alignment via Joint Knowledge Embeddings." IJCAI. Vol. 17. 2017.

### ITransE – Knowledge Embeddings

• TransE: relations as translating vectors



- Loss function:  $L(h, r, t) = \sum_{(h', r', t') \in T^{-}} [\gamma + E(h, r, t) E(h', r', t')]_{+}$
- Negative samples:  $T^- = \{(h', r, t) | h' \in E\} \cup \{(h, r, t') | t' \in E\}$  $\cup \{(h, r', t) | r' \in R\}, (h, r, t) \in T.$
- PTransE: to encode multi-step relation path  $E(p,r) = ||\mathbf{p} \mathbf{r}|| = ||\mathbf{p} (\mathbf{t} \mathbf{h})|| = E(h, p, t)$

located in

# **ITransE – Joint Embeddings**

- Key idea: to join embeddings in a unified space
- Translation-based model:
  - Key idea: view alignment as a special relation
  - Formulation: given  $e_1 \in E_1$ ,  $e_2 \in E_2 \rightarrow e_1 + r^{(E_1 \rightarrow E_2)} \approx e_2$  $E(e_1, e_2) = ||\mathbf{e}_1 + \mathbf{r}^{(E_1 \rightarrow E_2)} - \mathbf{e}_2||$
- Linear transformation model:
  - Key idea: embedding space can be transformed linearly
  - Formulation: transformation matrix  $M^{(E_1 \rightarrow E_2)}$

$$E(e_1, e_2) = ||\mathbf{M}^{(E_1 \to E_2)} \mathbf{e}_1 - \mathbf{e}_2||$$

## **ITransE – Iterative Alignment**

- Key idea: iteratively adding newly aligned entities
- Soft alignment:
  - Reliability scores of newly aligned entities

$$R(e_1, e_2) = \sigma \left( k(\theta - E(e_1, e_2)) \right)$$

• Score function for soft alignment

$$\mathcal{I}_{S} = \sum_{(e_{1}, e_{2}) \in \mathbb{M}} R(e_{1}, e_{2}) (\mathcal{H}_{(e_{1}, e_{2})} + \mathcal{H}_{(e_{2}, e_{1})}),$$
$$\mathcal{H}_{(e_{1}, e_{2})} = \sum_{(e_{1}, r, t)} U(e_{2}, r, t) + \sum_{(h, r, e_{1})} U(h, r, e_{2}),$$

 Limit # of newly aligned entities to a threshold in each alignment procedure

# **ITransE – Experimental Results**

- Dataset: DFB1, DFB2, DFB3 from FB15K
- Entity alignment performance
  - ITransE: iterative alignment w/ TransE
  - IPTransE: iterative alignment w/ PTransE

Matria	DFB-1			DFB-2			DFB-3		
Meure	Hits@1	Hits@10	Mean Rank	Hits@1	Hits@10	Mean Rank	Hits@1	Hits@10	Mean Rank
MTransE (LT)	38.9	61.0	237.7	12.3	33.8	419.2	6.5	22.0	699.8
MTransE (TB)	13.6	35.1	547.7	13.9	35.4	675.7	4.5	16.1	1255.5
TransE + PS	61.9	79.2	105.2	41.1	67.0	154.9	12.2	34.6	431.9
ITransE (HA)	62.6	78.9	100.0	41.2	66.9	151.9	12.3	33.7	432.3
ITransE (SA)	67.1	83.1	80.1	57.7	77.7	109.3	16.2	40.9	367.2
PTransE + PS	65.8	83.4	62.9	46.3	72.1	96.8	15.8	40.2	346.9
IPTransE (HA)	66.1	83.3	59.1	46.2	72.6	94.2	15.1	39.7	337.6
IPTransE (SA)	71.7	86.5	49.0	63.5	82.2	67.5	20.4	47.4	281.0

#### **Observations:**

- IPTransE performs better than ITransE
- Soft alignment performs better than hard alignment

Zhu, Hao, et al. "Iterative Entity Alignment via Joint Knowledge Embeddings." IJCAI. Vol. 17. 2017.

#### **ITransE – Experimental Results**

• Effectiveness of soft alignment strategy



**Observation:** the performance of all methods increase with iterations.

#### Knowledge Graph Alignment via Graph Convolutional Networks

- Key idea: use GCNs to embed entities where aligned entities are expected to be as close as possible.
- Assumptions:
  - Equivalent entities tend to have similar attributes
  - Equivalent entities are neighbored by other equivalent entities
- Embedding framework:

$$\begin{split} & [H_s^{(l+1)}; H_a^{(l+1)}] \\ & = \sigma \left( \hat{D}^{-\frac{1}{2}} \hat{A} \hat{D}^{-\frac{1}{2}} [H_s^{(l)} W_s^{(l)}; H_a^{(l)} W_a^{(l)}] \right) \end{split}$$

Wang, Zhichun, et al. "Cross-lingual knowledge graph alignment via graph convolutional networks." Proceedings of the 2018 Conference on Empirical Methods in Natural Language Processing. 2018.

### **GCN-Align – Construct Adjacency Matrix**

- KGs are relational multi-graphs (i.e., typed relations)
- Key idea: two measures on relations

Relation functionality:  $fun(r) = \frac{\#Head\_Entities\_of\_r}{\#Triples\_of\_r}$ 

Inverse functionality: 
$$ifun(r) = \frac{\#Tail\_Entities\_of\_r}{\#Triples\_of\_r}$$

• Edge weight: influence of *i*-th entity over *j*-th entity

$$a_{ij} = \sum_{\langle e_i, r, e_j \rangle \in G} ifun(r) + \sum_{\langle e_j, r, e_i \rangle \in G} fun(r)$$



Wang, Zhichun, et al. "Cross-lingual knowledge graph alignment via graph convolutional networks." Proceedings of the 2018 Conference on Empirical Methods in Natural Language Processing. 2018.

# **GCN-Align – Alignment Prediction**

- Model training:
  - Margin-based rank loss for both  $h_s$  and  $h_a$
  - **h**<sub>s</sub>: structure embedding
  - **h**<sub>a</sub>: attribute embedding
- Small distance for aligned entities for prediction

$$D(e_{i}, v_{j}) = \beta \frac{\|\boldsymbol{h}_{s}(e_{i}) - \boldsymbol{h}_{s}(v_{j})\|_{1}}{d_{s}} + (1 - \beta) \frac{\|\boldsymbol{h}_{a}(e_{i}) - \boldsymbol{h}_{a}(v_{j})\|_{1}}{d_{a}}$$

- $d_s$ ,  $d_a$ : dimensions of structure and attribute embedding
- $\beta$ : hyperparameter balancing importance of two embeddings
- For each entity  $e_i$ , return a list of candidate entities in KG<sub>2</sub>

Wang, Zhichun, et al. "Cross-lingual knowledge graph alignment via graph convolutional networks." Proceedings of the 2018 Conference on Empirical Methods in Natural Language Processing. 2018.

# **GCN-Align – Experimental Results**

• Datasets: DBP15K from DBpedia with different languages

$DBP15K_{IA-EN}$		$JA \rightarrow EN$			$EN \to JA$			
			Hits@10	Hits@50	Hits@1	Hits@10	Hits@50	
*JE		18.92	39.97	54.24	17.80	38.44	52.48	
*MTransE		27.86	57.45	75.94	23.72	49.92	67.93	
*JAPE	SE w/o neg. SE SE + AE	33.10 34.27 36.25	63.90 66.39 68.50	80.80 83.61 85.35	29.71 31.40 38.37	56.28 60.80 67.27	73.84 78.51 82.65	
JAPE'	SE w/o neg. SE SE + AE	28.90 29.35 31.06	60.61 63.31 64.11	80.03 82.76 81.57	25.34 26.37 32.45	53.36 57.35 62.21	71.94 76.87 79.08	
GCN	SE SE + AE	38.21 <b>39.91</b>	72.49 <b>74.46</b>	82.69 <b>86.10</b>	36.90 <b>38.42</b>	68.50 <b>71.81</b>	79.51 <b>83.72</b>	
DBP15KED EN								
	$15K_{EB-EN}$		$FR \rightarrow EN$	T		$EN \rightarrow FI$	2	
	$15K_{FR-EN}$	Hits@1	$FR \rightarrow EN$ Hits@10	/ Hits@50	Hits@1	$EN \rightarrow FI$ Hits@10	? Hits@50	
DBP	$15K_{FR-EN}$ *JE	Hits@1	$FR \rightarrow EN$ Hits@10 38.84	7 Hits@50 56.50	Hits@1 14.61	$EN \rightarrow FH$ Hits@10 37.25	R Hits@50 54.01	
	$15K_{FR-EN}$ *JE /TransE	Hits@1 15.38 24.41	$FR \rightarrow EN$ Hits@10 38.84 55.55	Hits@50 56.50 74.41	Hits@1 14.61 21.26	$EN \rightarrow FH$ Hits@10 37.25 50.60	R Hits@50 54.01 69.93	
DBP:       *N   *JAPE	$15K_{FR-EN}$ *JE ATransE SE w/o neg. SE SE + AE	Hits@1 15.38 24.41 29.55 29.63 32.39	$FR \rightarrow EN$ Hits@10 38.84 55.55 62.18 64.55 66.68	7 Hits@50 56.50 74.41 79.36 81.90 83.19	Hits@1 14.61 21.26 25.40 26.55 32.97	$EN \rightarrow FF$ Hits@10 37.25 50.60 56.55 60.30 65.91	R         Hits@50         54.01         69.93         74.96         78.71         82.38	
DBP:     *N   *JAPE   JAPE'	$15K_{FR-EN}$ *JE ATransE SE w/o neg. SE + AE SE w/o neg. SE SE + AE SE w/o neg. SE	Hits@1 15.38 24.41 29.55 29.63 32.39 28.23 27.58 30.21	$FR \rightarrow EN$ Hits@10 38.84 55.55 62.18 64.55 66.68 60.99 62.03 65.81	T           Hits@50           56.50           74.41           79.36           81.90           83.19           78.47           79.98           82.57	Hits@1 14.61 21.26 25.40 26.55 32.97 24.68 24.93 31.42	$EN \to FF$ Hits@10 37.25 50.60 56.55 60.30 65.91 55.25 58.95 63.86	R         Hits@50         54.01         69.93         74.96         78.71         82.38         74.19         77.79         80.95	



Wang, Zhichun, et al. "Cross-lingual knowledge graph alignment via graph convolutional networks." Proceedings of the 2018 Conference on Empirical Methods in Natural Language Processing. 2018.

#### **Overview of Part I**





### **Multi-layered Networks**

• An example of multi-layered networks



#### Infrastructure networks

**Biological system networks** 



#### **Cross-Layer Dependency Inference**

- Given: a multi-layered network
  - Layer-layer dependency matrix G;
  - Within-layer connectivity matrices  $\mathcal{A} = \{A_1, \cdots, A_g\}$ ;
  - Observed cross-layer dependency matrices  $\mathcal{D} = \{ \boldsymbol{D}_{ij} \}$
- Find: true cross-layer dependency matrices  $\{\widetilde{\pmb{D}}_{ij}\}$
- To link different types of nodes (alignment links same)



- **A**<sub>1</sub> for chemical network, etc.
- G(1,2) = 1, G(1,3) = 0;
- *D*<sub>12</sub> are represented by solid arrows between *G*<sub>1</sub> and *G*<sub>2</sub>



#### **Fascinate – Formulation**

- Key idea: as a collective collaborative filtering problem
  - Within-layer networks as user-user network, item-item similarity network, etc.
  - Cross-layer dependency as user-item ratings
- Optimization problem:

$$\min_{\mathbf{F}_{i} \geq \mathbf{0}(i=1,...,g)} J = \underbrace{\sum_{i,j: \mathbf{G}(i,j)=1} \|\mathbf{W}_{i,j} \odot (\mathbf{D}_{i,j} - \mathbf{F}_{i}\mathbf{F}_{j}')\|_{F}^{2}}_{\text{C1: Matching Observed Cross-Layer Dependencies}} + \alpha \underbrace{\sum_{i=1}^{g} \text{tr}(\mathbf{F}_{i}'(\mathbf{T}_{i} - \mathbf{A}_{i})\mathbf{F}_{i})}_{\text{C2: Node Homophily}} + \beta \underbrace{\sum_{i=1}^{g} \|\mathbf{F}_{i}\|_{F}^{2}}_{\text{C3: Regularization}}$$

## **Fascinate – Optimization Algorithm**

Block coordinate descent method

0.7

• For each  $F_i$ , use multiplicative update method



### Fascinate – Experimental Setups

• Datasets:

Dataset	# of Layers	# of Nodes	# of Links	# of CrossLinks
SOCIAL	3	125,344	214,181	188,844
BIO	3	35,631	253,827	75,456
INFRA-5	5	349	379	565
INFRA-3	3	15,126	29,861	28,023,500

Abstract dependency structure





# **Fascinate – Experimental Results**

• Effectiveness of dependency inference on BIO

Methods	MAP	R-MPR	HLU	AUC	Prec@10
Fascinate	0.0660	0.2651	8.4556	0.7529	0.0118
Fascinate-Clust	0.0667	0.2462	8.2160	0.7351	0.0108
MulCol	0.0465	0.2450	6.0024	0.7336	0.0087
PairSid	0.0308	0.1729	3.8950	0.6520	0.0062
PairCol	0.0303	0.1586	3.7857	0.6406	0.0056
PairNMF	0.0053	0.0290	0.5541	0.4998	0.0007
PairRec	0.0056	0.0435	0.5775	0.5179	0.0007
FlatNMF	0.0050	0.0125	0.4807	0.5007	0.0007
FlatRec	0.0063	0.1009	0.6276	0.5829	0.0009



## **Fascinate – Experimental Results**

• Effectiveness of dependency inference on INFRA-5

Methods	MAP	R-MPR	HLU	AUC	Prec@10
Fascinate	0.5040	0.3777	67.2231	0.8916	0.2500
FASCINATE-CLUST	0.4297	0.3220	56.8215	0.8159	0.2340
MulCol	0.4523	0.3239	59.8115	0.8329	0.2413
PairSid	0.3948	0.2392	49.5484	0.7413	0.2225
PairCol	0.3682	0.2489	48.5966	0.7406	0.2309
PairNMF	0.1315	0.0464	15.7148	0.5385	0.0711
PairRec	0.0970	0.0099	9.4853	0.5184	0.0399
FlatNMF	0.3212	0.2697	44.4654	0.7622	0.1999
FlatRec	0.1020	0.0778	11.5598	0.5740	0.0488



#### **Overview of Part I**





### **Cross-Network Node Associations**

• Goal: to find node associations across different networks



#### Node Correspondence

#### **Users Purchase Products**



# **Limitations of Traditional Methods**

Linear and/or consistency assumptions



Embedding space disparity issue



#### **Cross-Network Transformation**

- Given: (1) Source and target networks  $G_1 = \{V_1, A_0, X_0\}, G_2 = \{V_2, B_0, Y_0\}$ ; Observed cross-network node associations L
- **Output:** (1) Cross-network transformation function g, s.t.  $g(\mathcal{G}_1) \approx \mathcal{G}_2$ ; (2) Node association function  $g_{node}$



#### **NetTrans – Model Overview**

- Key idea: encoder-decoder architecture
  - Encoder: to coarsen source network at different resolutions
  - Decoder: to reconstruct target network at different resolutions



#### **NetTrans – Encoder**

- Key component: TransPool as a pooling layer
- Supernode selection
  - Self-attention-based pooling



#### **NetTrans – Encoder**

- Supernode representation learning
  - Attention-based message passing
  - Aggregation by node-to-supernode assignment



#### **NetTrans – Encoder**

- Node-to-supernode assignment
  - Gumbel softmax to approximate **P**
  - Supernode candidate pruning


### **NetTrans – Encoder**

- Supernode connections
  - Use auxiliary connections  $\widehat{A}_l$

$$A_l = \frac{1}{2} \left( A_{l-1}(I,I) + \widehat{A}_l \right)$$



### **NetTrans – Decoder**

- Goal: to reconstruct target network
- Key idea: same latent meanings of supernodes
  - Part #1: leverage  $G_1$  by skip connections
  - Part #2: calibrate part #1 from supernodes to nodes



# **NetTrans – Experimental Results**

• Effectiveness of NetTrans for network alignment

	Cora1-Cora2				ACM-DBLI	)	Foursquare-Twitter		
	Hits@10	Hits@30	Accuracy	Hits@10	Hits@30	Accuracy	Hits@10	Hits@30	Accuracy
NetTrans	90.98%	97.51%	89.89%	84.09%	94.52%	58.21%	24.68%	34.58%	9.17%
FINAL-N	88.73%	90.77%	87.58%	82.91%	90.71%	54.39%	24.09%	33.80%	8.47%
FINAL-P	62.28%	80.01%	54.34%	69.70%	83.12%	36.34%	24.09%	33.80%	8.47%
REGAL	60.90%	69.20%	46.26%	63.68%	71.80%	41.78%	0.15%	2.20%	0.11%
IONE	73.03%	79.92%	42.29%	58.93%	84.19%	33.00%	13.44%	28.17%	4.13%
CrossMNA	59.06%	68.62%	33.26%	42.54%	49.69%	21.04%	3.37%	14.79%	2.48%

**Observation:** NetTrans outperforms all other baselines for network alignment task



# **NetTrans – Experimental Results**

• Effectiveness of NetTrans for social recommendation

	Ciao-0.2				Ciao-0.3		Ciao-0.5		
	Prec@10	Rec@10	Rec@50	Prec@10	Rec@10	Rec@50	Prec@10	Rec@10	Rec@50
NetTrans	13.87%	11.08%	29.90%	11.01%	13.23%	28.15%	10.87%	12.43%	39.02%
BPR	1.37%	0.6%	20.25%	1.38%	0.62%	20.18%	1.00%	0.37%	14.97%
wpZAN	11.99%	9.19%	20.77%	9.88%	10.33%	23.22%	9.85%	11.64%	26.04%
GraphRec	8.65%	6.62%	17.56%	8.42%	6.60%	18.07%	6.94%	6.63%	18.08%
SamWalker	4.94%	1.97%	5.98%	4.39%	2.07%	5.67%	2.48%	1.58%	4.05%
NGCF	2.77%	1.21%	3.26%	2.77%	1.48%	3.61%	3.17%	1.99%	4.77%

# **Observation:** NetTrans outperforms all other baselines for recommendation task



# RoadMap



- Motivations and Background
- Part I: Recent Network Alignment Algorithms
- Part II: Network Alignment Applications
- Part III: Future Research Directions



# **Overview of Part II**





# **Social Analysis – User Identity Linkage**

- User Identity Linkage
  - To identify the same physical user across social platforms



• Can be used for de-anonymization, information integration, etc.

# **User Identity Linkage**

- Existing methods:
  - Profile based [Zafarani'13, Zhang'14, Perito'11, Vosecky'09]
  - Network based [Zhou'16, Zhang'15, Liu'16]
  - Profile + network based [Zhang'15, Shen'14, Zhang''16]
- Network-based can be considered as network alignment w/o attributes.
- Profile + network-based methods can be viewed as network alignment w/ attributes.



# **Social Analysis - Recommendation**

- Friend recommendation:
  - For two social networks, if we know
    - User  $u_1$  is a friend of user  $u_2$  in  $\mathcal{G}_1$
    - User v<sub>1</sub> in G<sub>2</sub> and user u<sub>1</sub> in G<sub>1</sub> are same person
    - User  $v_2$  in  $\mathcal{G}_2$  and user  $u_2$  in  $\mathcal{G}_2$  are same person



- But user  $v_1$  and user  $v_2$  are not friend in  $\mathcal{G}_2$
- Then, we can recommend  $v_1$  to user  $v_2$

Yan, Ming, et al. "Friend transfer: Cold-start friend recommendation with cross-platform transfer learning of social knowledge." *2013 IEEE International Conference on Multimedia and Expo (ICME)*. IEEE, 2013. Nelakurthi, Arun Reddy, and Jingrui He. "Finding cut from the same cloth: Cross network link recommendation via 153 joint matrix factorization." Thirty-First AAAI Conference on Artificial Intelligence. 2017.

# **Cross-Site Friend Recommendation**

- Think of it as a cross-site link prediction problem
- Given two incomplete social networks, we jointly solve network alignment and link prediction problems



## **CENALP – Network Embedding**

- DeepWalk-based network embedding
  - Key idea: build a world-view graph

$$\mathbf{W} = \begin{bmatrix} q \cdot \mathbf{P}_{\mathcal{G}} & (1-q) \cdot \mathbf{P}_{\mathcal{G}\mathcal{G}'} \\ (1-q) \cdot \mathbf{P}_{\mathcal{G}'\mathcal{G}} & q \cdot \mathbf{P}_{\mathcal{G}'} \end{bmatrix}$$

- Within-network node sampling with a probability of q, and cross-network sampling with (1 q)
- Allows for cross-network Skip-gram embedding
- Construction of  $P_{\mathcal{G}\mathcal{G}'}$  by structure and attribute

$$dist = \left| \min_{d \in s_k(u)} \log(d+1) - \min_{d \in s_k(u')} \log(d+1) \right| + \\ \left| \max_{d \in s_k(u)} \log(d+1) - \max_{d \in s_k(u')} \log(d+1) \right|.$$

$$sim_{attr}(u, u') = \frac{\mathbf{y}_u^\top \cdot \mathbf{y}_{u'}}{||\mathbf{y}_u||_2 \cdot ||\mathbf{y}_{u'}||_2},$$

#### **CENALP – Network Alignment and Link Prediction**

- Greedy alignment by embedding-based similarity
  - Given embeddings of u, u' in two networks

$$\operatorname{sim}_{\operatorname{emb}}(u, u') = \frac{\mathbf{x}_u^\top \cdot \mathbf{x}_{u'}}{||\mathbf{x}_u||_2 \cdot ||\mathbf{x}_{u'}||_2}$$

Greedy-based alignment objective

 $u^*, u'^* = \underset{u,u'}{\operatorname{arg\,max}} \quad \operatorname{sim}_{\operatorname{emb}}(u, u')$ 

• Embedding for link prediction



$$\begin{aligned} \operatorname{layer}_{0}(\mathcal{I}) &= \operatorname{concatenate}_{\substack{\mathbf{x}_{u}, \, \mathbf{x}_{v} \,\in \, \mathcal{X}(\mathcal{I}) \\ \mathbf{x}_{u} \,\neq \, \mathbf{x}_{v}}} (\mathbf{x}_{u} \circ \mathbf{x}_{v}), \\ \operatorname{layer}_{1}(\mathcal{I}; w, b) &= w \cdot \operatorname{layer}_{0}(\mathcal{I}) + b \triangleq \hat{w} \cdot \operatorname{layer}_{0}(\mathcal{I}), \\ \operatorname{layer}_{2}(\mathcal{I}; \hat{w}) &= \sigma \left[ \operatorname{layer}_{1}(\mathcal{I}; \hat{w}) \right] = \frac{1}{1 + e^{-\operatorname{layer}_{1}(\mathcal{I}; \hat{w})}}, \end{aligned}$$

# **CENALP – Algorithm**

Objective function



# **CENALP – Experimental Results**

• AUC score of link prediction

Dataset	Mathad	Training rate.									
Dataset	Method	95%	90%	85%	80%	75%	70%	65%	60%	55%	50%
	JC [11]	92.28%	90.93%	90.37%	88.44%	85.43%	84.12%	80.51%	77.99%	74.81%	72.16%
	AA [12]	92.33%	91.01%	90.30%	88.32%	85.44%	84.07%	80.48%	77.94%	74.82%	72.14%
	SC [13]	78.84%	78.89%	78.68%	78.54%	74.72%	77.21%	76.83%	75.87%	73.91%	74.40%
DBLP	n2v [22]	78.40%	81.34%	78.72%	78.32%	75.01%	74.30%	73.32%	71.60%	70.56%	68.61%
\$	n2v+LR	95.58%	95.44%	94.30%	94.30%	92.37%	93.07%	90.86%	90.80%	89.25%	88.08%
disturbed copy	CLF [8]	96.92%	96.55%	95.70%	95.69%	94.43%	94.28%	92.95%	92.93%	92.23%	90.68%
	MNN [43]	98.13%	97.76%	97.57%	97.28%	97.10%	96.78%	96.38%	96.44%	96.03%	95.86%
	CE-CLF	98.37%	98.29%	97.88%	97.80%	97.34%	96.74%	96.75%	96.36%	96.09%	95.86%
	CELP	98.48%	98.39%	98.36%	98.57%	98.28%	98.49%	98.58%	98.31%	98.38%	98.27%
	CENALP	99.65%	<b>99.27%</b>	99.35%	99.38%	<b>99.36%</b>	99.08%	99.01%	<b>99.29%</b>	99.25%	99.06%
	JC [11]	74.76%	77.89%	76.94%	75.64%	73.15%	72.63%	70.48%	68.90%	67.25%	65.12%
	AA [12]	74.77%	77.54%	76.57%	75.76%	73.36%	72.68%	71.09%	68.84%	67.19%	65.18%
	SC [13]	84.39%	83.39%	86.88%	84.53%	83.83%	83.79%	81.56%	80.80%	81.81%	77.61%
Facebook	n2v [22]	75.62%	78.94%	78.23%	79.36%	76.18%	75.25%	74.64%	74.86%	74.49%	71.16%
\$	n2v+LR	82.20%	85.58%	83.04%	84.51%	81.64%	82.07%	81.17%	81.02%	80.08%	78.04%
Twitter	CLF [8]	84.88%	85.02%	86.18%	86.70%	84.00%	83.99%	82.95%	82.43%	81.96%	80.75%
	MNN [43]	95.72%	96.44%	96.28%	96.30%	96.21%	96.25%	96.07%	95.88%	95.47%	95.23%
	CE-CLF	96.52%	96.84%	96.37%	96.34%	96.30%	95.69%	94.92%	94.31%	93.11%	92.00%
	CELP	97.29%	97.52%	97.46%	97.85%	<b>97.99%</b>	97.56%	97.23%	97.15%	96.66%	96.14%
	CENALP	97.31%	<b>97.77%</b>	97.51%	97.24%	97.60%	97.86%	97.34%	96.47%	96.74%	96.16%



# **Social Analysis - Recommendation**

- Cross-site product recommendation:
  - Intuition: if users are aligned, purchase histories can be combined for better recommendation
  - Key idea: leverage cross-site actions to improve user modeling
  - Benefits: may mitigate issues, e.g., cold start, etc.





# JUMA – Approach

- Key idea: use a probabilistic graphical model for joint user modeling over aligned sites
  - User's site-specific preference  $P_i^q$  is transferred from universal preference  $U_i$  by transferring model  $T^q$ .
  - User conducts actions  $A_i^q$ based on  $P_i^q$  and site-specific item models  $\{\phi_k^q\}$ .





# JUMA – Approach

- Joint user modeling over aligned sites
  - For item-based site (Douban), use matrix factorization method.
  - For text-based site (Weibo), use Latent Dirichlet Allocation (LDA) to model topic distributions for microblogs.





### **JUMA – Experimental Results**

• Effectiveness of recommendation

TARGET	ALGS	AUC SCORE, VARYING TRAINING INFORMATION RATIO								
IARGET		0.4	0.5	0.6	0.7	0.8	0.9			
	LDA	$0.6514 \pm 0.0017$	$0.6605 \pm 0.0015$	$0.6694 \pm 0.0016$	$0.6769 \pm 0.0018$	$0.6839 \pm 0.0015$	$0.6928 \pm 0.0014$			
Text-Based (Weibo)	JUMA	$0.6824 \pm 0.0014$	$0.6892 \pm 0.0016$	$0.6976 \pm 0.0014$	$0.7058 \pm 0.0017$	$0.7120 \pm 0.0012$	$0.7194 \pm 0.0013$			
	CTR	$0.7021 \pm 0.0021$	$0.7133 \pm 0.0017$	$0.7262 \pm 0.0018$	$0.7352 \pm 0.0017$	$0.7432 \pm 0.0016$	$0.7532 \pm 0.0015$			
	JUMA <sup>+</sup>	$0.7338 \pm 0.0017$	$0.7420 \pm 0.0015$	$0.7502 \pm 0.0018$	$0.7592 \pm 0.0015$	$0.7670 \pm 0.0015$	$0.7743 \pm 0.0014$			
	PMF	$0.7275 \pm 0.0016$	$0.7323 \pm 0.0013$	$0.7384 \pm 0.0015$	$0.7428 \pm 0.0016$	$0.7485 \pm 0.0014$	$0.7521 \pm 0.0013$			
Item-Based (Douban)	SVD++	$0.7856 \pm 0.0012$	$0.7929 \pm 0.0010$	$0.7986 \pm 0.0016$	$0.8055 \pm 0.0012$	$0.8089 \pm 0.0013$	$0.8112 \pm 0.0011$			
	TMF	$0.7872 \pm 0.0015$	$0.7946 \pm 0.0012$	$0.8001 \pm 0.0013$	$0.8071 \pm 0.0019$	$0.8102 \pm 0.0014$	$0.8132 \pm 0.0012$			
	mmTM	$0.6929 \pm 0.0019$	$0.6940 \pm 0.0011$	$0.6943 \pm 0.0012$	$0.6963 \pm 0.0015$	$0.7034 \pm 0.0010$	$0.7064 \pm 0.0018$			
	JUMA	$0.8127 \pm 0.0017$	$0.8172 \pm 0.0016$	$0.8219 \pm 0.0013$	$0.8235 \pm 0.0011$	$0.8243 \pm 0.0015$	$0.8259 \pm 0.0013$			

**Observation:** JUMA performs best for both textbased site Weibo and item-based site Douban.



### **JUMA – Experimental Results**

• Effectiveness of addressing cold-start



# **Observation:** Improvements are higher when dealing with cold users than non-cold users.



# **Social Analysis – Information Diffusion**

- Motivations
  - Users can post messages in multiple platforms;
  - Information thus propagates within-network and across networks.





## M&M – Approach

- Goal: multi-aligned multi-relational network influence maximizer
- Key idea: to extends traditional linear threshold to depict diffusion across networks
- Activation probability functions:
  - For intra-network relation *i*

$$g_{v,i}^{(1)}(t+1) = \frac{\sum_{u \in \Gamma_{in}(v,i)} \phi_{(u,v)}^{i} \varphi(u,t)}{\sum_{u \in \Gamma_{in}(v,i)} \phi_{(u,v)}^{i}}$$

• For inter-network relation *j* 

$$h_{v,j}^{(1)}(t+1) = \frac{\sum_{u \in \Gamma_{in}(v,j)} \phi_{(u,v)}^{j} \varphi(u,t)}{\sum_{u \in \Gamma_{in}(v,j)} \phi_{(u,v)}^{j}}$$



Zhan, Qianyi, et al. "Influence maximization across partially aligned heterogenous social networks." Pacific-Asia Conference on Knowledge Discovery and Data Mining. Springer, Cham, 2015.

### **M&M – Experimental Results**

- Effectiveness of influence maximization
- Metric: # of activated users by the seed users





Zhan, Qianyi, et al. "Influence maximization across partially aligned heterogenous social networks." Pacific-Asia Conference on Knowledge Discovery and Data Mining. Springer, Cham, 2015.

## **Overview of Part II**





# **Bioinformatics – Knowledge Transfer**

- Motivations:
  - Traditional methods are based on sequence alignment
  - Network data and sequence data provide complementary insights
  - Restricting to sequences may limit knowledge transfer
- Network alignment to identify functional orthologs
  - Benefits: insightful for knowledge of aging and other biological processes.



Faisal, Fazle E., et al. "The post-genomic era of biological network alignment." EURASIP Journal on Bioinformatics and Systems Biology 2015.1 (2015): 3.

### **Knowledge Transfer – Evolutionary Relationships Discovery**

- Goal: using network alignment to guide biological knowledge transfer
  - From well-studied species to less well-studied species
- Methods:
  - GRAAL and H-GRAAL: focused on phylogenetic tree inference based on metabolic networks
  - MI-GRAAL:
    - Used these PPI network data to infer evolutionary relationships
    - Considered five herpesviruses based on their network similarities.



### Knowledge Transfer – Human Aging Discovery

- Motivations:
  - Susceptibility to diseases increases with age
  - Important to study molecular mechanisms behind aging and aging-associated diseases
- Traditional methods:
  - Transferring knowledge from well-studied species to human between conserved sequence regions
- Network alignment-based methods:
  - MI-GRAAL and IsoRankN: align well known aging-related network parts of one species to known aging-related network parts of other species



Faisal, Fazle E., et al. "The post-genomic era of biological network alignment." EURASIP Journal on Bioinformatics and Systems Biology 2015.1 (2015): 3.

## **Overview of Part II**





# **Knowledge Completion**

- Goal: to complete a triple (*h*, *r*, *t*) when one of *h*, *r*, *t* is missing
- Application scenario by entity alignment:
  - Two sets of triplets (i.e., KGs) for training
  - One set of triplets for testing
  - Two training KGs can be aligned
- Methods:
  - Basically can be any KG alignment methods
  - ITransE/IPTransE for example

## **ITransE – Experimental Results**

• Effectiveness of ITransE for knowledge completion

		Entity P	rediction	Relation Prediction				
Metric	Mean Rank		Hits@10		Mean	Rank	Hits@1	
	Raw	Filter	Raw	Filter	Raw	Filter	Raw	Filter
MTransE (LT)	240.8	131.3	36.4	47.3	37.2	36.9	48.3	56.9
MTransE (TB)	851.3	759.7	9.4	10.8	293.7	293.4	27.4	27.7
TransE	246.1	131.6	42.5	54.3	55.9	55.6	44.2	50.7
TransE + Aux	232.8	121.5	43.3	54.9	50.1	49.8	44.4	50.9
ITransE (SA)	209.2	101.0	44.2	55.1	19.8	19.6	54.2	60.7
PTransE	213.0	97.2	50.9	72.1	2.33	1.96	67.4	86.9
PTransE + Aux	206.3	80.4	52.7	80.7	2.34	1.93	<b>68.8</b>	90.5
IPTransE (SA)	197.5	70.6	53.0	80.8	2.03	1.62	68.6	90.8

**Observation:** By successfully leveraging the auxiliary information (i.e., second KG by alignment), ITransE and IPTransE perform better than other baseline methods.



Zhu, Hao, et al. "Iterative Entity Alignment via Joint Knowledge Embeddings." IJCAI. Vol. 17. 2017.

## **Overview of Part II**





# **Security – Modeling Adversarial Activities**

- Background:
  - Networks are natural structure to model adversarial activities
    - Smuggling
    - Illegal arm dealing
    - Illicit drug production
  - But such activities are often embedded in different domains





Xu, Jiejun, et al. "GTA3 2018: Workshop on Graph Techniques for Adversarial Activity Analytics." Proceedings of the Eleventh ACM International Conference on Web Search and Data Mining. 2018.

# MAA – Challenges

- Domain heterogeneity
  - Communication networks
    - Phone call, emails, text, etc.
  - People who call each other may unlikely text often
  - Similarly, email network is structurally distinct from phone call network
- Spatial-temporal challenge
  - Relations contain much spatial-temporal information
    - Who calls whom at which location and at what time
- Very large-scale networks



# MAA – Approaches

- Any scalable network alignment methods
  - w/o attribute: only based on connections
  - w/ attribute: view spatial-temporal information as attributes
- Encode temporal information:
  - Count # of connections in certain time window
  - Values at all time windows form node attributes
  - Can be used as attribute-based prior similarity matrix
  - And/or as the attributes in attributed alignment methods (e.g., FINAL)



# RoadMap



- Motivations and Background
- Part I: Recent Network Alignment Algorithms
- Part II: Network Alignment Applications
- Part III: Future Research Directions

# **Big Network Alignment – 4Vs**

• 4V characteristics also hold for networks





# **Big Network Alignment – Volume**

- Real-world networks are very large-scale
  - Facebook, Instagram, Twitter have billions of users
- Challenge: most of existing methods have at least  $O(n^2)$  complexity
  - Some recent consistency-based and embedding-based methods reduce the complexity to linear
  - Complexity may be even larger if we handle multiple networks collectively
- **Question:** how to efficiently do network alignment?
- **Possible directions:** (1) leverage approximation techniques, (2) parallelizable algorithm


## **Big Network Alignment – Variety**

- Real-world networks have rich information
  - Node/edge attributes, text descriptions, temporal information
- Methods exist to handle attribute information
  - But few can handle temporal relation information
  - Who called whom at what time, etc.
- **Question:** how to better incorporate side-information into network alignment?
- **Possible directions:** heterogeneous network alignment, temporal network alignment, etc.



# **Big Network Alignment – Variety**

- Network heterogeneity
  - Networks to be aligned carry different types of information
  - Even same user may behave differently in different networks
- Existing methods explicitly or implicitly build upon consistency assumptions
  - But network heterogeneity may easily violate this assumption

#### • Questions:

- How to align different types of networks (e.g., LinkedIn vs. FB)?
- How to adaptively control consistency assumption?
- Possible directions: Deep learning methods that are highly learnable.

# **Big Network Alignment – Velocity**

- Networks are dynamically changing over time.
- Dynamic network alignment
  - Simple solution: run from scratch at each timestamp
  - Limitation: time consuming; can't capture dynamics

### Questions:

- How to efficiently handle alignment over dynamic networks?
- How to leverage the dynamics (e.g., smoothness)?
- Possible directions:
  - Matrix approximation to avoid unnecessary re-computations.
  - Dynamic network embedding-based alignment methods.



# **Big Network Alignment – Veracity**

- Real-world networks are often noisy and incomplete.
  - Missing connections
  - Missing nodes
  - Missing attribute information
- Existing methods:
  - Jointly solve network alignment and link prediction
  - Benefit: if handled properly, they mutually benefit each other
- Challenge: error propagation
  - If alignment or imputed edges are not correct, the performance will be hurt.



### **Adversarial Network Alignment**

- Improve the alignment effectiveness and robustness
- Noise/adversarial attacks can mislead alignment





## **Adversarial Network Alignment**

### • Background:

- Existing adversarial attacks on network alignment are based on derivative-based importance score
- But no work exits on adversarial defense

### Challenge:

 Compared to adversarial attack/defense in single network, multiple networks may further complicate the defense process.

#### Possible direction:

 Graph neural network-based adversarial learning on network alignment



## **Integrated Network Alignment**

- Explainable network alignment
  - Background: there exist explainable network mining tasks
    - Network embedding
    - Graph neural networks
    - Ranking, clustering, etc.
  - Problem goal:
    - Explain why two nodes should be aligned or not
  - Possible directions:
    - Extend explainable network embedding to embeddingbased network alignment



## **Integrated Network Alignment**

- Fair network alignment
  - Background:
    - Fairness has been studied recently in many machine learning and data mining tasks
    - Fairness in graphs has attracted attentions very recently, but for single network
  - Problem goal:
    - To debias the network alignment
  - Possible direction:
    - Extend fairness in single network mining to multiple networks first, then combine the specific objective of network alignment



### Summary

- Background and motivation
  - Network alignment aims to find node correspondence across networks
  - A key step to many mining tasks across multiple networks
- Recent network alignment algorithms
  - Pairwise network alignment
  - Collective network alignment
  - Higher-order network alignment
  - Other related tasks
- Network alignment applications
- Future directions



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