

# High-order Joint Embedding for Multi-Level Link Prediction

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\*This is a joint work with Yubai Yuan (Penn State)

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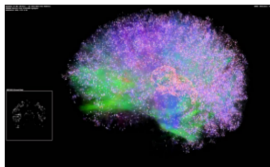


# Network Data

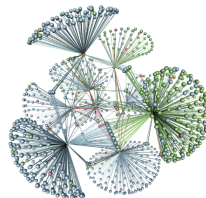
social networks



brain networks



HIV protein interaction networks



- Traditional network data: collection of two-way relation
  - ▶ interactions between a pair of nodes
  - ▶ two-way relations are **independent** to each other
  - ▶ Real world complex network: multi-way (subgroup) interaction

# Motivation: Ego Network in Social Media

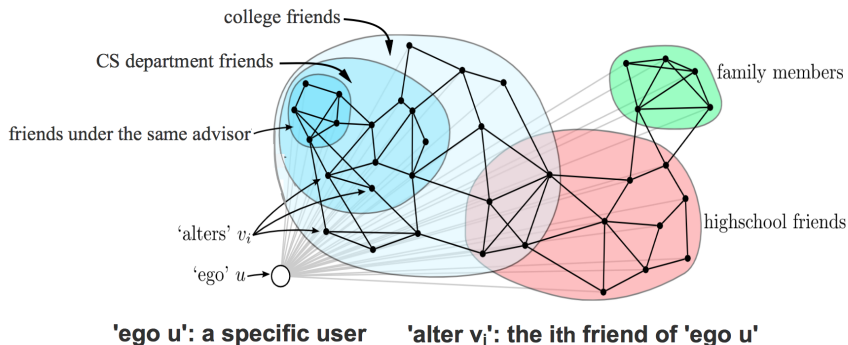


Fig. 1: Facebook Ego-network, adapted from McAuley and Leskovec (2012)

- Two-way relations: friendships among people
- **Social circles**: multi-way relations among people

# Network Beyond Two-way Relation

- **Multi-way relations:** protein complex, social circle, authorship, ...
  - ▶ relations among a group of nodes
  - ▶ capture **higher-order** interactions among nodes
  - ▶ subgroup information in network
- Two-way and multi-way relations **coexist** among the same set of nodes

# Model Multi-Way Relations as Hyperlink

- **Hyperlink:** **links to connect** nodes in a subgroup
- *M*-**order hyperlink:** links connecting *M* nodes

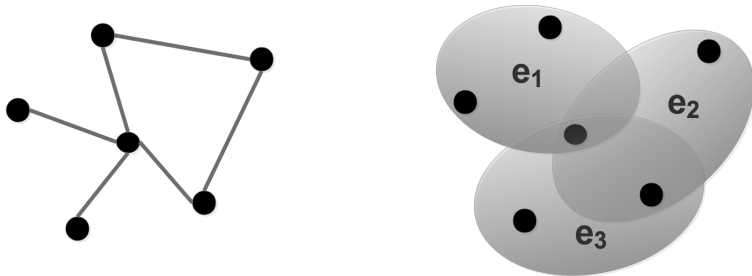


Fig. 2: Left: pairwise links; Right: three 3-order hyperlinks

- A pairwise link is a special case: 2-order hyperlink

# Hyperlink Encodes Subgroup Similarity

- Capture nodes' similarity at different levels
- Pairwise link:
  - ▶ common features shared by **two nodes** only
- Hyperlink:
  - ▶ common features shared by **all nodes** in a subgroup

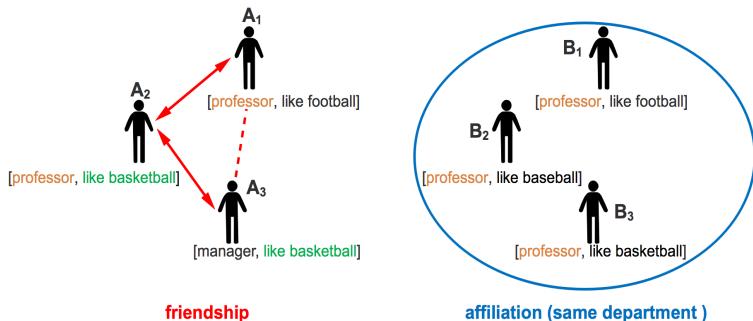
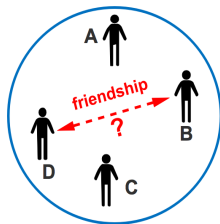


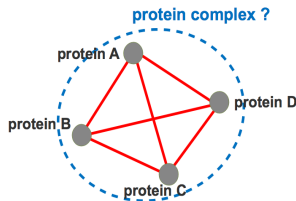
Fig. 3: Differences between pairwise similarity and subgroup similarity

# Dependency among Pairwise Links and Hyperlinks

- Dependency between pairwise links and hyperlinks
  - ▶ sharing the same set of nodes
  - ▶ high-order relations arise from specific connection patterns
- Incorporate mutual information



observe {A, B, C, D} in the  
same department



observe pairwise interaction clique  
among protein {A, B, C, D}

Fig. 4: B and D are more likely to be friends or enemies given that they are **in the same department**; protein A, B, C, and D are more likely to form a protein complex given that they are **pairwisely interacted with each other**



# Goal: Link Prediction

- Informal scoring methods (Adamic and Adar, 2003; Katz, 1953; Kossinet, 2006)
- Exponential-family random graph models (Holland and Leinhardt, 1981; Hunter et al., 2012)
- Latent variable models (Hoff et al., 2002; Handcock et al., 2007; Kim et al., 2018)
- Embedding-based methods:
  - ▶ matrix factorization (Ahmed et al., 2013; Cao et al., 2015)
  - ▶ random walk (Grover and Leskovec, 2016; Perozzi et al., 2014)
  - ▶ graph neural networks (Scarselli et al., 2009)
- **Our goals**
  - ▶ **Predict pairwise links and hyperlinks jointly**
  - ▶ **Borrow information between pairwise links and hyperlinks**

# Network Embedding

- **Embedding**: map nodes into latent factors  $\mathbf{Z}_i \in R^r$ ,  $\mathbf{Z} = \{\mathbf{Z}_i\}_{i=1}^N$
- $\mathbf{Z}_{ir}$  represents **hidden features** for node  $i$

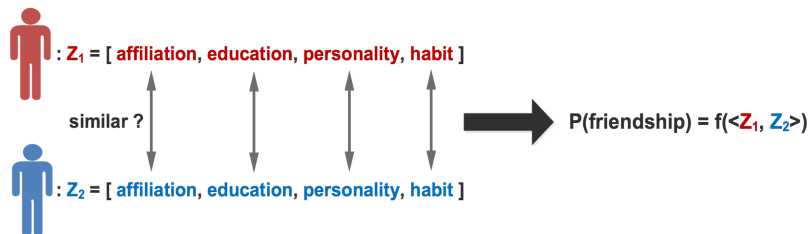


Fig. 5: The probability of potential link depends on the concordance via inner product between latent factors  $\mathbf{Z}_1$ ,  $\mathbf{Z}_2$ , and  $f(\cdot)$  is a link function.

- **Measure concordance among nodes**: transform a binary link to a continuous probability

# Proposed Embedding Framework

- Observed data:
  - ▶  $\mathcal{V}$ : a set of nodes  $\{v_i\}_{i=1}^N$
  - ▶  $\Omega_{\mathbf{A}}$ : a set of pairwise links and non-links on  $\mathcal{V}$
  - ▶  $\Omega_{\mathcal{A}}$ : a set of hyperlinks and non-hyperlinks on  $\mathcal{V}$
  - ▶  $|\Omega_{\mathbf{A}}|$ ,  $|\Omega_{\mathcal{A}}|$ : cardinality of  $\Omega_{\mathbf{A}}$  and  $\Omega_{\mathcal{A}}$
- Obtain latent factors  $\mathbf{Z} = \operatorname{argmin}_{\mathbf{Z}} \operatorname{Loss}(\mathbf{Z}; \Omega_{\mathbf{A}}, \Omega_{\mathcal{A}})$

$$\operatorname{Loss}(\mathbf{Z}; \Omega_{\mathbf{A}}, \Omega_{\mathcal{A}}) = \textcolor{blue}{\operatorname{Loss}_{\text{pair}}}(\mathbf{Z}; \Omega_{\mathbf{A}}) + \textcolor{red}{\operatorname{Loss}_{\text{hyper}}}(\mathbf{Z}; \Omega_{\mathcal{A}}) + \lambda \operatorname{Penalty}(\mathbf{Z})$$

- $\textcolor{blue}{\operatorname{Loss}_{\text{pair}}}$ : mismatch between observed and predicted pairwise links
- $\textcolor{red}{\operatorname{Loss}_{\text{hyper}}}$ : mismatch between observed and predicted hyperlinks
- $\operatorname{Penalty}$ : regularizations to filter out spurious links
- Integrate different-order moment information of  $\mathbf{Z}$

# Encode Pairwise Links

- Pairwise link network  $\Rightarrow$  **adjacent matrix**  $A = \{-1, 0, 1\}^{N^2}$

$$A_{ij} = A_{ji} = \begin{cases} 1, & i \text{ and } j \text{ are connected} \\ 0, & i \text{ and } j \text{ are not connected} \\ -1, & \text{not observed} \end{cases}$$

- Minimize  $Loss_{pair}(\mathbf{Z})$  by encouraging **concordance between embeddings** of connected nodes:

$$Loss_{pair}(\mathbf{Z}) = \frac{1}{|\Omega_{\mathbf{A}}|} \sum_{A_{ij} \in \Omega_{\mathbf{A}}} \left( \underbrace{A_{ij}}_{\text{observed}} - \underbrace{f[\mathbf{z}_i^T \mathbf{z}_j]}_{P(A_{ij}=1)} \right)^2$$

where  $f(\cdot)$  is a link function, such as logit

- If  $v_i$  and  $v_j$  are connected  $\iff$  a larger  $\mathbf{z}_i^T \mathbf{z}_j$
- Preserve observed **pairwise similarity** in latent space

$$(*\Omega_{\mathbf{A}} = \{A_{ij} | A_{ij} \in \{0, 1\}\})$$

# Tensor Modeling for Hyperlink Network

- A  $m$ -order tensor representation  $\mathcal{A} = \{-1, 0, 1\}^{N^m}$ :

$$\mathcal{A}_{i_1 \dots i_m} = \begin{cases} 1, \text{hyperlink among } \{i_1, \dots, i_m\} \\ 0, \text{non-hyperlink among } \{i_1, \dots, i_m\} \\ -1, \text{not observed} \end{cases}$$

- No order among nodes in hyperlink:  $\mathcal{A}$  is **supersymmetric**

$$\mathcal{A}_{i_1 \dots i_m} = \{\mathcal{A}_{\sigma(i_1) \dots \sigma(i_m)} | \sigma(\cdot) \text{ is any index permutation}\}$$

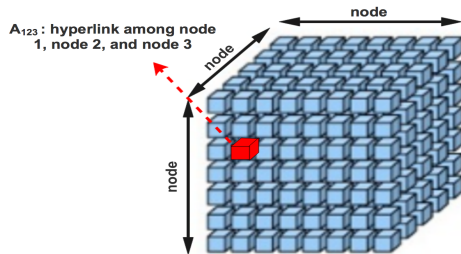


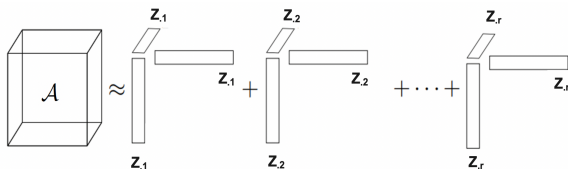
Fig. 6: A 3-uniform hypergraph formulates as a third-order tensor.

# Tensor Decomposition

- CANDECOMP/PARAFAC decomposition (Hitchcock, 1927):

$$\mathcal{A} = \sum_{k=1}^r \underbrace{\mathbf{Z}_{\cdot k} \circ \mathbf{Z}_{\cdot k} \cdots \circ \mathbf{Z}_{\cdot k}}_m,$$
$$\implies \mathcal{A}_{i_1 i_2 \dots i_m} = \sum_{k=1}^r Z_{i_1 k} \times Z_{i_2 k} \times \cdots \times Z_{i_m k},$$

where  $\mathbf{Z}_{\cdot k} (k = 1, \dots, r)$  are  $N$ -dimensional vectors,  $\circ$  is the outer product, and  $r$  is the rank of tensor



- Need to incorporate dependency between pairwise links and hyperlinks

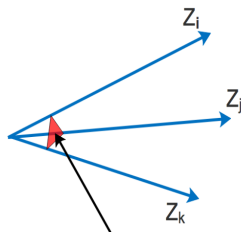


# High-Order Concordance Modeling

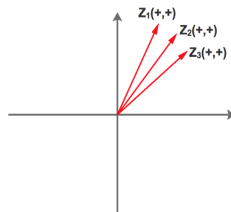
$$P_Z(\mathcal{A}_{i_1 i_2 \dots i_m} = 1) = f \left( \begin{array}{c} \text{pairwise concordance} \\ \text{on } \{Z_{i_1}, \dots, Z_{i_m}\} \end{array} + \begin{array}{c} \text{high-order concordance} \\ \text{on } \{Z_{i_1}, \dots, Z_{i_m}\} \end{array} \right)$$

$$\text{m-order concordance} = \sum_{k=1}^r \psi_k |Z_{i_1 k} \times Z_{i_2 k} \times \dots \times Z_{i_m k}|,$$

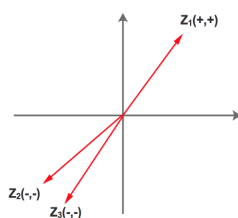
$$\psi_k = \begin{cases} 1, & \text{signs of } Z_{i_1 k}, Z_{i_2 k}, \dots, Z_{i_m k} \text{ are the same} \\ -1, & \text{otherwise} \end{cases}$$



high-order concordance among  $Z_i$ ,  $Z_j$ , and  $Z_k$



3-order concordance  $> 0$



3-order concordance  $< 0$

- $\psi_k$  captures the common latent features

(\*| · | is absolute value)

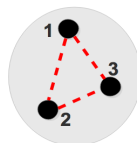
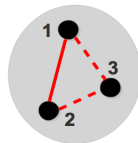
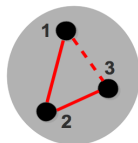
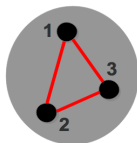


# Dependency between Pairwise Link and Hyperlink

$$P_Z(\mathcal{A}_{i_1 i_2 \dots i_m} = 1) = f \left( \underbrace{\sum_{(i,j) \in \{i_1 i_2 \dots i_m\}} Z_i^T Z_j}_{\text{pairwise concordance on } \{Z_{i_1}, \dots, Z_{i_m}\}} + \text{high-order concordance on } \{Z_{i_1}, \dots, Z_{i_m}\} \right)$$

- Density of **pairwise connections** within  $\{Z_{i_1}, \dots, Z_{i_m}\}$
- Model **dependency** between pairwise link and hyperlink

— linked      - - - not linked



$$P(A_{123}=1 | \text{Diagram 1}) > P(A_{123}=1 | \text{Diagram 2}) > P(A_{123}=1 | \text{Diagram 3}) > P(A_{123}=1 | \text{Diagram 4})$$

# Embed Hyperlinks

- Represent observed hyperlink statuses on latent space by minimizing

$$Loss_{hyper}(\mathbf{Z}; \Omega_{\mathcal{A}}) = \frac{1}{|\Omega_{\mathcal{A}}|} \sum_{(i_1 i_2 \dots i_m) \in \Omega_{\mathcal{A}}} \left\{ \underbrace{\mathcal{A}_{i_1 i_2 \dots i_m}}_{\text{observed}} - \underbrace{\mathbf{P}_{\mathbf{Z}}(\mathcal{A}_{i_1 i_2 \dots i_m} = 1)}_{\text{predicted prob.}} \right\}^2$$

- If  $\mathcal{A}_{i_1 i_2 \dots i_m} = 1$ , encourage large concordance among  $\{\mathbf{Z}_{i_1}, \mathbf{Z}_{i_2} \dots \mathbf{Z}_{i_m}\}$
- Size of subgroup  $\mathbf{m}$ : features shared by all  $\mathbf{m}$  nodes
- Decompose hyperlink tensor  $\{\mathbf{P}(\mathcal{A}_{i_1 i_2 \dots i_m} = 1)\}$  on  $\mathbf{Z}$

# Predict Hyperlinks and Pairwise Links

- Obtain embedding representation of nodes via  $\hat{\mathbf{Z}}$ :

$$\hat{\mathbf{Z}} = \operatorname{argmin}_{\mathbf{Z}} \textcolor{blue}{Loss}_{pair}(\mathbf{Z}; \Omega_{\mathcal{A}}) + \textcolor{red}{Loss}_{hyper}(\mathbf{Z}; \Omega_{\mathcal{H}}) + \lambda \|\mathbf{Z}\|_F^2$$

- Predict probability of a pairwise link:

$$\hat{P}(A_{ij} = 1) = f\left(\textcolor{blue}{\hat{\mathbf{Z}}}_i^T \textcolor{blue}{\hat{\mathbf{Z}}}_j\right)$$

- Predict probability of a  $m$ -order hyperlink:

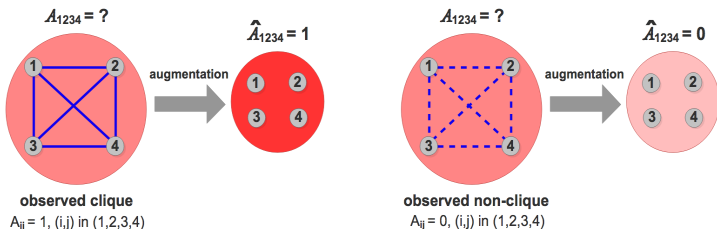
$$\hat{P}(\mathcal{A}_{i_1 i_2 \dots i_m} = 1) = f\left(\sum_{(i,j) \in \{i_1 i_2 \dots i_m\}} \textcolor{red}{\hat{\mathbf{Z}}}_i^T \textcolor{red}{\hat{\mathbf{Z}}}_j + \sum_{k=1}^r \psi_k |\textcolor{red}{\hat{\mathbf{Z}}}_{i_1 k} \textcolor{red}{\hat{\mathbf{Z}}}_{i_2 k} \dots \textcolor{red}{\hat{\mathbf{Z}}}_{i_m k}| \right)$$

- Joint link embedding (JLE) estimator:

$$\hat{\Theta} = \{\hat{P}(A_{ij} = 1), \hat{P}(\mathcal{A}_{i_1 i_2 \dots i_m} = 1)\}$$

# Hyperlink Augmentation from Observed Networks

- Hyperlinks might be sparse: infer unobserved hyperlink statuses
- Observed network + **clique dependency** = **augmented** training data



- **clique dependency**

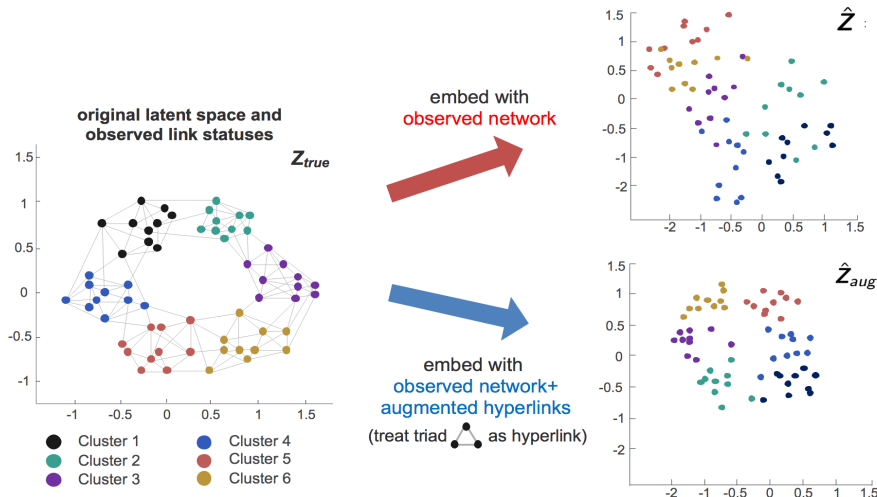
$$P(\mathcal{A}_{i_1, \dots, i_m} = 1 | \text{clique}, Z) - P(\mathcal{A}_{i_1, \dots, i_m} = 1 | \text{non-clique}, Z) > 0$$

- Augmented Embedding: embedding with a set of **augmented** hyperlink statuses  $\Omega_{\hat{\mathcal{A}}}$

$$\hat{Z}_{aug} = \operatorname{argmin}_Z \operatorname{Loss}(Z; \Omega_{\mathbf{A}}, \Omega_{\mathcal{A}}, \Omega_{\hat{\mathcal{A}}})$$

# Augmentation as Regularization on Embedding

- Hyperlink augmentation as **implicit regularization** on latent space
- Shrink distances among within-subgroup nodes: increase dependence between **hyperlinks** and **cliques**



# Asymptotic Property of Augmented JLE

- Goal: recover  $\Theta_0 = \{P(A_{ij} = 1), P(\mathcal{A}_{i_1 i_2 \dots i_m} = 1)\}$  via observed links
- $\rho := P(\mathcal{A}_{i_1 \dots i_m} = 1 | \text{clique}, \mathbf{Z}) - P(\mathcal{A}_{i_1 \dots i_m} = 1 | \text{no clique}, \mathbf{Z})$
- $|\Omega_{\hat{\mathcal{A}}}|$ : number of inferred hyperlinks from hyperlink augmentation procedure

## Theorem 1

Under regularity conditions, we establish the convergence rate for  $\hat{\Theta}_{aug}$ :

$$P\left(\frac{\|\hat{\Theta}_{aug} - \Theta_0\|_F}{\sqrt{n_{N,m}}} \geq \eta\right) \leq 11 \exp\left\{-c \frac{|\Omega_{aug}|}{(1 + C_0 \rho)^2} \left(1 + c_1 + c_1 \frac{\delta^2}{\epsilon^2}\right)^{-1} \eta^2\right\}$$

where  $|\Omega_{aug}| = |\Omega_{\mathbf{A}}| + |\Omega_{\mathcal{A}}| + |\Omega_{\hat{\mathcal{A}}}|$ ,  $n_{N,m} = \binom{N}{2} + \binom{N}{m}$ ,  $\epsilon$  is prediction MSE from *Aug JLE*, and  $\eta = \max(\epsilon, \lambda^{1/2})$ .

- Hyperlink augmentation accelerates convergence rate of prediction MSE  $\epsilon$ :
  - ▶ pairwise links + hyperlinks + augmentation:  $\epsilon \sim \frac{1 + C_0 \rho}{(|\Omega_{\mathbf{A}}| + |\Omega_{\mathcal{A}}| + |\Omega_{\hat{\mathcal{A}}}|)^{1/2}}$
  - ▶ pairwise links + hyperlinks:  $\epsilon \sim \frac{1 + C_0 \rho}{(|\Omega_{\mathbf{A}}| + |\Omega_{\mathcal{A}}|)^{1/2}}$
  - ▶ pairwise links only:  $\epsilon \sim \frac{1}{|\Omega_{\mathbf{A}}|^{1/2}}$

# Simulation Study

- Comparing methods

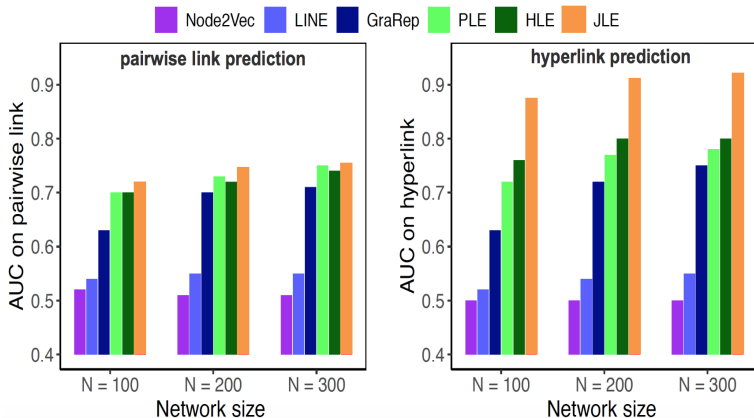
- ▶ **JLE**: the **proposed** joint pairwise and hyperlink embedding
- ▶ **Aug JLE**: the **proposed** JLE incorporating augmented hyperlinks
- ▶ **PLE**: embedding only through pairwise links  $Loss_{pair}(\mathbf{Z})$
- ▶ **HLE**: embedding only through hyperlinks  $Loss_{hyper}(\mathbf{Z})$
- ▶ **GraRep**: graph representations with global structural information (Cao et al., 2015)
- ▶ **LINE**: large-scale information network embedding (Tang et al., 2015)
- ▶ **Node2Vec** (Grover et al., 2016)

- Performance criterion

- ▶ AUC: Area under the ROC Curve

# Comparison under Conditional Independent Model

- $\{A_{ij}\}$  and  $\{\mathcal{A}_{ijk}\}$  are **independent** conditioning on  $\mathbf{Z}$
- Training on observed networks (without augmented hyperlink)
- **AUC** of link prediction on pairwise link and hyperlink testing sets



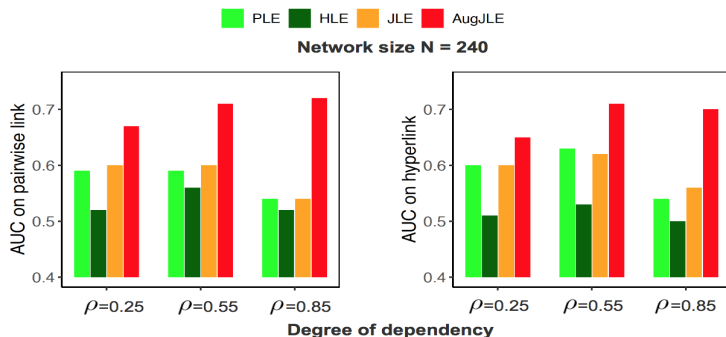


# Comparison under Conditional Dependent Model (Cont.)

- Incorporate **clique structure dependency**

$$\rho = P(\mathcal{A}_{ijk} = 1 | \text{clique}, Z) - P(\mathcal{A}_{ijk} = 1 | \text{no clique}, Z) > 0$$

- $\{\mathcal{A}_{ij}\}$  and  $\{\mathcal{A}_{ijk}\}$  are **dependent** conditioning on  $Z$
- Utilize hyperlink augmentation (Aug JLE)



- Performances using observed networks are poor with large  $\rho$
- Improvement from Aug JLE increases as  $\rho$  increases

# Real Data: Facebook Ego-Network

- Ego-Network: social network among user's friends
- Social circles
  - ▶ categorization of users sharing similar features
  - ▶ **multi-way relations among users**
- Applications on detecting underlying social circles
  - ▶ online advertising
  - ▶ recommendation/content filtering
  - ▶ personalized social network organization
- Current methods: organize manually or by pre-specified attributes
  - ▶ time consuming
  - ▶ not update automatically
  - ▶ missing user profiles

# Ego-Network Summary

- 224 people ( $N = 224$ )
- 6384 friendships (**two-way relations**)
- 14 social circles (**multi-way relations**)
  - ▶ defined by the ego user
  - ▶ describe different social relations: family, classmates, colleges

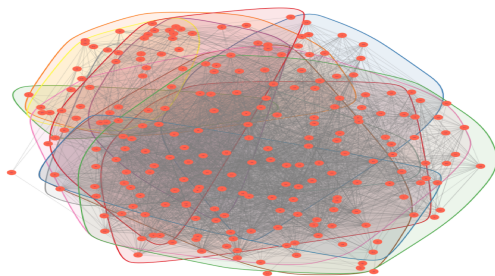


Fig. 7: The ego network in the Facebook dataset, where the social circles are marked as polygons with different colors.

# Prediction Results

- Prediction

- ▶ pairwise friendship (pairwise link)
- ▶ whether users  $\{i_1, i_2, \dots, i_M\} (M = 6, 10)$  belong to the same circle (M-order hyperlink)

Table 1: **AUC** of link prediction for ego-network

	Link Prediction		
	Pairwise Link	6-order Hyperlink	10-order Hyperlink
<b>Aug JLE</b>	<b>0.80</b>	<b>0.95</b>	<b>0.97</b>
<b>JLE</b>	0.79	0.91	0.89
HLE	0.57	0.89	0.82
PLE	0.80	0.62	0.63
GraRep	0.79	0.77	0.51
LINE	0.62	0.51	0.75
Node2Vec	0.49	0.49	0.48

# Concluding Remarks

- Hierarchical modeling for **multi-way** relations
  - ▶ detect subgroup structures and high-order interactions
  - ▶ capture nodes' similarities at different network levels
- Joint embedding of two-way and multi-way links
  - ▶ borrow **mutual** information for predictions
  - ▶ increase prediction performance
- Hyperlink augmentation
  - ▶ model structural dependency between pairwise and hyperlinks in latent space
  - ▶ infer potential unobserved hyperlinks
  - ▶ achieve fast convergence rate of estimation

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# Appendix

- Proportion of hyperlinks with high certainty:

$$f_{\text{clique}}(\varphi), f_{\text{non-clique}}(\varphi): [0, 1] \rightarrow [0, 1]$$

$$f_{\text{clique}}(\varphi) = \frac{|\{Y_{i_1 i_2 \dots i_m} \in \Omega_{\text{clique}} | P(Y_{i_1 i_2 \dots i_m} = 1 | \mathbf{Z}) \in [1 - \varphi, 1)\}|}{|\Omega_{\text{clique}}|}$$

$$f_{\text{non-clique}}(\varphi) = \frac{|\{Y_{i_1 i_2 \dots i_m} \in \Omega_{\text{non-clique}} | P(Y_{i_1 i_2 \dots i_m} = 1 | \mathbf{Z}) \in (0, \varphi]\}|}{|\Omega_{\text{non-clique}}|}$$

- Size from augmented hyperlinks  $|\Omega_{\hat{\mathcal{A}}}(\epsilon_{\text{aug}}, \rho)| = |\Omega_{\text{link}}| + |\Omega_{\text{non-link}}|$

$$|\Omega_{\text{link}}| = f_{\text{clique}} \left( \min \left\{ \frac{\epsilon}{1 - \rho}, 1 \right\} \right) |\Omega_{\text{clique}}|$$

$$|\Omega_{\text{non-link}}| = f_{\text{non-clique}} \left( \min \left\{ \frac{\epsilon}{1 - \rho}, 1 \right\} \right) |\Omega_{\text{non-clique}}|$$

# Appendix: Hyperlink Augmentation Procedure

- Hyperlink augmentation procedure on three-order hyperlinks
- Infer  $\{\mathcal{A}_{ijk}\} \in \Omega_{\mathcal{A}}^c$  based on  $\{\{\mathcal{A}_{ijk}\} \in \Omega_{\mathcal{A}}, \{A_{ij}\} \in \Omega_{\mathbf{A}}\}$
- **Step 1:** construct candidate for hyperlink status:  $\Omega_{\text{clique}}$  and  $\Omega_{\text{non-clique}}$

$$\text{(hyperlink)} \quad \Omega_{\text{clique}} : \{(i, j, k) | A_{ij} = A_{ik} = A_{jk} = 1\} \cap \Omega_{\mathcal{A}}^c$$

$$\text{(non-hyperlink)} \quad \Omega_{\text{non-clique}} : \{(i, j, k) | A_{ij} = A_{ik} = A_{jk} = 0\} \cap \Omega_{\mathcal{A}}^c$$

- $|\Omega_{\text{clique}}|$  and  $|\Omega_{\text{non-clique}}|$ : estimable from observed network
- Use hierarchical dependency prior, not involve network model



# Appendix: Hyperlink Augmentation Procedure (Continue)

- **Step 2:** select candidate hyperlink status with **high certainty**

- 1 obtain  $\{\hat{P}(\mathcal{A}_{i_1 i_2 i_3})\}$  via JLE based on **observed networks**
- 2 construct the set of augmented hyperlink statuses as

$$\hat{\mathcal{A}}_{ijk} = \begin{cases} 1, & (i, j, k) \in \Omega_{\text{clique}} \text{ and } \hat{P}(\mathcal{A}_{ijk}) \geq 1 - \delta, \\ 0, & (i, j, k) \in \Omega_{\text{non-clique}} \text{ and } \hat{P}(\mathcal{A}_{ijk}) \leq \delta. \end{cases}$$

- Augmented hyperlink  $\Omega_{\hat{\mathcal{A}}} := \{\hat{\mathcal{A}}_{ijk}\}$ :  $|\Omega_{\hat{\mathcal{A}}}| = f(\delta, \rho, |\Omega_{\text{clique}}|, |\Omega_{\text{non-clique}}|)^1$

- ▶ larger  $\delta$  (require higher inference certainty)  $\implies$  smaller  $|\Omega_{\hat{\mathcal{A}}}(\delta, \rho)|$
- ▶ larger  $\rho$  (stronger hierarchical dependency)  $\implies$  larger  $|\Omega_{\hat{\mathcal{A}}}(\delta, \rho)|$   
(larger  $\rho \implies$  smaller  $|P(\mathcal{A}_{ijk} = 1|\mathbf{Z}) - P(\Delta_{ijk} = 1|\mathbf{Z})|$ )

- **Step 3:** embedding with **augmented** hyperlinks

$$\hat{\mathbf{Z}}_{aug} = \underset{\mathbf{Z}}{\operatorname{argmin}} \operatorname{Loss}(\mathbf{Z}; \Omega_{\mathbf{A}}, \Omega_{\mathcal{A}}, \Omega_{\hat{\mathcal{A}}})$$

<sup>1</sup>detailed  $|\Omega_{\hat{\mathcal{A}}}|$  is provided in paper

# Appendix: Model Setup for Theoretical Analysis

- Hierarchical link generation  $(\mathcal{A}, \mathbf{A}) \sim \mathbf{P}_{\mathbf{Z}}(\mathcal{A}, \mathbf{A}) = \mathbf{P}_{\mathbf{Z}}(\mathcal{A}|\mathbf{A})\mathbf{P}_{\mathbf{Z}}(\mathbf{A})$
- Pairwise link  $\mathbf{P}_{\mathbf{Z}}(\mathbf{A})$ :  $A_{ij} \sim \text{Bern}(P(A_{ij} = 1|\mathbf{Z}))$
- Hyperlink  $\mathbf{P}_{\mathbf{Z}}(\mathcal{A}|\mathbf{A})$ :  $\mathcal{A}_{i_1 \dots i_m} \sim \text{Bern}(P(\mathcal{A}_{i_1 \dots i_m} = 1|\Delta, \mathbf{Z}))$ 
  - ▶  $P(\mathcal{A}_{i_1 \dots i_m} = 1|\Delta, \mathbf{Z})$ : dependent on  $\mathbf{A}$  via clique indicator  $\Delta_{i_1 \dots i_m}$

$$\Delta_{i_1 \dots i_m} = \begin{cases} 1, & \text{if } A_{ij} = 1, (i, j) \in \{i_1, \dots, i_m\}, \\ 0, & \text{otherwise.} \end{cases}$$

- ▶ functional form of  $P(\mathcal{A}_{i_1 \dots i_m} = 1|\Delta, \mathbf{Z})$  is not specified
- ▶ degree of structural dependency

$$\rho_{i_1 \dots i_m} := P(\mathcal{A}_{i_1 \dots i_m} = 1|\Delta_{i_1 \dots i_m} = 1, \mathbf{Z}) - P(\mathcal{A}_{i_1 \dots i_m} = 1|\Delta_{i_1 \dots i_m} = 0, \mathbf{Z})$$

- ▶  $\rho_{i_1 \dots i_m} = 0$ : conditional independent,  $\rho_{i_1 \dots i_m} > 0$ : conditional correlated

# Appendix: Simulation Settings

- Hierarchical network generation
- Latent position  $\mathbf{Z} = \{Z_i = (Z_{ir})_{r=1}^5\}_{i=1}^N$ ,  $N$ : number of nodes

$$Z_{ir} \sim \mu \times \text{Unif}(-1, -0.6) + (1 - \mu) \times \text{Unif}(0.6, 1), \mu \sim \text{Bern}(1, 0.5)$$

- Pairwise links  $\mathbf{A}$ :  $\{Z_i^{(\alpha)} = Z_i \odot \alpha\}_{i=1}^N$ ,  $\alpha = (1, 1, 1, 0.2, 0.2)$

$$A_{ij} \sim \text{Bern}(\sigma(Z_i^{(\alpha)T} Z_j^{(\alpha)})), \sigma(\cdot) \text{ is logistic function}$$

- Hyperlinks  $\mathcal{A}$ :  $\{Z_i^{(\beta)} = Z_i \odot \beta\}_{i=1}^N$ ,  $\beta = (0.2, 0.2, 0.2, 1, 1)$

$$\mathcal{A}_{ijk} \sim \text{Bern}(\theta_{ijk}), \theta_{ijk} = \sigma\left(\sum_{(s,t) \in \{i,j,k\}} Z_s^{(\beta)T} Z_t^{(\beta)} + \sum_{r=1}^5 \psi_r |Z_{ir}^{(\beta)} Z_{jr}^{(\beta)} Z_{kr}^{(\beta)}|\right)$$

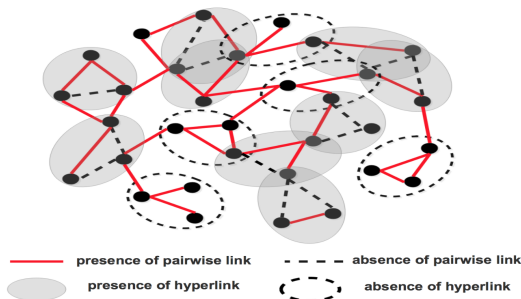
- $\{A_{ij}\}$  and  $\{\mathcal{A}_{ijk}\}$  are **independent** conditioning on  $\mathbf{Z}$

(\*  $\odot$  denotes element-wise multiplication)

# Appendix: Simulated Multi-Level Network

- Randomly split  $\mathbf{A}$ 
  - ▶ training set ( $\Omega_{\mathbf{A}}$ ): 60%
  - ▶ validation and testing set: 20% and 20%
- Sampling for hyperlinks:  $\Omega_{\text{pool}} = \{\mathcal{A}_{ijk} | A_{ij} \in \Omega_{\mathbf{A}}, A_{ik} \in \Omega_{\mathbf{A}}, A_{jk} \in \Omega_{\mathbf{A}}\}$ 
  - ▶ sample 5% from  $\Omega_{\text{pool}}$  as a training set  $\Omega_{\mathcal{A}}$
  - ▶ split  $\Omega_{\text{pool}} \cap \Omega_{\mathcal{A}}^c$  into validation (50%) and testing (50%) set

Observed pairwise link and hyperlink status



# Appendix: Comparison of Conditional Dependent Model

- Incorporate **structural dependency**

$$\rho = P(\mathcal{A}_{ijk} = 1 | \text{clique}, Z) - P(\mathcal{A}_{ijk} = 1 | \text{no clique}, Z) > 0$$

- Hyperlink generating model

$$P(\mathcal{A}_{ijk} = 1 | \text{clique}) = \theta_{ijk} + \rho \left\{ 1 - \prod_{(p,q) \in \{ijk\}} \theta_{pq} \right\}$$

$$P(\mathcal{A}_{ijk} = 1 | \text{no clique}) = \theta_{ij} - \rho \left\{ \prod_{(p,q) \in \{ijk\}} \theta_{pq} \right\}$$

- $\{A_{ij}\}$  and  $\{\mathcal{A}_{ijk}\}$  are **dependent** conditioning on  $\mathbf{Z}$

# Appendix: Asymptotic Results of the Proposed Estimator

## Theorem 2

Denote  $n_{N,m} := \binom{N}{2} + \binom{N}{m}$  as the number of possible pairwise and hyperlinks, under regularity conditions, we establish the convergence rate for a **JLE** estimator  $\hat{\Theta}$  using **observed network**. That is,

$$P \left( \frac{\|\hat{\Theta} - \Theta_0\|_F}{\sqrt{n_{N,m}}} \geq \eta \right) \leq 11 \exp \left( -c \frac{|\Omega_{\mathbf{A}}| + |\Omega_{\mathbf{A}}|}{(1 + C_0 \rho)^2} \eta^2 \right),$$

where  $\|\cdot\|_F$  indicates the Frobenius norm,  $\eta = \max(\varepsilon, \lambda^{1/2})$ , and  $\lambda$  is the penalty parameter,  $c \geq 0$  is a constant,  $C_0$  is the degree of link overlap, and the best possible rate is  $\varepsilon \sim \left( \frac{1+C_0\rho}{(|\Omega_{\mathbf{A}}|+|\Omega_{\mathbf{A}}|)^{1/2}} \right)$  when  $\lambda \asymp \varepsilon^2$ .