ICDM 2021
IEEE International Conference on Data Mining
7 – 10 DECEMBER 2021
AUCKLAND NEW ZEALAND

Roles Analytics in Networks
Foundations, Methods and Applications

Yulong Pei
Akrati Saxena
George Fletcher
Mykola Pechenizkiy
TU Eindhoven, the Netherlands

Pengfei Jiao
Xuan Guo
Tianjin University, China

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

天津大学 Tianjin University

Outline

- What is and Why Role Analytics?
- Equivalence Relations
- Taxonomy of Role Analytics Methods
- Role-oriented Network Embedding
- Challenges and Outlook

Outline

- What is and Why Role Analytics?
- Equivalence Relations
- Taxonomy of Role Analytics Methods
- Role-oriented Network Embedding
- Challenges and Outlook

What Roles Are

Role [Cambridge Dictionary]
1) the position or purpose that someone or something has a situation, organization, society, or relationship
2) the duty or use that someone or something usually has or is expected to have
3) an actor's part in a film or play

Different notions of roles in computer science:
sematic roles, social roles, structural roles, etc.

https://all-free-download.com/free-vector/download/user-role-icon-vector_152771.html

Semantic Roles (linguistics perspective)

also known as thematic relations, are the various roles that a noun phrase may play with respect to **the action** or **state** described by a governing verb, i.e the sentence's main verb.

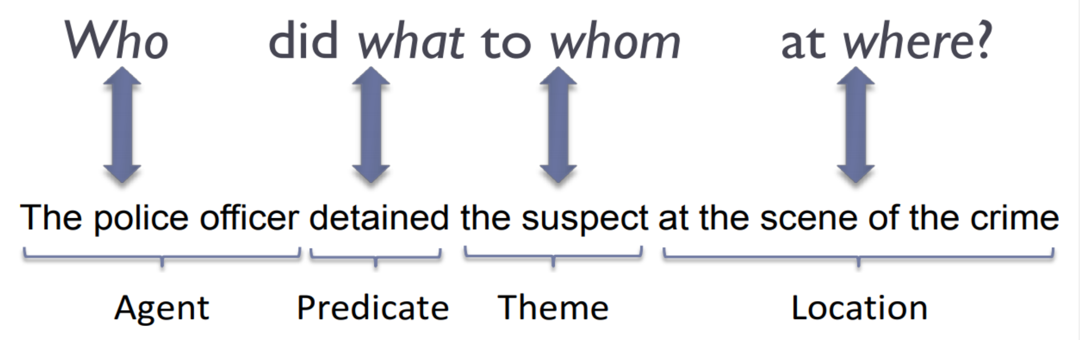
For example,

"The police officer detained the suspect
at the scene of the crime",

- *The police officer* is the doer of detaining – an agent;
- *the suspect* is the people that is detained – a theme.

Common roles include

- Agent, Experiencer, Stimulus, Theme, Patient, Location, Time, Beneficiary, etc.



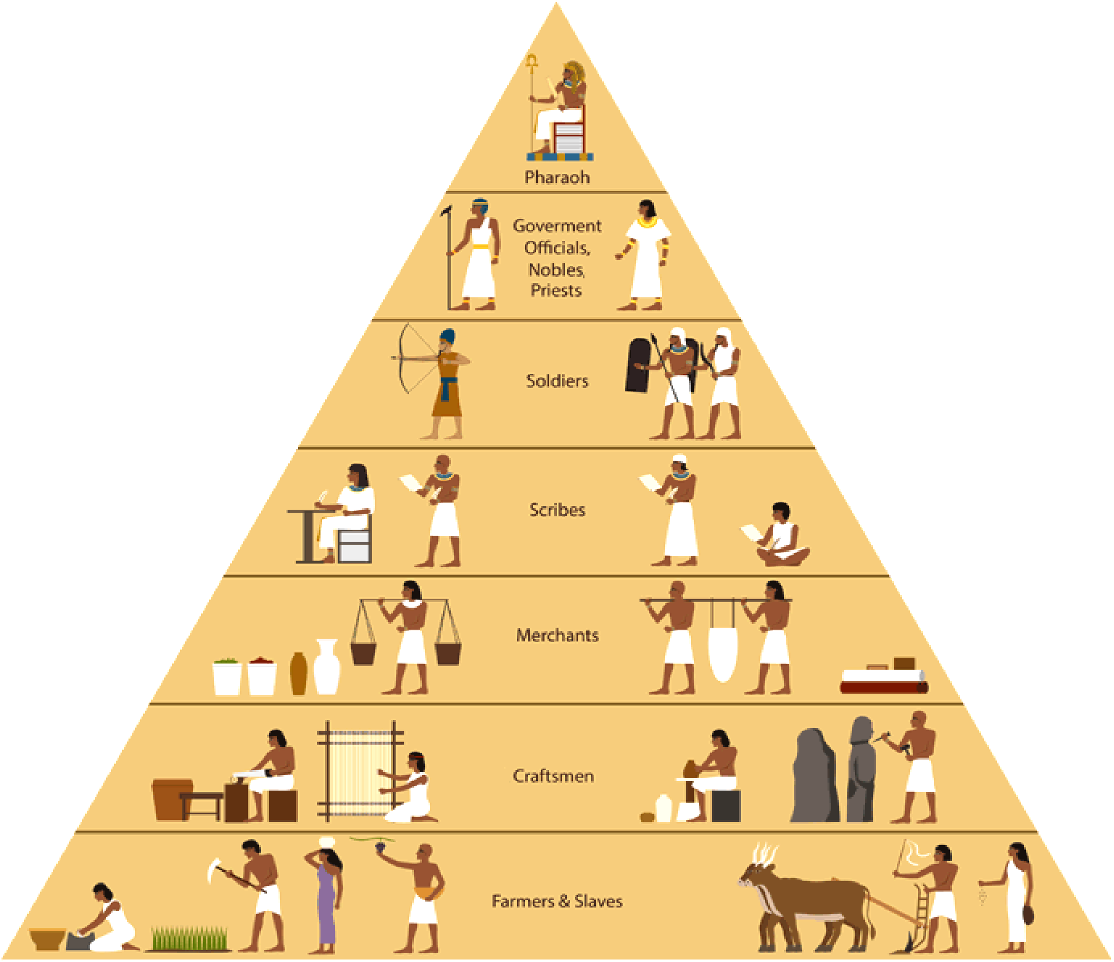
https://web.stanford.edu/~jurafsky/slp3/slides/22_SRL.pdf

Social Roles (sociology perspective)

connected behaviors, rights, obligations, beliefs, and norms as conceptualized by people in a social situation

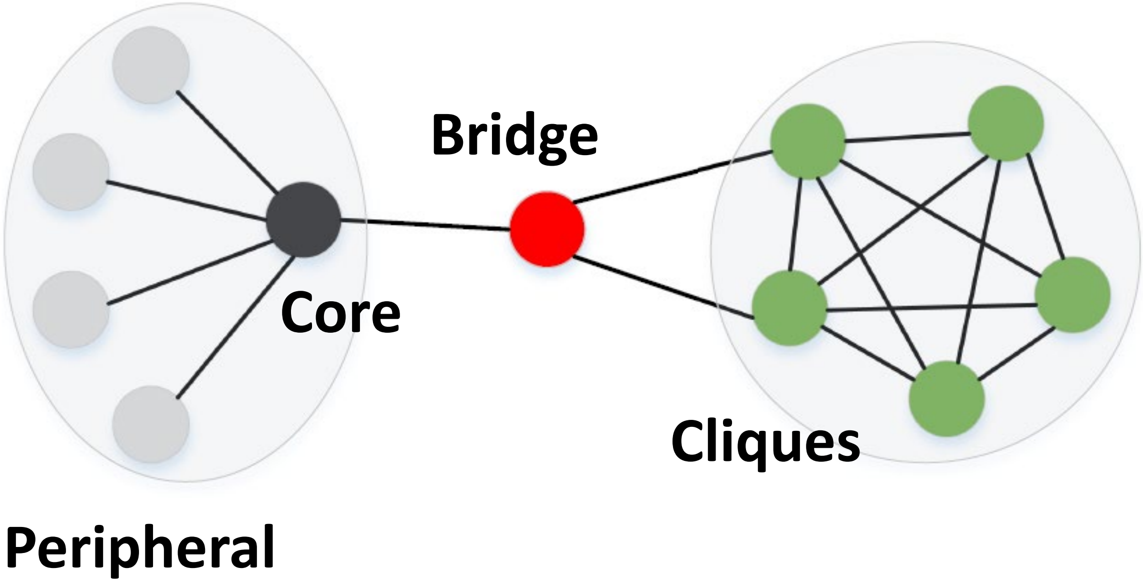
Role development can be influenced by different factors:

- Societal influence
- Genetic predisposition
- Cultural influence
- Situational influence



https://www.ancient-egypt-online.com/

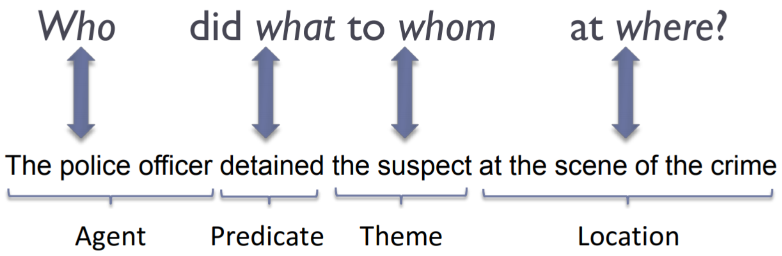
Structural Roles (network perspective)



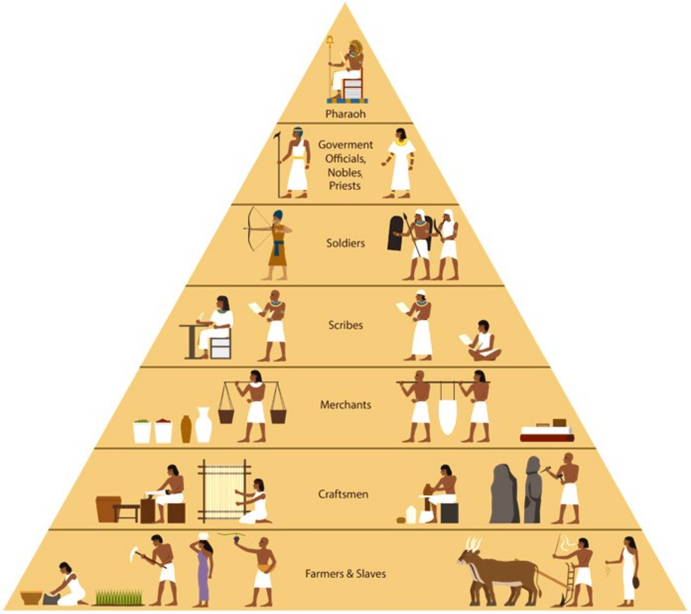
- capture functions that nodes play in a network through node-level connectivity patterns such as core, peripheral, cliques and bridges, e.g.
- Bridges connect multiple communities and could be useful on maximizing the spread of influence over communities
- Cliques are the nodes who connect to each other inside a community

Target in This Tutorial

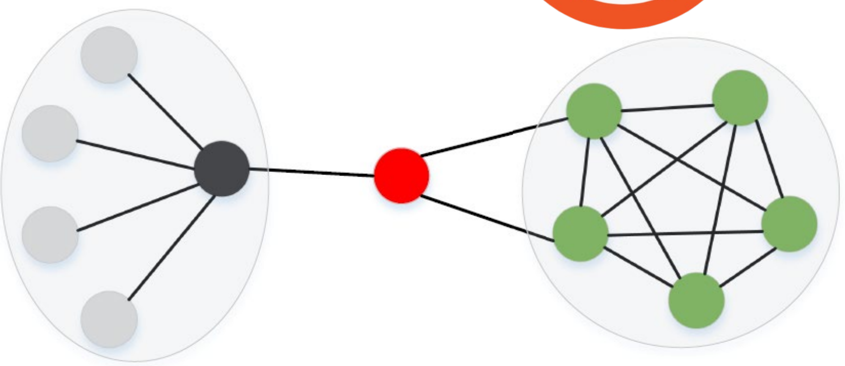
Semantic Roles



Social Roles



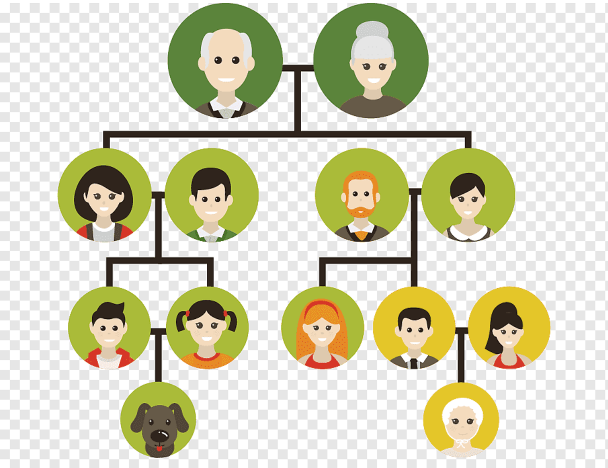
Structural Roles

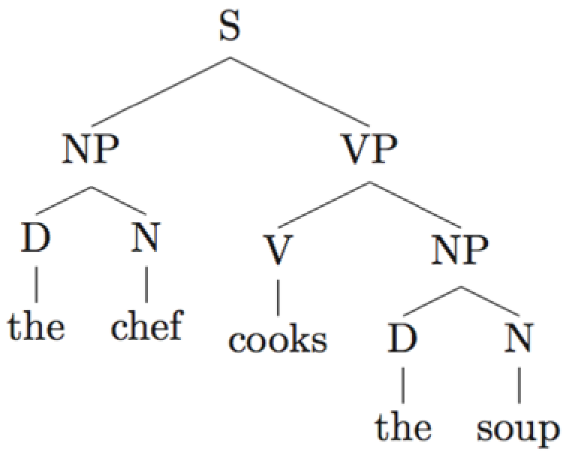


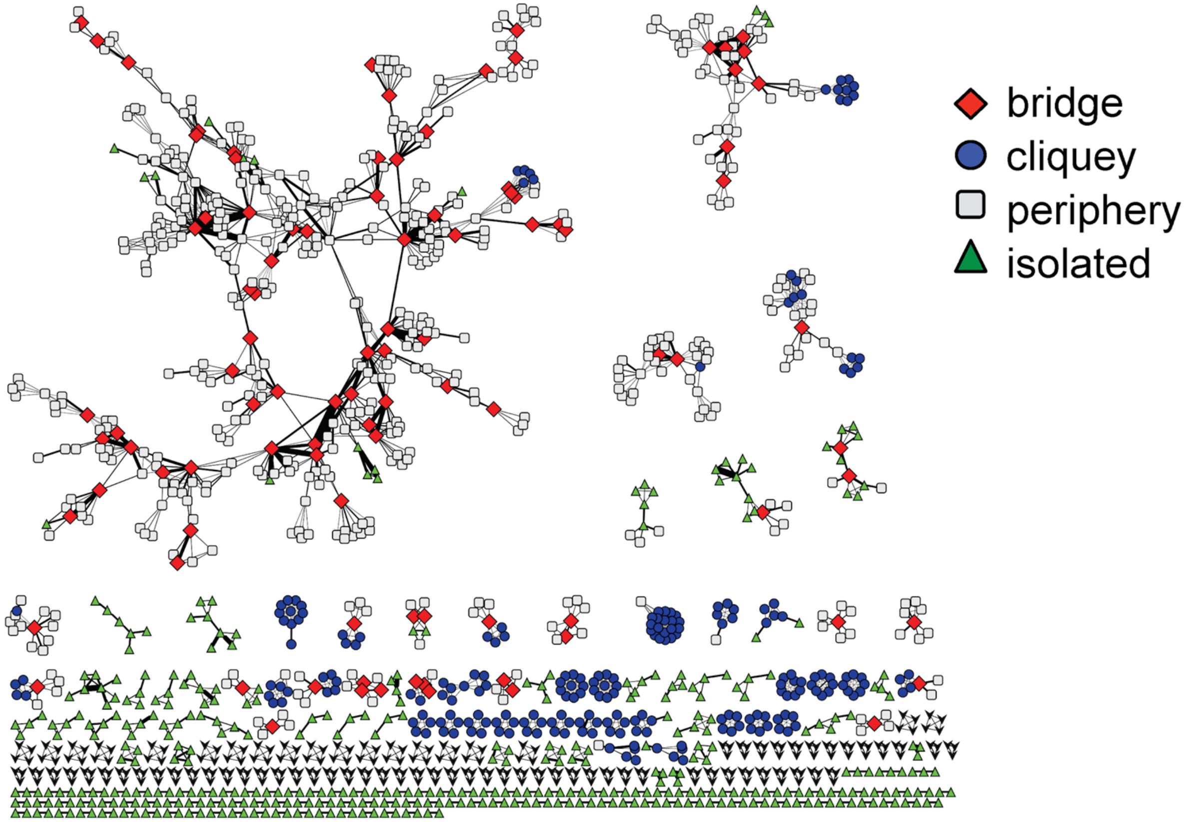
Roles in Networks

Roles represent node-level connectivity patterns, e.g., bridge, cliquey, isolated.

Structural roles can also reflect other types of roles







Node and Graph Similarity: Theory and Applications, ICDM 2014 Tutorial

What is Role Analytics in Networks?

Role analytics is about identifying the roles that different nodes play in the network of interest.

We need to define what roles are

- similar in structual features
- equivalent in some relation
- labeled data
- prior knowledge

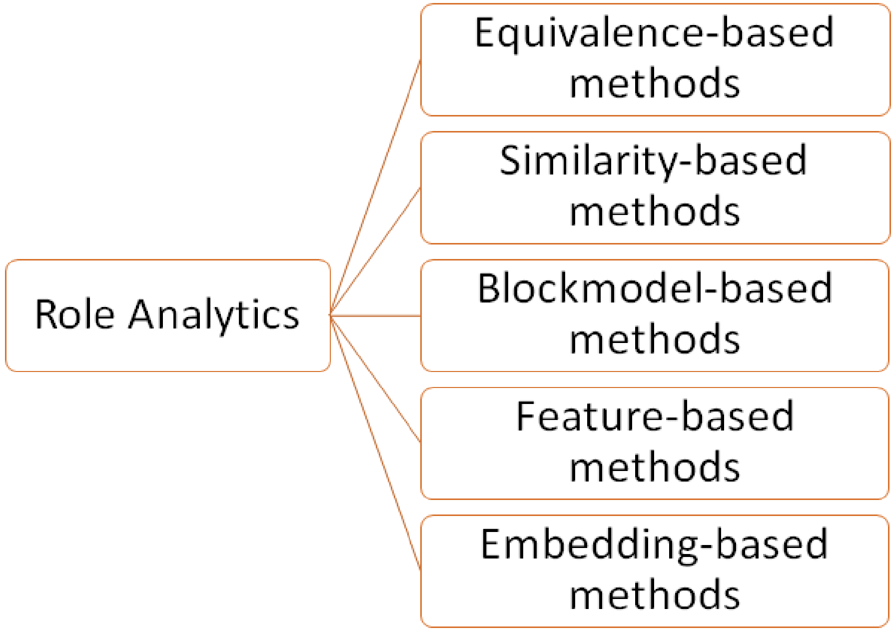
Role Analytics Methods

Role analytics can be solved using:

- Node classification (if labeled data is available)
- Node clustering (with role theories and/or representative features)

Classification and clustering techniques can be applied in role analytics if they

- follow certain role theories, e.g., equivalence relations; or
- capture features which are representative in distinguishing different roles.



Problem Formulation

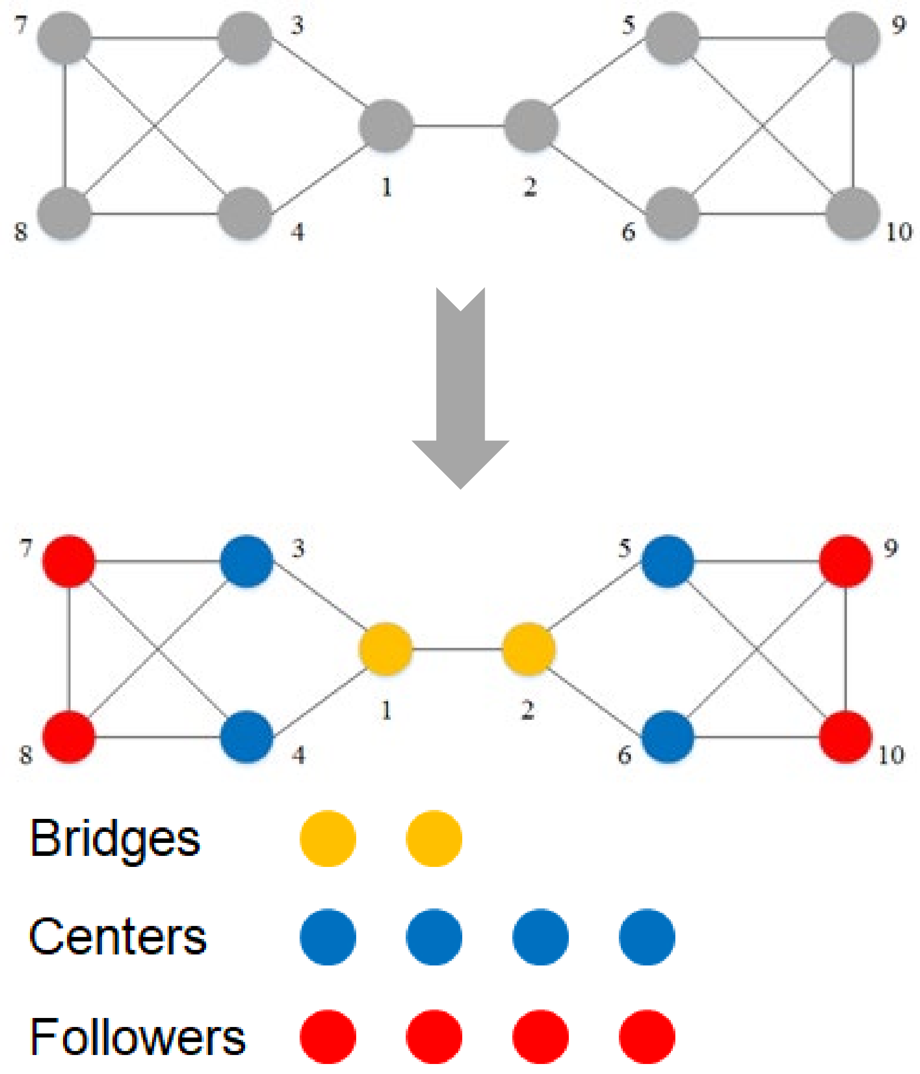
Input

A graph *G*={*V*, *E*} where *V* is the set of nodes and *E* is the set of edges.

Other types of graphs, e.g., temporal, attributed Signed, heterogeneous networks.

Output

- Discovery: 1) assignment of role of each node in *G* and 2) groups of nodes where each group contains nodes belonging to the same role.
- Analysis: 1) interpretation of each role and/or 2) transition of roles in temporal/dynamic networks

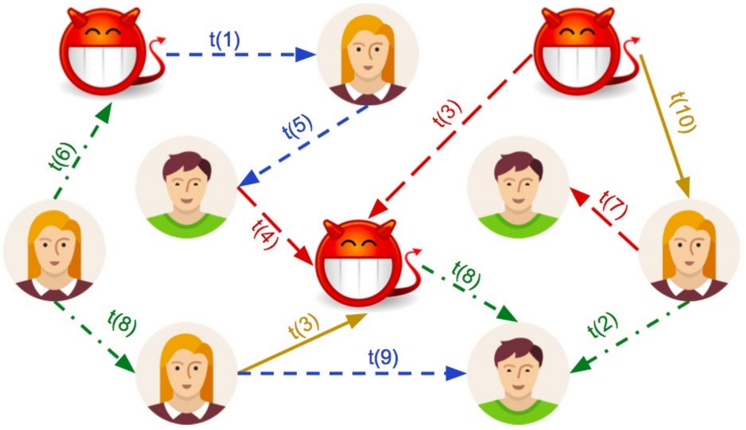


Why Role Analytics in Networks?

- Social science: how to identify and understand the social positions of individuals from social networks which consist of cyber or physical social interactions
- Network science: how to study the structural representations of complex networks, e.g. social or biological networks
- Graph mining in computer science: how to group nodes into clusters where nodes inside a cluster share similar structural information

Applications of Role Analytics

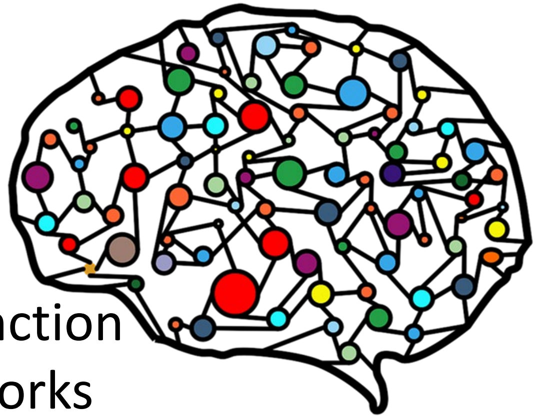
Hub in
transportation networks



Spammer in social networks
[Fakhraei el al., KDD 2015]

Opinion leader and information spread in social networks

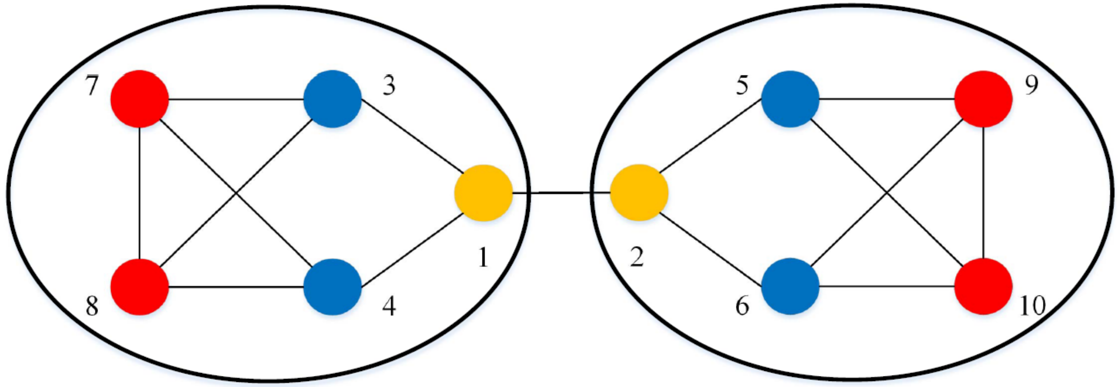
https://all-free-download.com/free-vector/download/social-network-concept-human-icons-connected-in-circle_6826089.html



Structural function in brain networks

https://neurosciencenews.com/brain-network-structure-14435/

Roles VS Communities



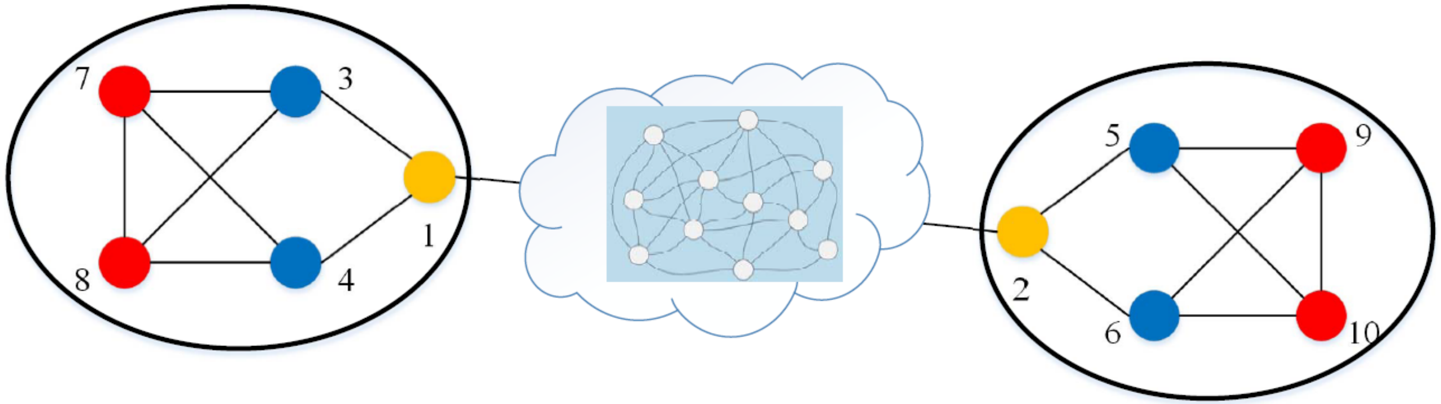
Roles VS Communities:

- Roles shown in different colors
  - E.g., yellow nodes are bridges
- Communities shown inside the ellipses
  - Denser internal connections inside each community

Global structure. It reflects the topological properties of graphs through the *unbounded* observation of the input graph as an entirety

Local structure. It captures the topological properties of graphs by observing a *bounded* part of the input graph

Roles VS Communities: Spatial Perspective



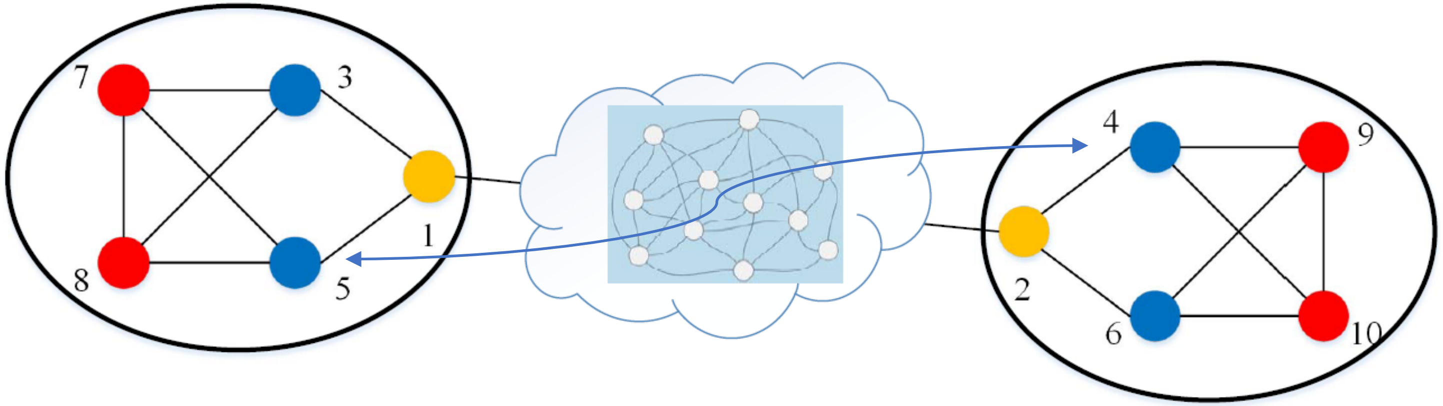
Roles

- For role discovery, we need to have a *global view* of this graph.
- Node 1 and 2 may not be bridges after adding these nodes and edges between them

Communities

- To detect each community, what we need to know is the *local structural information.*
- Detecting the left community does not require the information of the right community

Roles VS Communities: Perturbation Perspective



Roles

- Role of node 4 and 5 does not change because their global structural information stays the same.

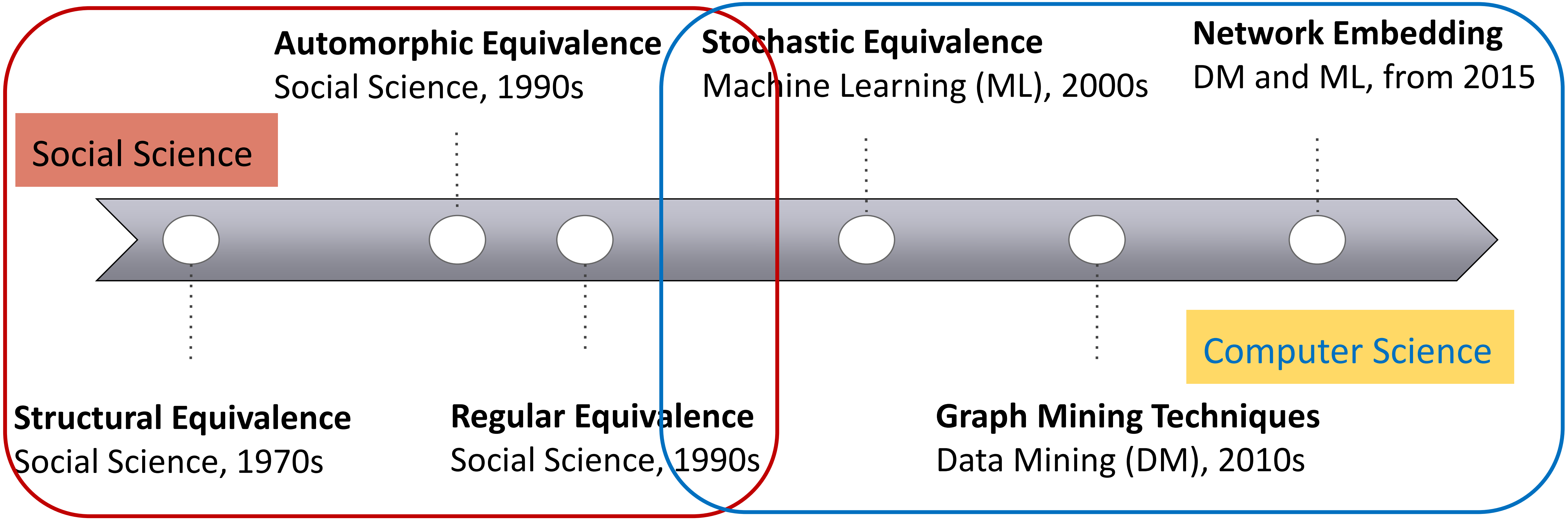
Communities

- The communities of node 4 and 5 are changed, because their local structures are different. E.g., the neighbors of node 4 are different.

Outline

- What is and Why Role Analytics?
- Equivalence Relations
- Taxonomy of Role Analytics Methods
- Role-oriented Network Embedding
- Challenges and Outlook

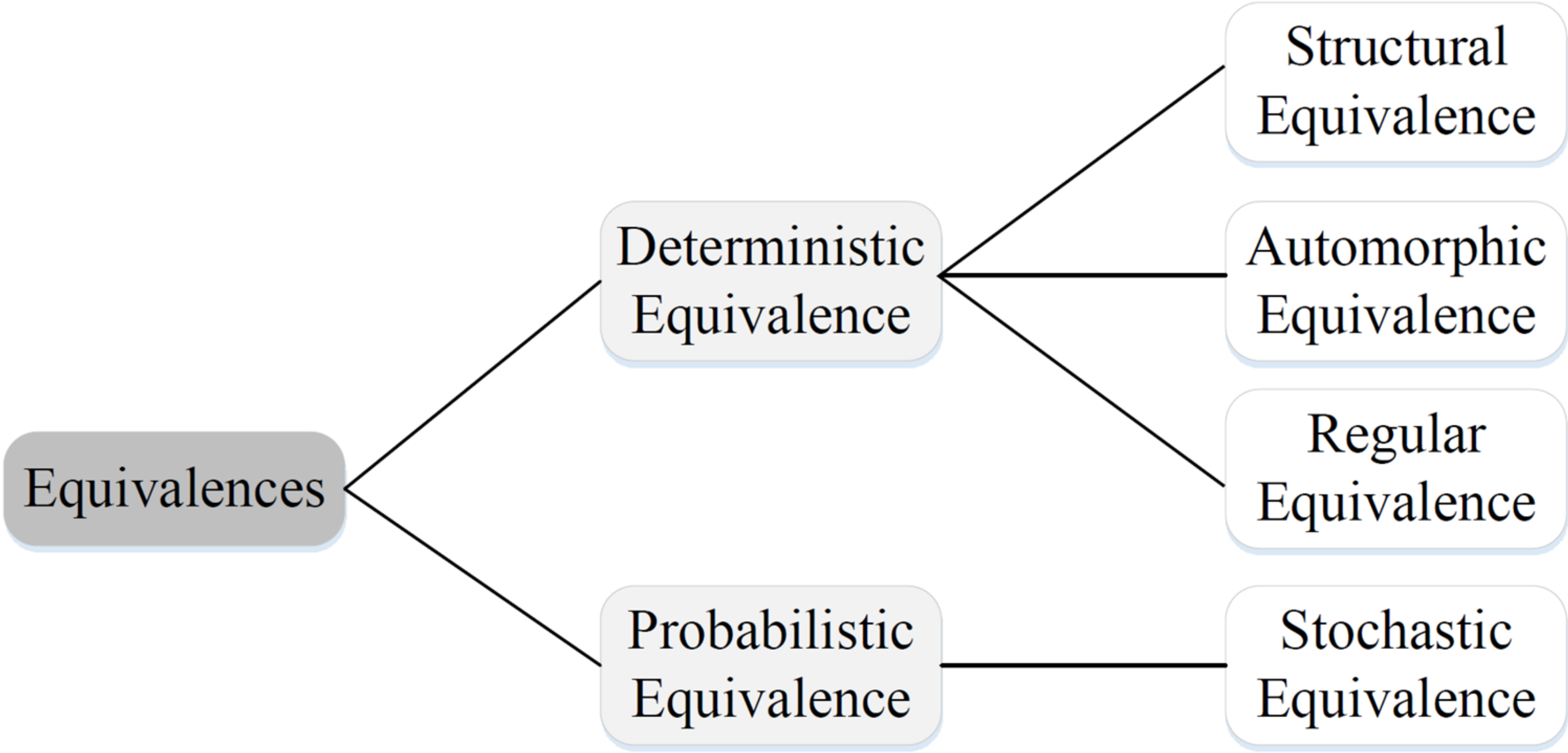
Role Analytics Research Timeline



Equivalence Relation

- Formally, an equivalence relation E is any relation that satisfies these three conditions:
  - *Transitivity*: $(a,b), (b,c) \in E \Rightarrow (a,c) \in E$
  - *Symmetry*: $(a,b) \in E \Leftrightarrow (b,a) \in E$
  - *Reflexivity*: $(a,a) \in E$
- Two nodes that have the same role are in an *equivalence relation*.
- Structural, automorphic, regular and stochastic equivalence

Taxonomy of Equivalence Relations

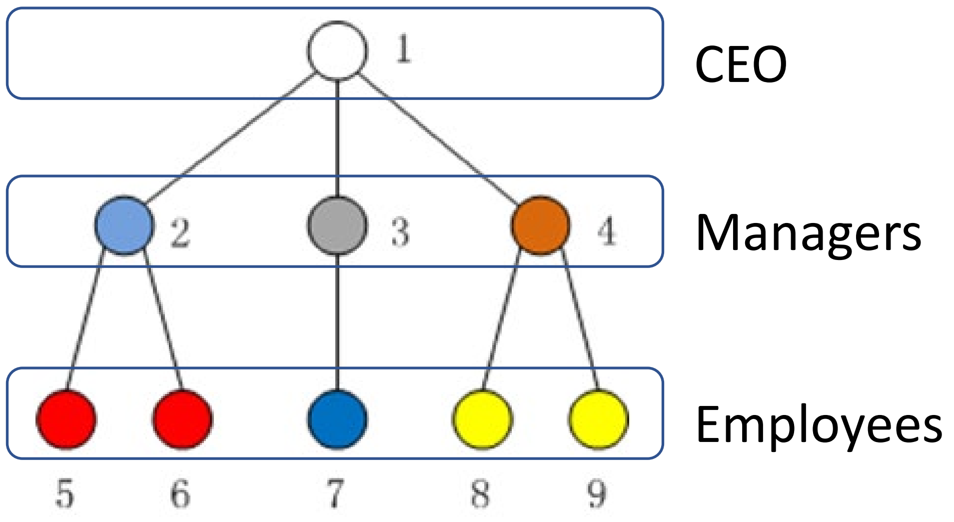


Structural Equivalence

- Two nodes u and v are structurally equivalent
  - if, for all nodes, k=1,2,...,n ($k \neq u, v$), node u has an edge to k, if and only if v also has an edge to k, and
  - u has an edge from k if and only if v also has an edge from k.

- Two nodes u and v are structurally equivalent if they have the **same relationships** to **all other nodes**
- Rarely appears in real-world networks

Structural Equivalence



Seven structurally equivalent groups:

{5, 6}, {8, 9}

{1}, {2}, {3}, {4}, {7}

Two structurally equivalent nodes should have exactly the same relationships, e.g., node 5 and 6

Automorphic Equivalence

- Two nodes are automorphically equivalent if all the nodes can be re-labeled to form an isomorphic graph with the labels of u and v interchanged.
- An isomorphism of graphs G and H is a bijection between the node sets of G and H: f: V(G) → V(H)
  - such that any two nodes u and v of G are adjacent in G if and only if f(u) and f(v) are adjacent in H.

https://en.wikipedia.org/wiki/Similarity_(network_science)

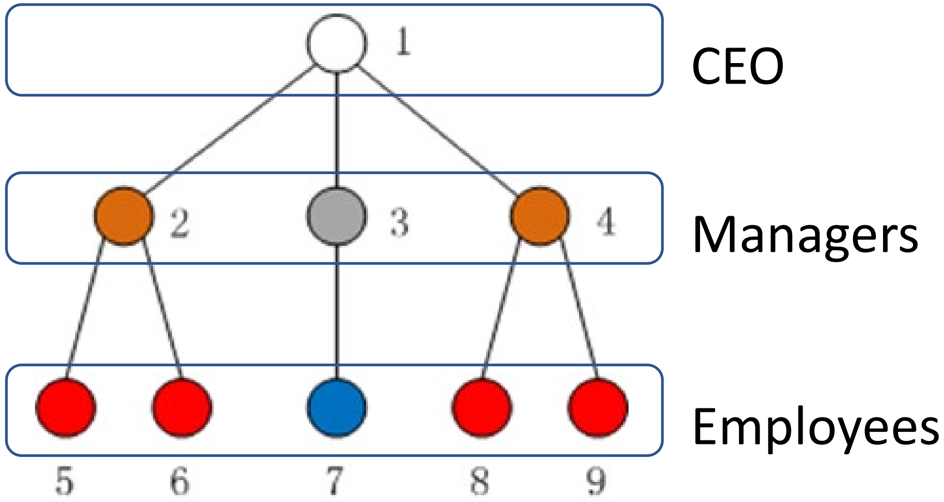
Automorphic Equivalence

- Two automorphically equivalent nodes share exactly the same label-independent properties.

- Nodes are automorphically equivalent if we can permute the graph in such a way that exchanging the two nodes has no effect on the distances among all nodes in the graph.

https://en.wikipedia.org/wiki/Similarity_(network_science)

Automorphic Equivalence



Five automorphically equivalent groups:

{5, 6, 8, 9}, {2, 4}, {1}, {3}, {7}

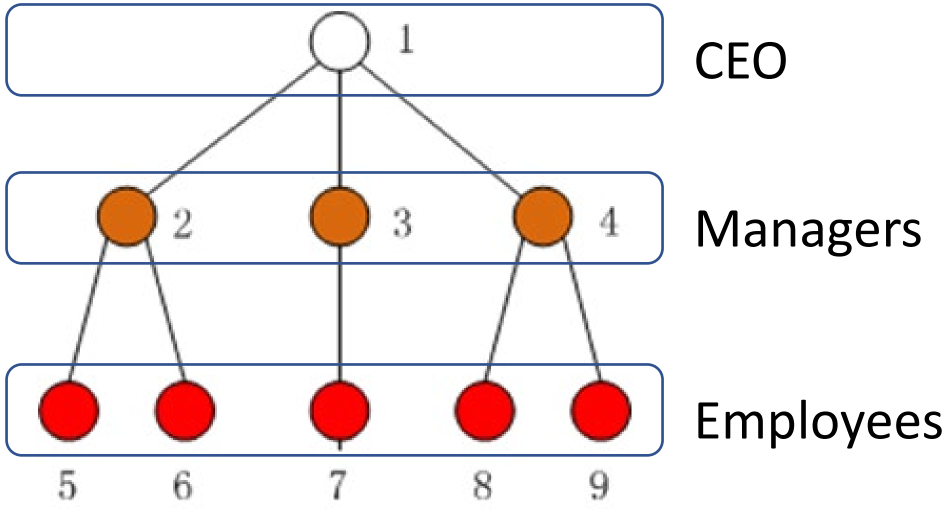
- Two nodes u and v are automorphically equivalent if they are exchangeable
- If we change node 2 and 4, the network structure will not be changed

Regular Equivalence

- Two nodes u and v are regularly equivalent if they are equally related to equivalent others

- Regular equivalence is defined in a recursive way that two regularly equivalent nodes have network neighbors which are also regularly equivalent.

Regular Equivalence



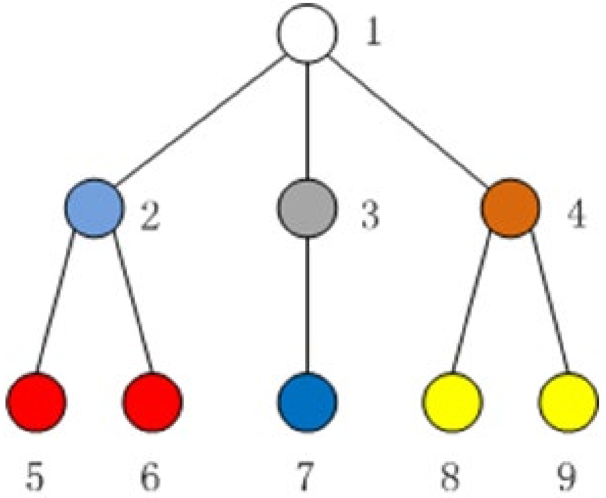
Three regularly equivalent groups:

{1}, {2, 3, 4}

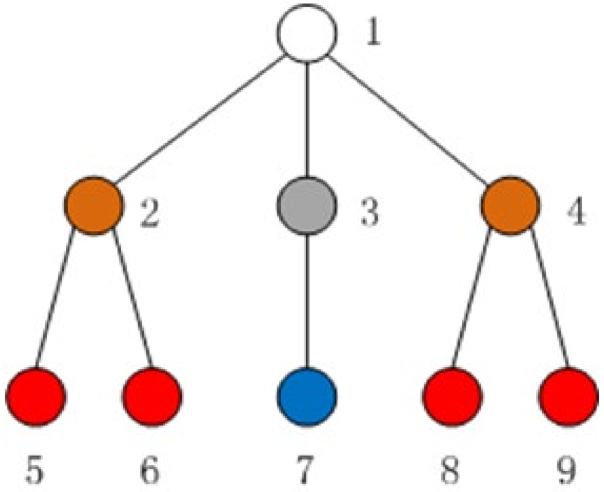
{5, 6, 7, 8, 9}

Two nodes *u* and *v*
are regularly equivalent if they
are equally related to equivalent others

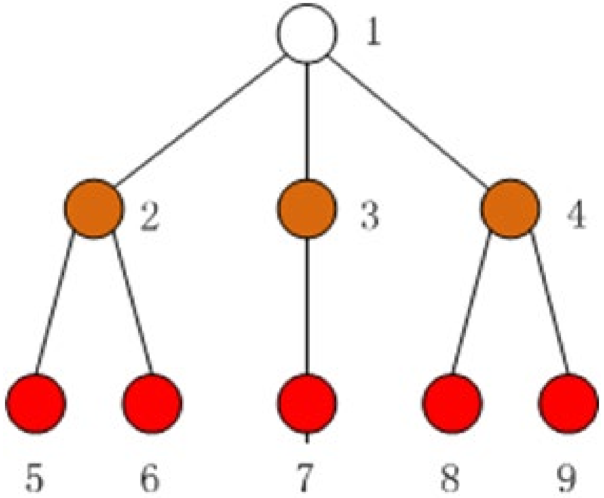
Summary of Deterministic Equivalence Relations



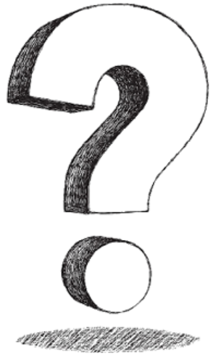
Structural equivalence



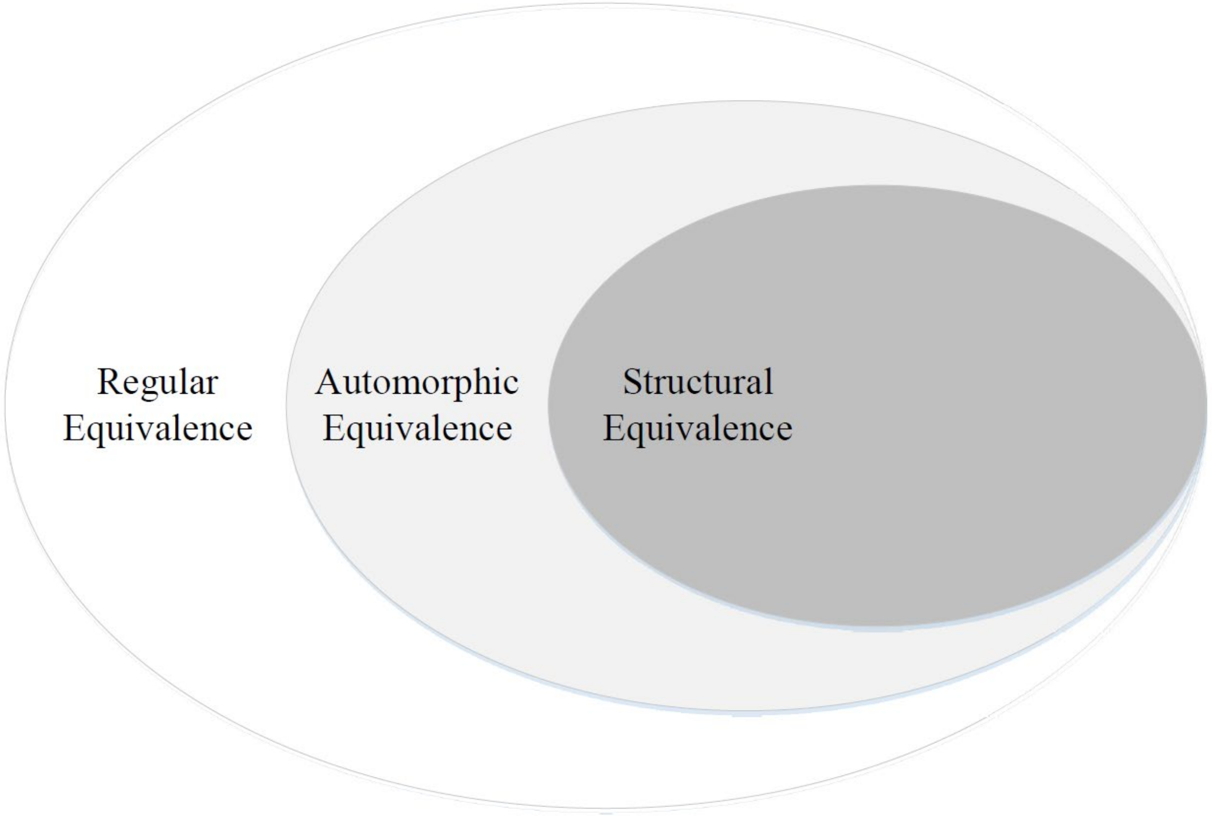
Automorphic equivalence



Regular equivalence



Summary of Deterministic Equivalence Relations



- Strictness of conditions:
- structural eq > automorphic eq > regular eq

- Practical values:
- regular eq > automorphic eq > structural eq

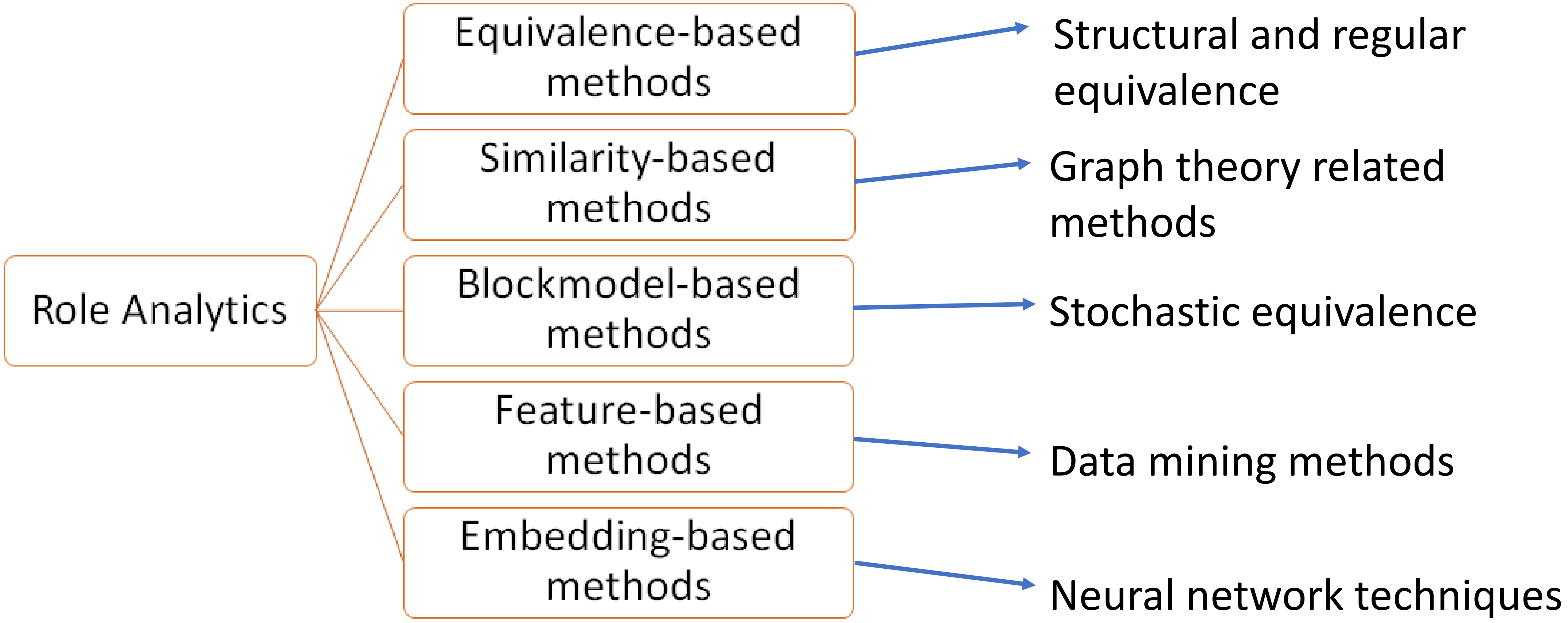
Stochastic Equivalence

- Probabilistic version of structural equivalence
- Two nodes *i* and *j* are stochastically equivalent if they are "exchangeable" w.r.t. a probability distribution
- The probability distribution of the graph must *remain the same* when equivalent nodes are exchanged.
- Stochastic blockmodel (and its variants) to discover roles based on stochastic equivalence

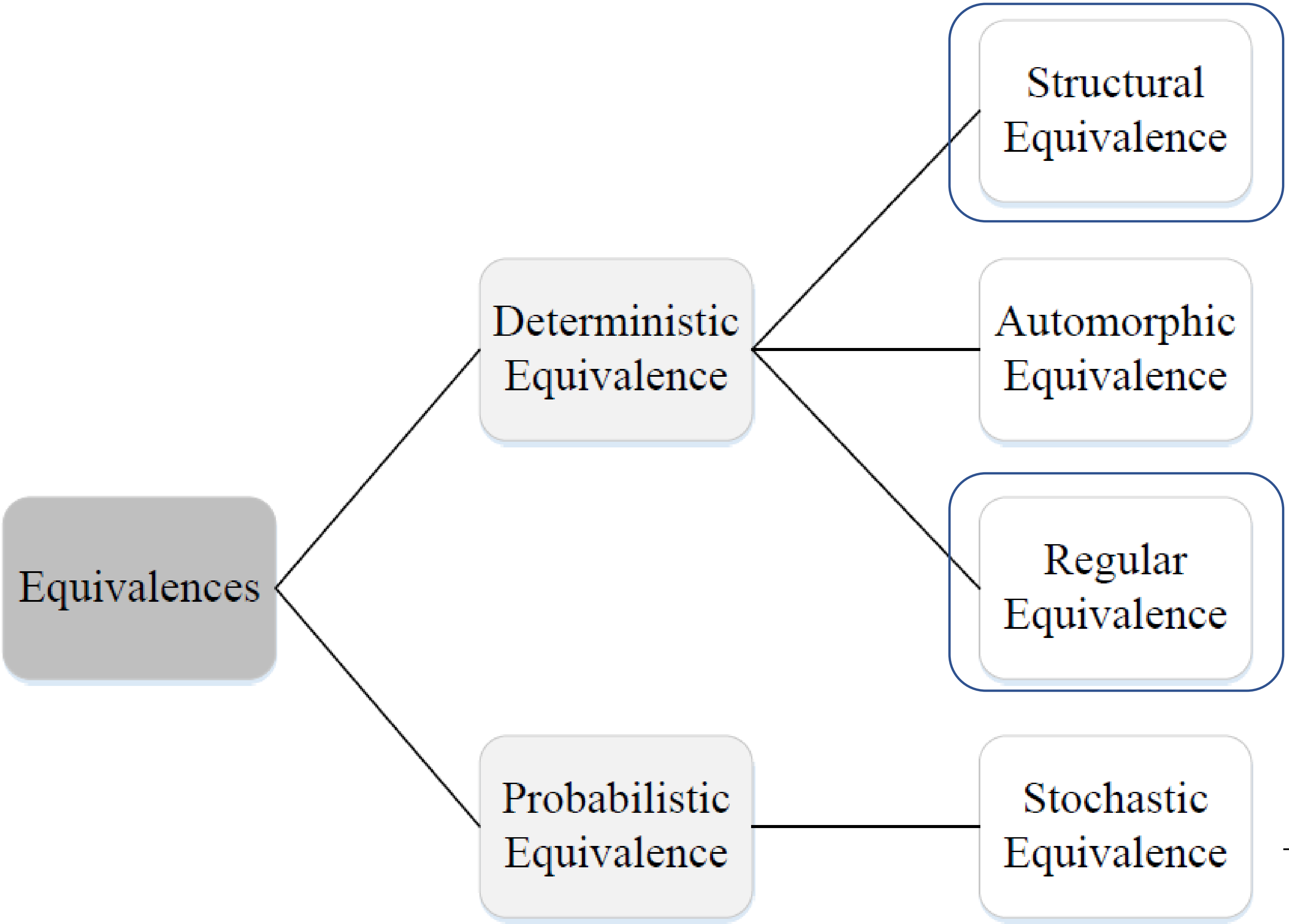
Outline

- What is and Why Role Analytics?
- Equivalence Relations
- Taxonomy of Role Analytics Methods
- Role-oriented Network Embedding
- Challenges and Outlook

Taxonomy of Role Analytics Methods

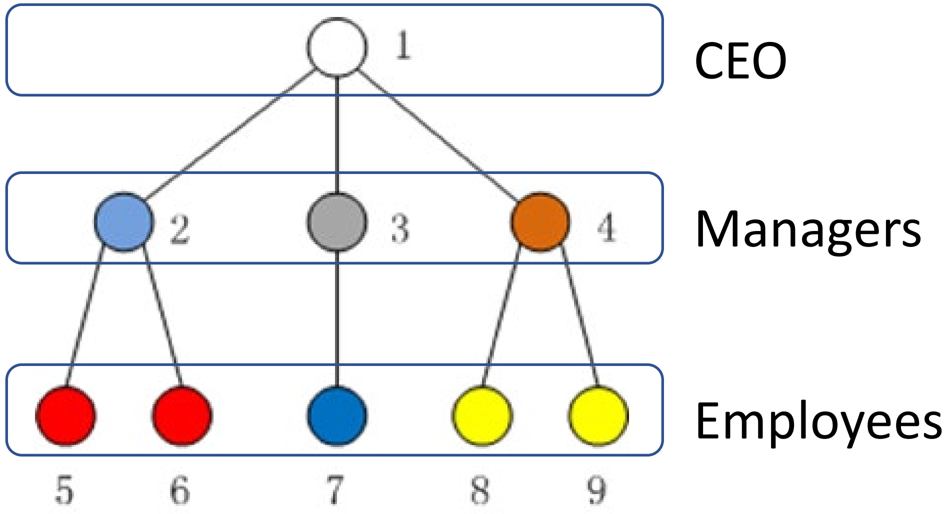


Equivalence-based Methods

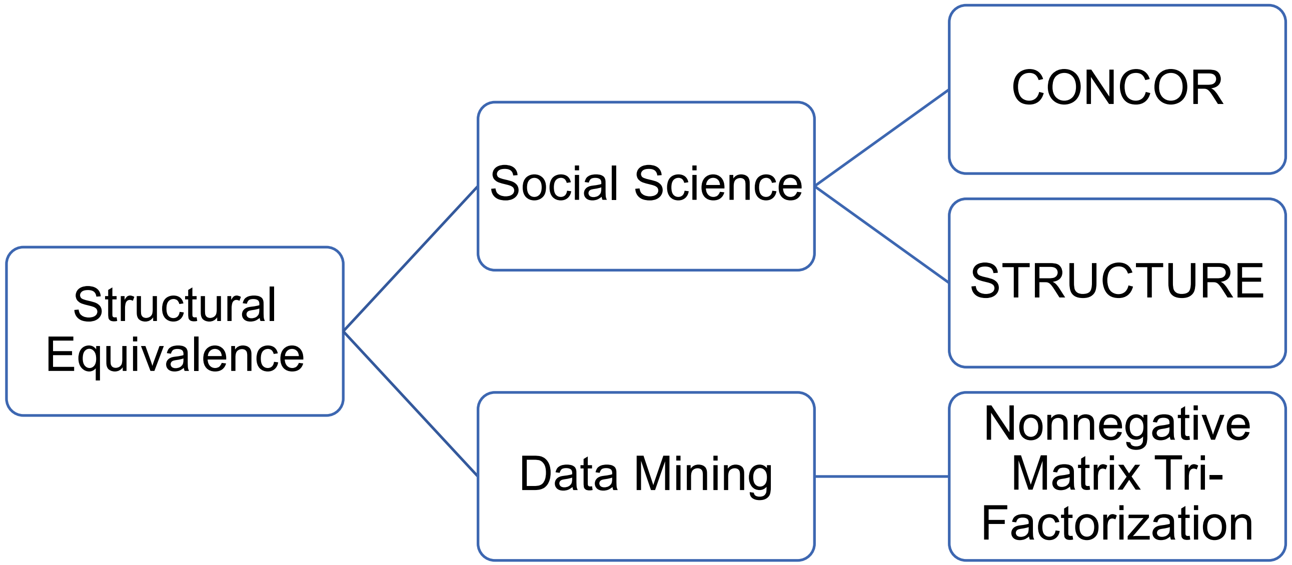


Blockmodel-based methods

Structural Equivalence



Two nodes are structurally equivalent if they have the **same relationships** to **all other nodes**



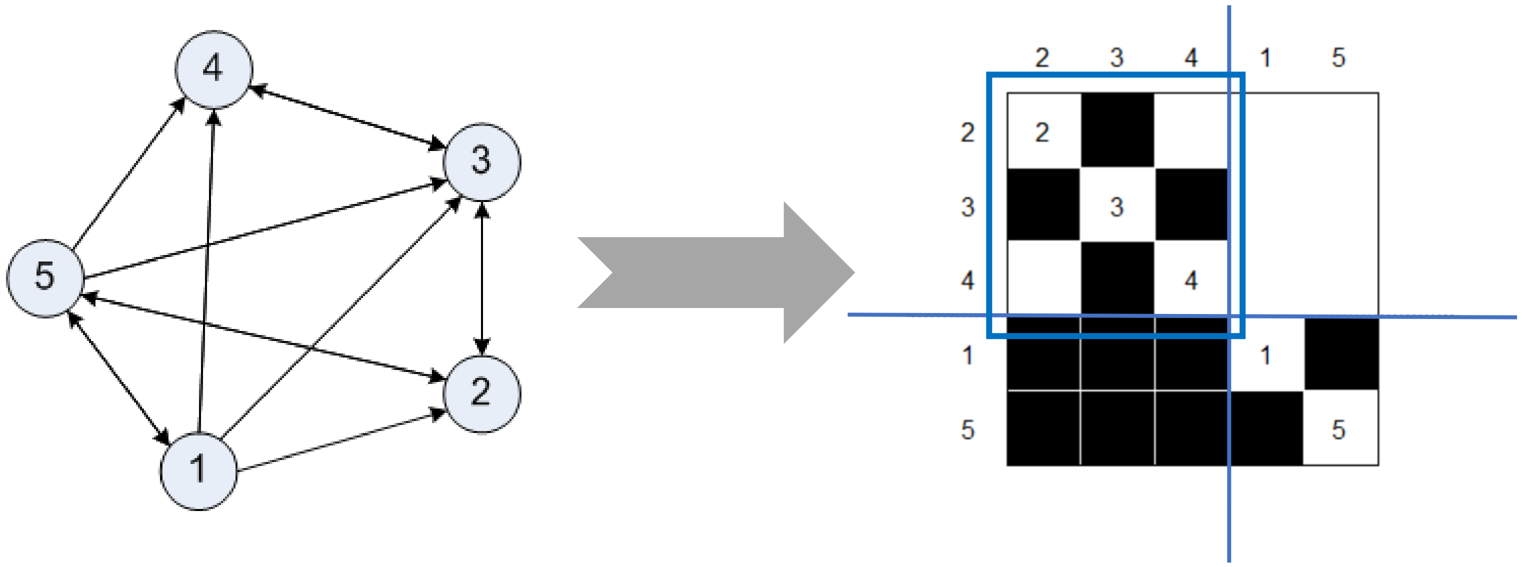
CONCOR

- CONvergence of iterated CORrelations (CONCOR) is a *hierarchical divisive* method to discover roles according to the definition of structural equivalence.
- Procedure:

1. Calculate correlations, e.g., Pearson correlation, between rows (or columns) repeatedly on the adjacency matrix until the resultant correlation matrix consists of +1 and -1 entries;
2. Split the last correlation matrix into two structurally equivalent submatrices (a.k.a. blocks): one with +1 entries, another with -1 entries.

CONCOR

- The split in the 2nd step can be further applied to submatrices in order to produce a hierarchy
- Nodes in the same submatrix belong to the same role



Procedure:

1. Compute correlations
2. Split the correlation matrix into blocks

STRUCTURE

STRUCTURE is a hierarchical agglomerative approach. It consists of three steps:

1. For each node u, create its feature vector by concatenating its row and column vectors from the adjacency matrix;
2. For each pair of nodes (u, v), measure the square root of sum of squared differences between the corresponding entries in their feature vectors;
3. Merge entries in hierarchical fashion until their difference is less than a predefined threshold.

CONCOR VS STRUCTURE

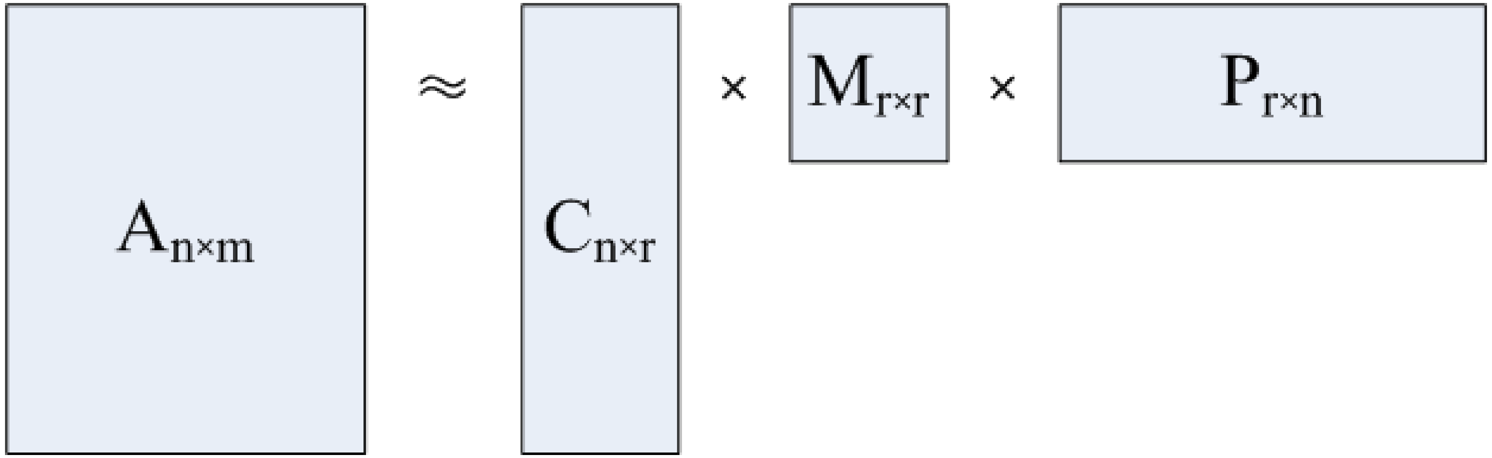
CONCOR

1. Calculate correlations between rows (or columns) repeatedly on the adjacency matrix
2. Split the last correlation matrix into two structurally equivalent blocks

STRUCTURE

1. Create its feature vector from the adjacency matrix;
2. Measure the square root of sum of squared differences between pairs of nodes;
3. Merge entries in hierarchical fashion until their difference is less than a predefined threshold.

Nonnegative Matrix Tri-Factorization (NMTF)



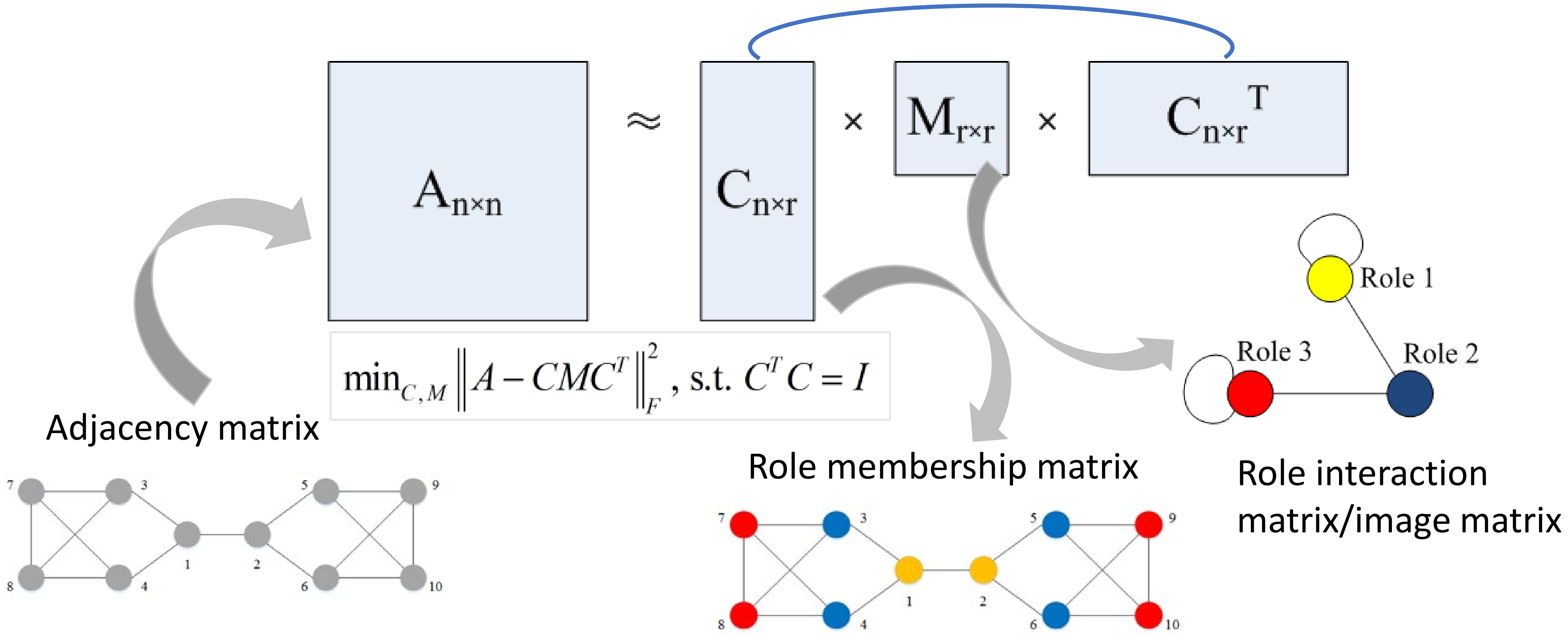
Objective:

$$\min_{C,M,P} \left\| A - CMP \right\|_F^2$$

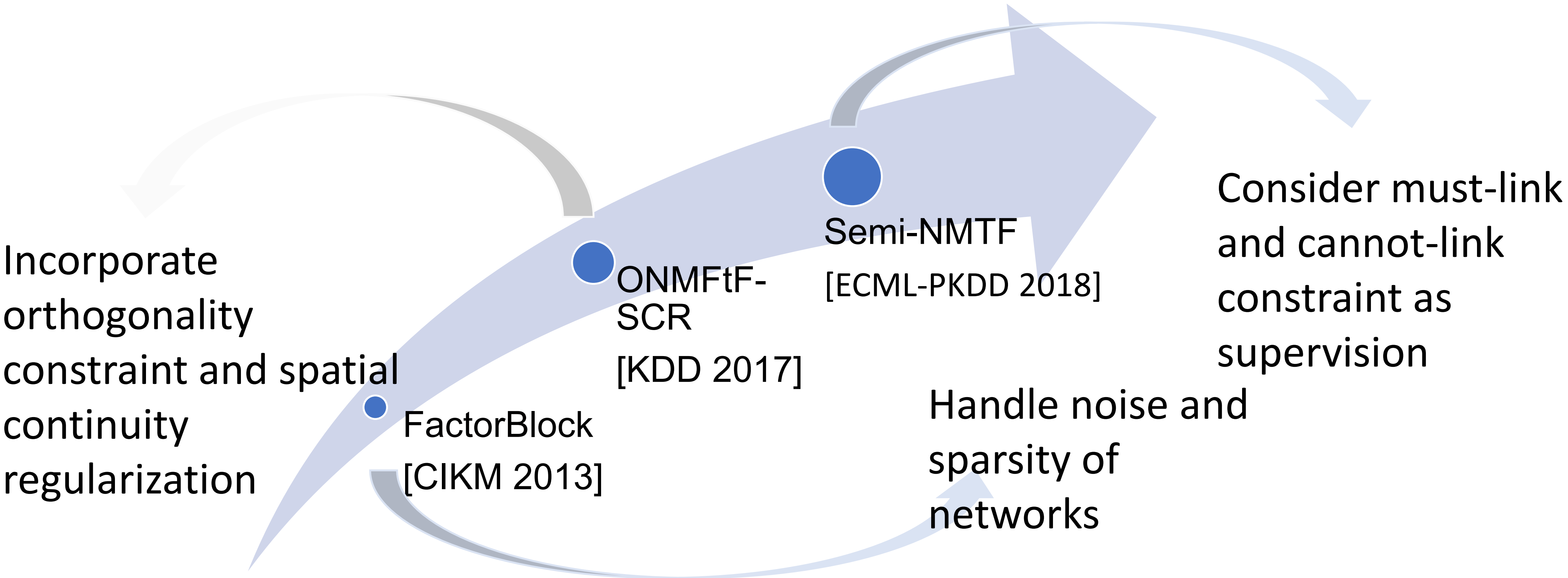
Optimization

- multiplicative update rule
- alternating direction method of multipliers (ADMM)

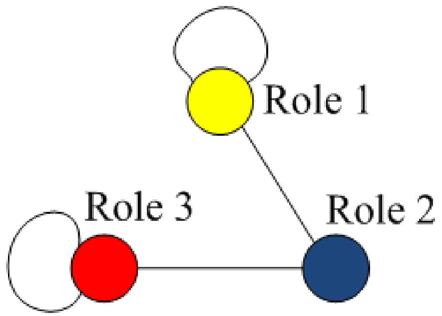
NMTF-based Role Analytics Method



NMTF Extensions



FactorBlock [Chan et al., CIKM 2013]



$$\min_{C,M} \left\| A - CMC^T \right\|_F^2 ,$$

in the ideal case, the densities of the image matrix entries should either be 0 or 1

use the density of the graph as
a background model

$$\min_{C,M} \left\| \boxed{\left(A - CMC^T\right)} \circ \boxed{U \Big\|_F^2} + \boxed{\left\| M_{ideal} - M \right\|_F^2} ,$$

s.t. $C^T C = I$

U=A-R, where A is the adj. matrix
And $R_{ij}=m/n^2$

Standard NMTF-based Role Analytics

Ideal image matrix M_{ideal} is approximately defined as

$$\mathrm{M_{ideal}} = \frac{1}{1+\gamma e^{-\upsilon(\mathrm{M}-\tau)}}$$

ONMFtF-SCR [Bai et al., KDD 2017]

- Model structural equivalence relation
- Incorporate orthogonality constraint and spatial continuity regularization
- Θ is a reciprocal Gaussian Kernel matrix for each pair of nodes, which is defined as

$$\min_{C,M} \left\| A - CMC^T \right\|_F^2$$

spatial continuity
regularization

$$\min_{C,M} \left\| A - CMC^T \right\|_F^2 + \beta \bullet Tr(C^T \Theta C),$$

$$\text{s.t. } C^T C = I$$

orthogonality c
onstraint

$$(\Theta)_{ij} = e^{\frac{\|\mathbf{v}_i - \mathbf{v}_j\|_2^2}{2\sigma^2}}$$

v_i indicates the
spatial location of node i

Semi-NMTF [Ganji et al., ECML-PKDD 2018]

$$\min_{C,M} \left\| A - CMC^T \right\|_F^2$$

- take advantage of the existing information that might be available about objects that are known to be similar

$$\min_{C,M} \left\| A - CMC^T \right\|_F^2 + \frac{1}{2}(1-C)\circ(Q_{ML}\bullet C) + \frac{1}{2}C\circ(Q_{CL}\bullet C)$$

- can help finding complex patterns, such as hierarchical or ring blockmodel structures

Q_{ML} and Q_{CL} are non-negative real valued matrices quantifying the cost of violating each of the must-link and cannot-link constraints respectively

NMTF Extensions

FactorBlock
[CIKM 2013]

Handle noise and sparsity of networks

ONMFtF-SCR
[KDD 2017]

Incorporate orthogonality constraint and spatial continuity regularization

Semi-NMTF
[ECML-PKDD 2018]

Consider must-link and cannot-link constraint as supervision

Roles in Networks - Foundations, Methods and Applications

Coffee/Tea Break

ICDM 2021
IEEE International Conference on Data Mining
7 – 10 DECEMBER 2021
AUCKLAND NEW ZEALAND

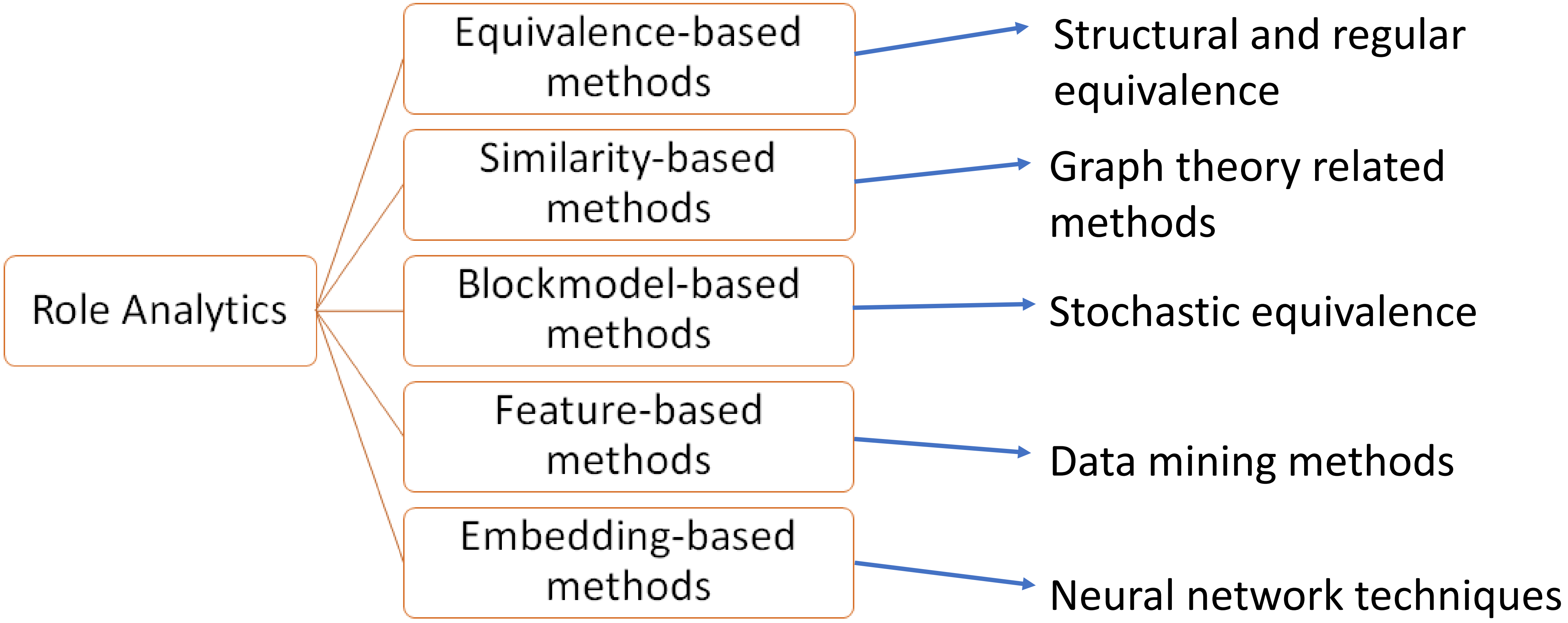
TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

天津大学 Tianjin University

Outline

- What is and Why Role Analytics?
- Equivalence Relations
- Taxonomy of Role Analytics Methods
- Role-oriented Network Embedding
- Challenges and Outlook

Taxonomy of Role Analytics Methods



Similarity-based Methods

Partition/Clustering → Similarity

Connection Sim

SimRank
[Jeh and Widom, KDD 2002]

MatchSim
[Lin et al., CIKM 2009]

RoleSim
[Jin et al., KDD 2011, TKDD 2014]

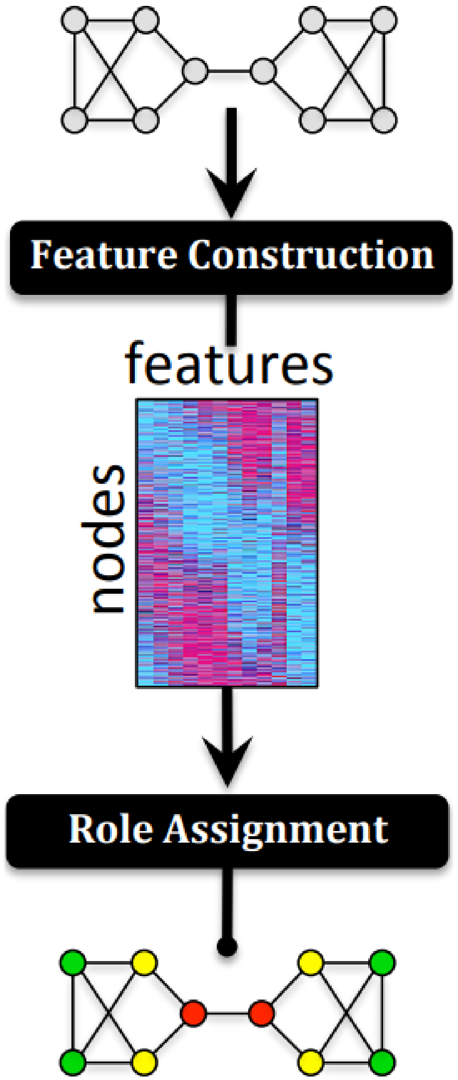
NED
[Zhu et al., VLDB 2017]

StructSim
[Chen et al. ICDE 2020]

Feature-based Methods

General framework of feature-based methods consists of two steps:

- feature extraction
- role assignment



Feature-based Methods: Feature Extraction

Features							
Graph Theories			Social Theories			Calculated Features	
1st order: e.g., degrees	2nd order: e.g., common neighbors	Higher order: e.g., centrality	Homophily	Triadic closure	Structural holes	product, sum, min, max, average	Network embedding

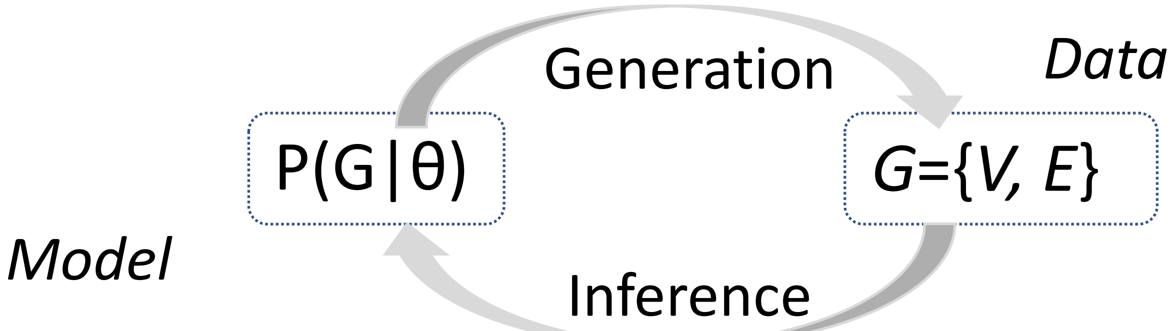
Blockmodel-based Methods

- Aim to solve the role analytics problem based on stochastic equivalence
  - Two nodes *i* and *j* are stochastically equivalent if they are “exchangeable” w.r.t. a probability distribution.
  - The probability distribution of the graph must remain the same when equivalent nodes are exchanged.
- Generative models based on Bayesian statistics

Stochastic Blockmodel (SBM) [Holland et al., Social Networks, 1983]

- A stochastic blockmodel (SBM) is a generative model that yields a probability distribution over the set of possible role assignments to nodes given the observed structure of a network.

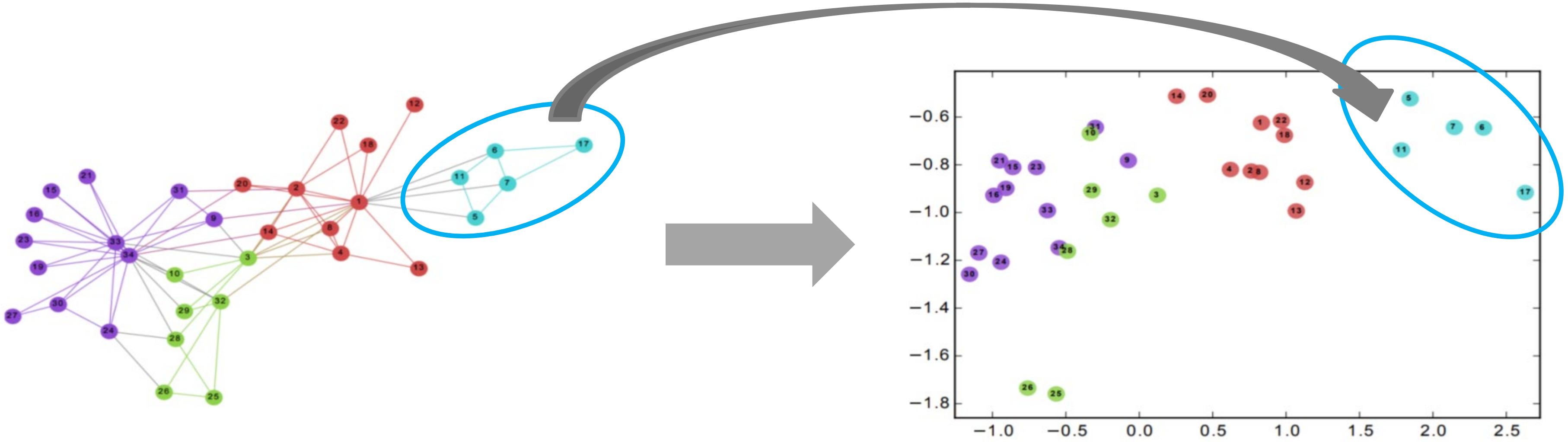
- a partition of the node set into disjoint subsets $C_1, C_2, \ldots, C_r$
- a symmetric matrix P_{r*r} of role interaction probabilities.



Embedding-based Methods

Network embedding methods aim at learning low-dimensional latent representations of nodes in a graph.

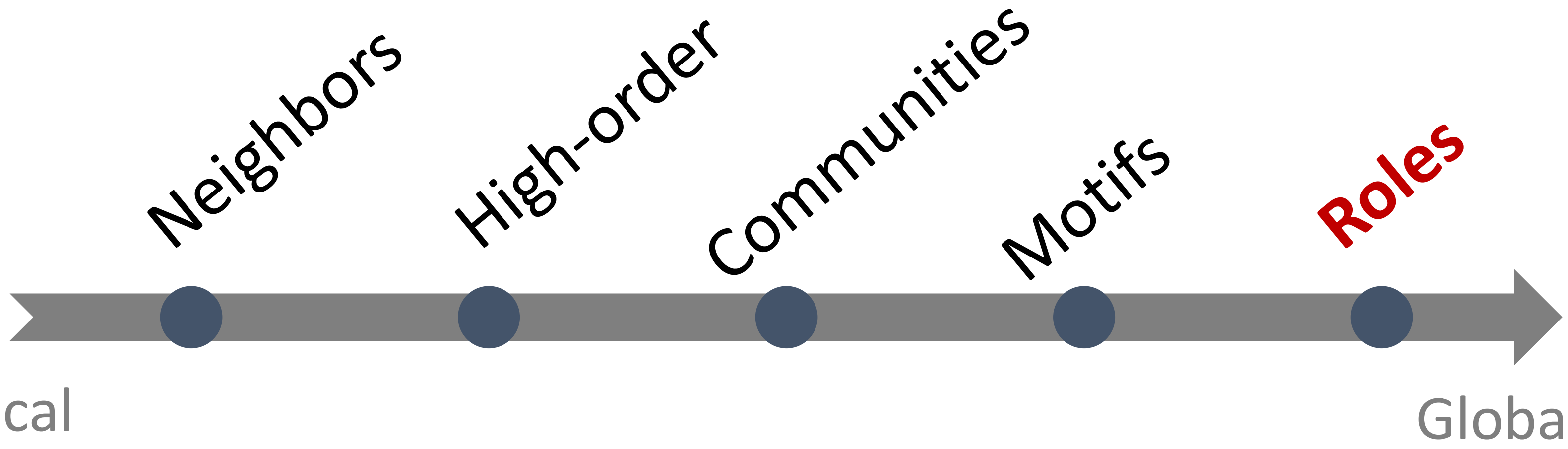
- preserve the graph structures
- can be used as features for downstream tasks



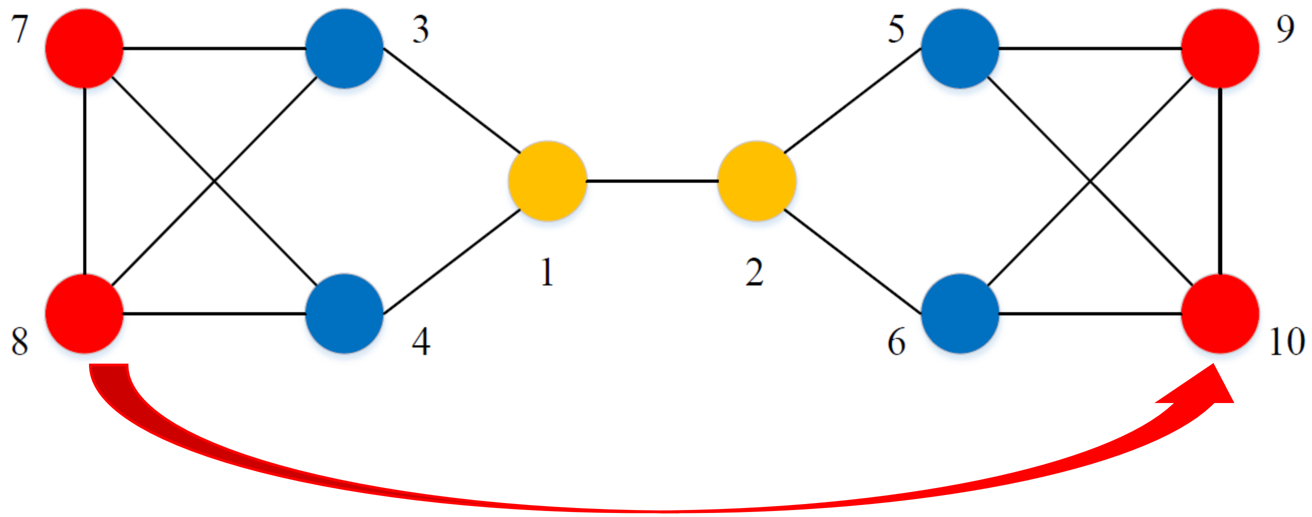
NRL: Preserving Structures

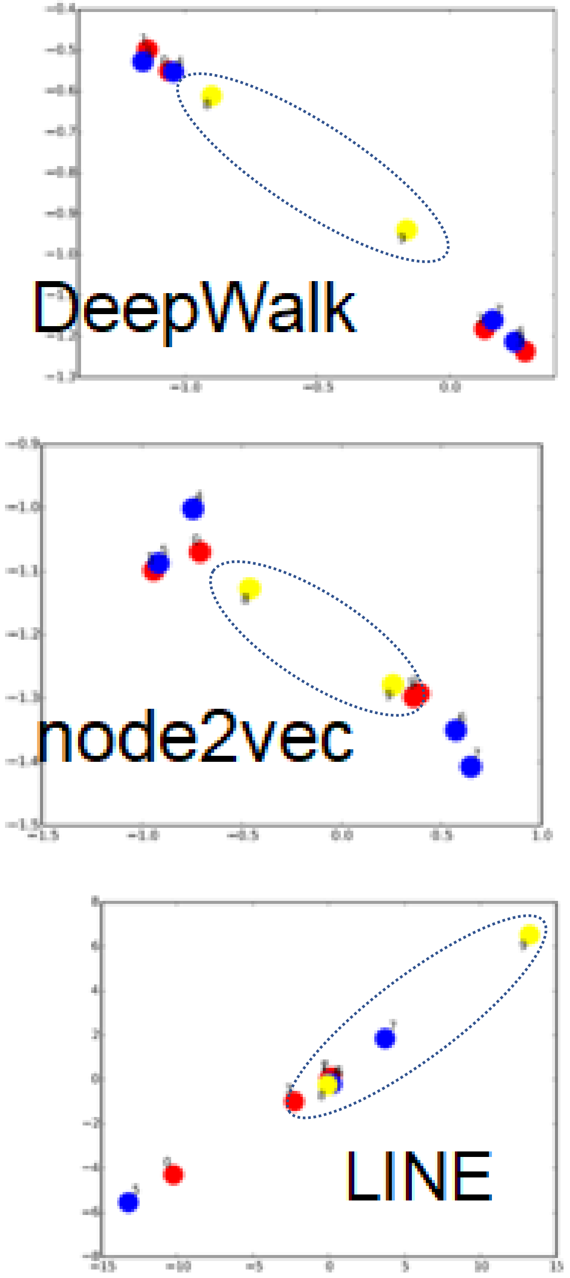
Network representation learning (NRL) aims at learning low-dimensional latent representations of nodes in a graph which can **preserve the graph structures**

What graph structures to preserve?



Network Embedding: Issues



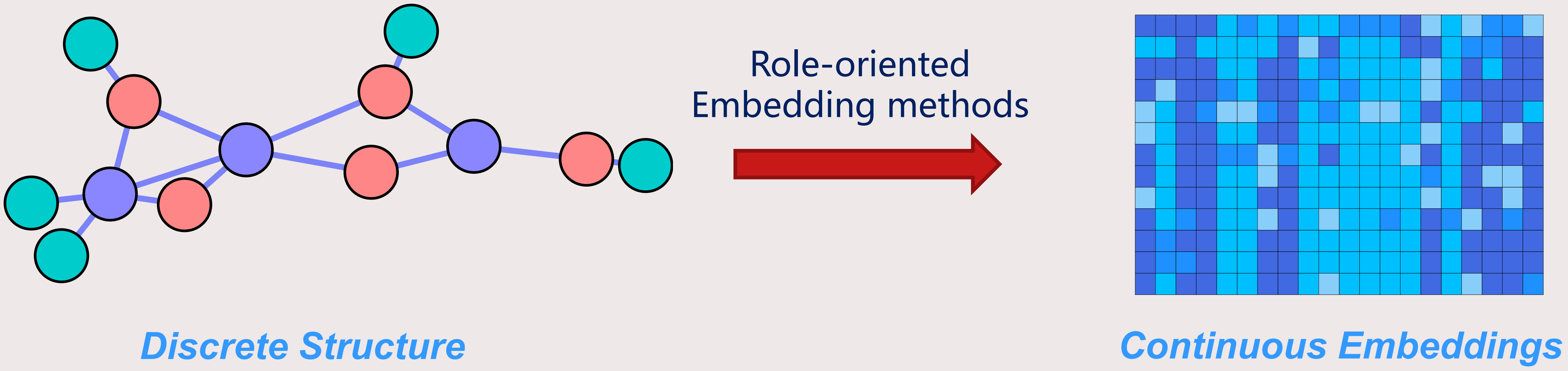


- Role: Global Structures

- Random Walk ?

The Taxonomy of RONE methods :

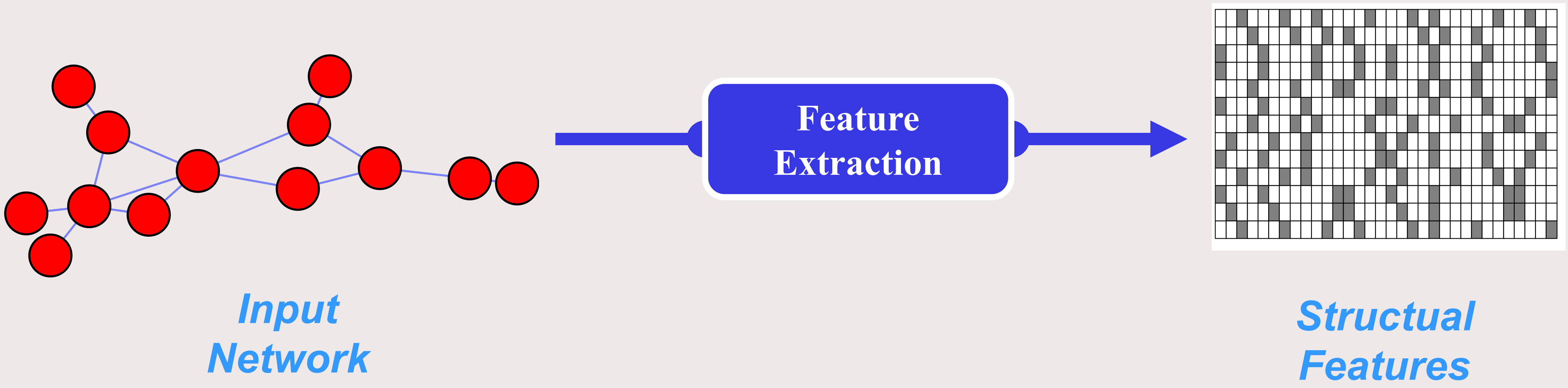
The Aim of Role-oriented Network Embedding (RONE) methods :



- The two-step process of RONE methods to bridge the gulf between two spaces :
  a. Structure Property Extraction
  b. Embeddings

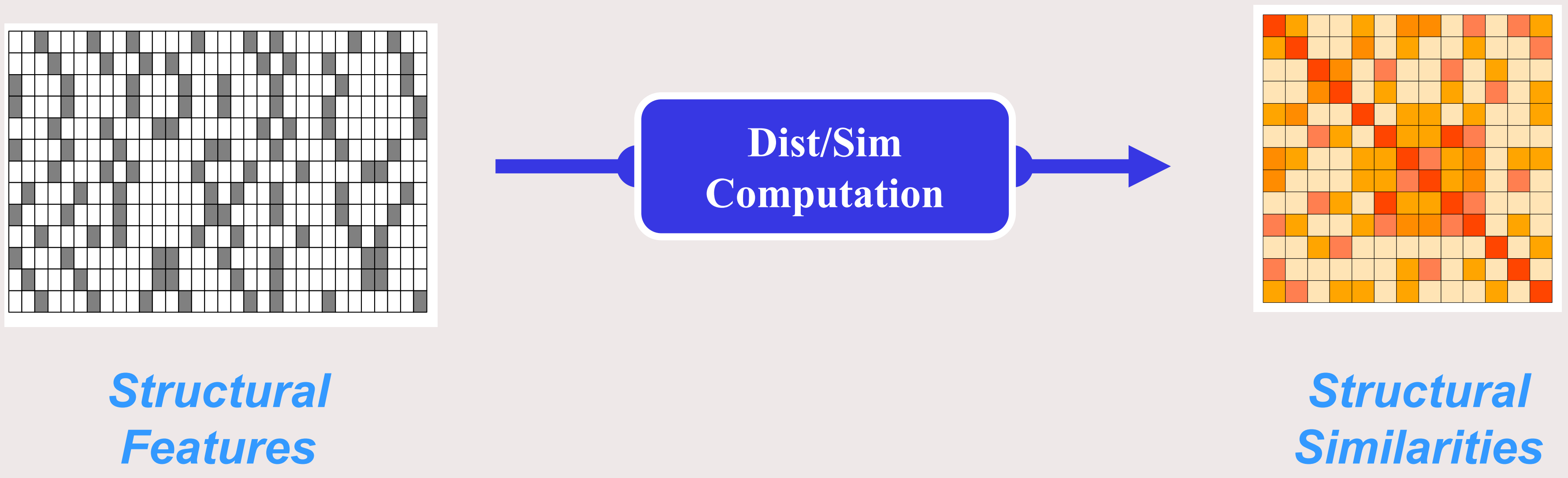
Tianjin University

a. Structure Property Extraction:
1.Some methods leverage structural features such as node degrees and triangle numbers. (RolX [1]; DRNE [2])



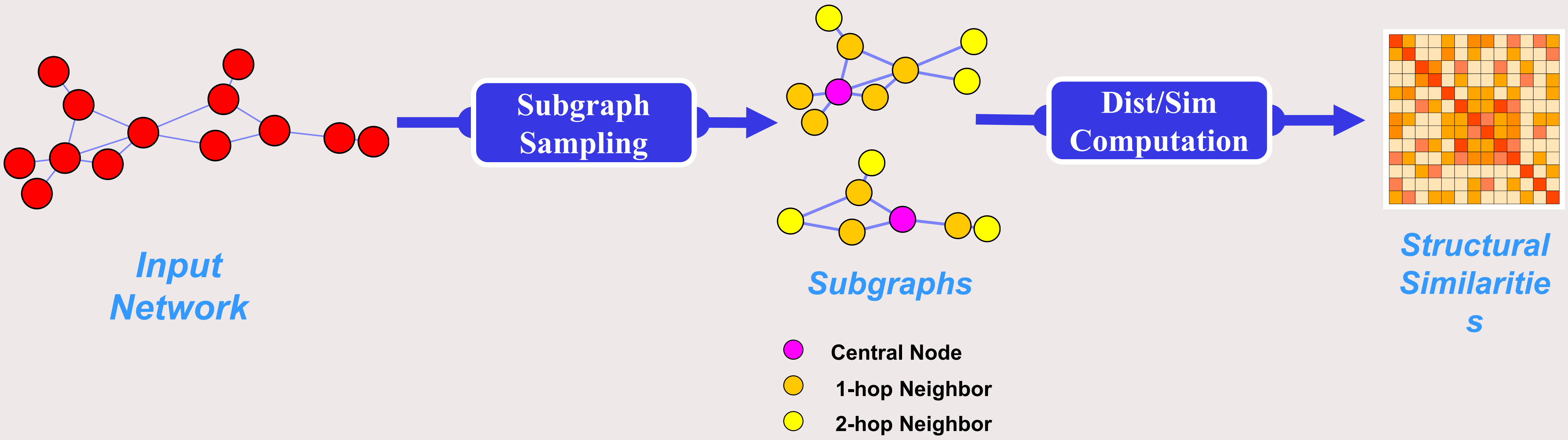
TU/e

a. Structure Property Extraction:
2.Some methods continue to transform the features into continuous distances or similarities. (SPINE [3])



Tianjin University

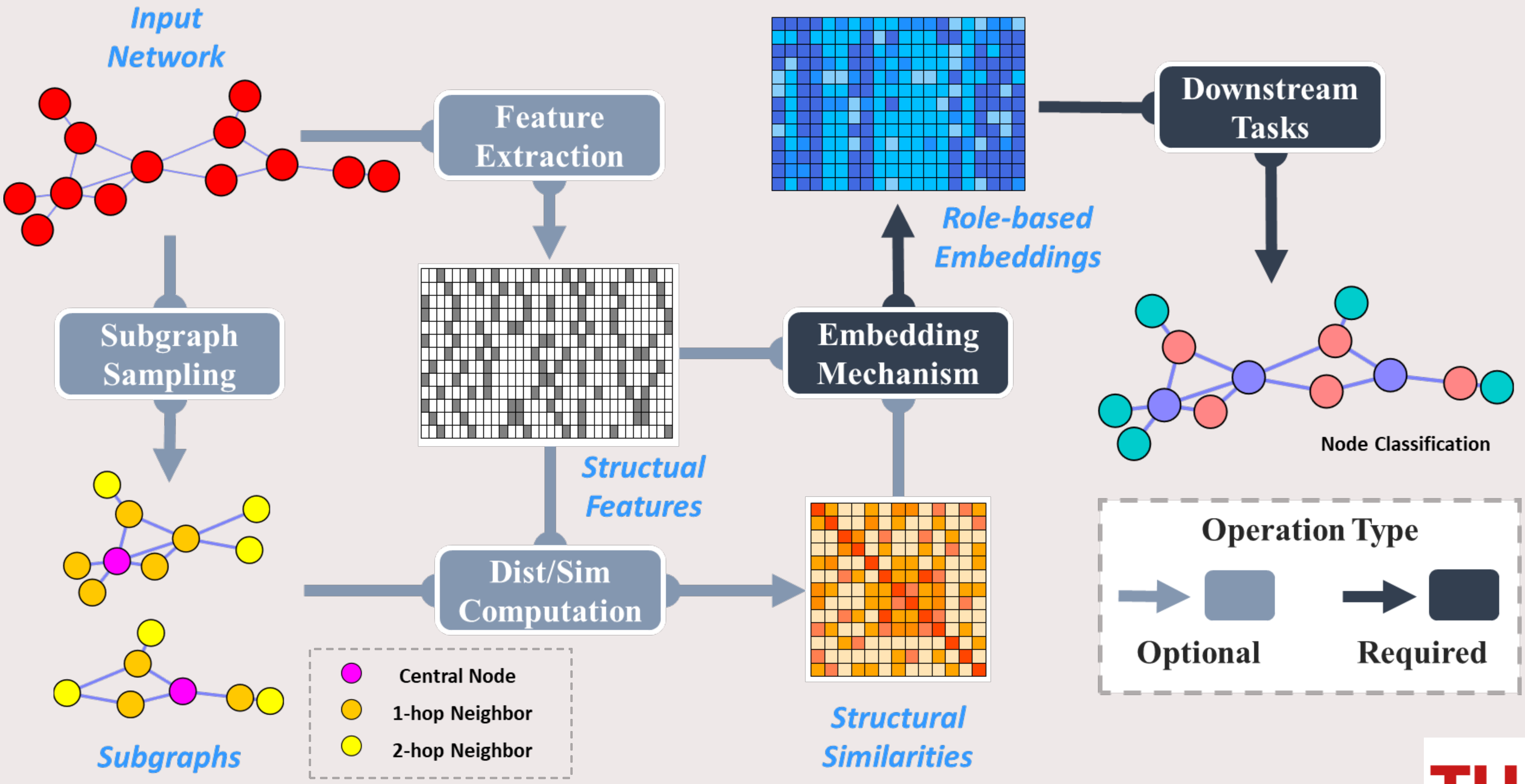
a. Structure Property Extraction:
3.Some methods captureing similarity between node-centric subgraphs. (struc2vec [4]; SEGK [5])



TU/e

The Taxonomy of RONE methods :

天津大学 Tianjin University



TU/e

Jiao, Pengfei, Xuan Guo, Ting Pan, Wang Zhang, and Yulong Pei. "A Survey on Role-Oriented Network Embedding." *arXiv preprint arXiv:2107.08379* (2021).

The new two-level categorization :

Method	Embedding Mechanism		Conducted Tasks				Year
			Vis	CLF/CLT	ER/NA/SS	LP	
RolX	low-rank matrix factorization	on structural feature matrix	✔	✔	✘	✘	2012
GLRD			✘	✘	✔	✘	2013
RIDεRs			✔	✔	✔	✘	2017
GraphWave			✔	✔	✘	✘	2018
HONE			✔	✘	✔	✔	2020
xNetMF		on structural similarity matrix	✘	✘	✔	✘	2018
EMBER			✘	✔	✔	✘	2019
SEGK			✔	✔	✔	✘	2019
REACT			✘	✔	✘	✘	2019
SPaE			✔	✔	✘	✘	2019
struc2vec	random walk-based methods	on similarity-biased random walks	✔	✔	✘	✘	2017
SPINE			✘	✔	✘	✘	2019
struc2gauss			✔	✔	✘	✘	2020
Role2Vec		on feature-based random walks	✘	✘	✘	✔	2019
RiWalk			✘	✔	✘	✘	2019
NODE2BITS			✘	✘	✔	✘	2019
DRNE	deep learning	via structural information reconstruction/guidance	✔	✔	✘	✘	2018
GAS			✔	✔	✘	✘	2020
RESD			✔	✔	✔	✘	2021
GraLSP			✔	✔	✘	✔	2020
GCC			✘	✔	✔	✘	2020
RDAA			✔	✔	✘	✘	2021
CNESE			✔	✔	✔	✘	2021

Jiao, Pengfei, Xuan Guo, Ting Pan, Wang Zhang, and Yulong Pei. "A Survey on Role-Oriented Network Embedding." *arXiv preprint arXiv:2107.08379* (2021).

The new two-level categorization :

Method	Embedding Mechanism		Conducted Tasks				Year
			Vis	CLF/CLT	ER/NA/SS	LP	
RolX	low-rank matrix factorization	on structural feature matrix	✓	✓	✗	✗	2012
GLRD			✗	✗	✓	✗	2013
RIDεRs			✓	✓	✓	✗	2017
GraphWave			✓	✓	✗	✗	2018
HONE			✓	✗	✓	✓	2020
xNetMF		on structural similarity matrix	✗	✗	✓	✗	2018
EMBER			✗	✓	✓	✗	2019
SEGK			✓	✓	✓	✗	2019
REACT			✗	✓	✗	✗	2019
SPaE			✓	✓	✗	✗	2019
struc2vec	random walk-based methods	on similarity-biased random walks	✓	✓	✗	✗	2017
SPINE			✗	✓	✗	✗	2019
struc2gauss			✓	✓	✗	✗	2020
Role2Vec		on feature-based random walks	✗	✗	✗	✓	2019
RiWalk			✗	✓	✗	✗	2019
NODE2BITS			✗	✗	✓	✗	2019
DRNE	deep learning	via structural information reconstruction/guidance	✓	✓	✗	✗	2018
GAS			✓	✓	✗	✗	2020
RESD			✓	✓	✓	✗	2021
GraLSP			✓	✓	✗	✓	2020
GCC			✗	✓	✓	✗	2020
RDAA			✓	✓	✗	✗	2021
CNESE			✓	✓	✓	✗	2021

Jiao, Pengfei, Xuan Guo, Ting Pan, Wang Zhang, and Yulong Pei. "A Survey on Role-Oriented Network Embedding." *arXiv preprint arXiv:2107.08379* (2021).

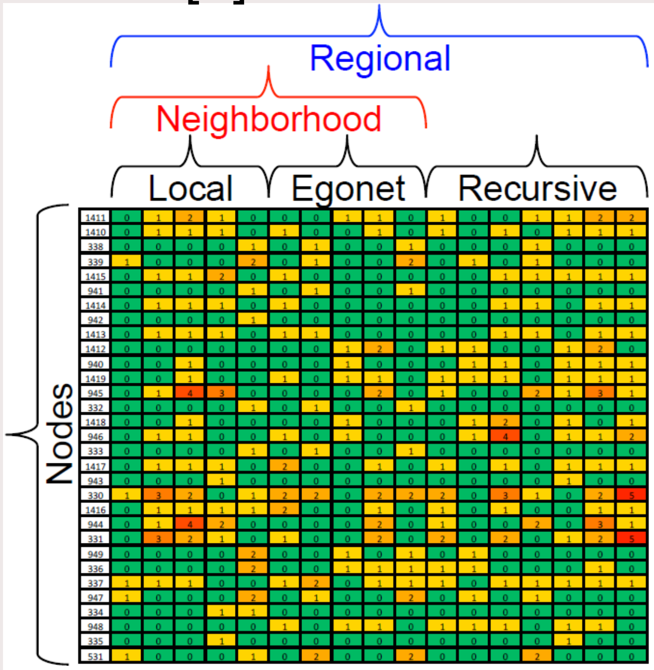
Low-rank matrix factorization based methods :

RolX (Role eXtraction) [1]:

Structural Feature
Matrix Factorization

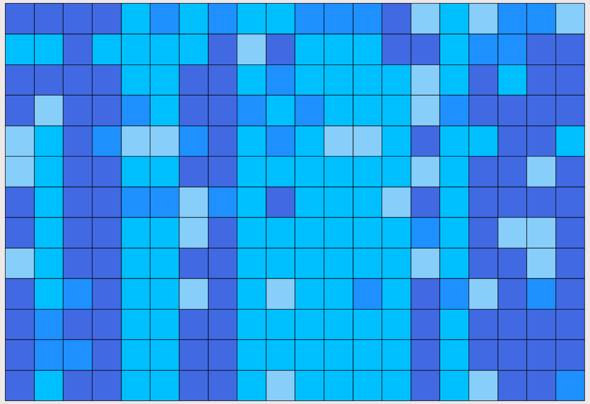
Feature matrix generated by ReFeX [6]:

- Neighborhood features
  - Local and egonet features, e.g., degrees
  - Representations of connectivity patterns
- Recursive Features
  - Calculated features
  - Generated using means, sums and pruning



Structural Features

NMF



Role-oriented Embeddings

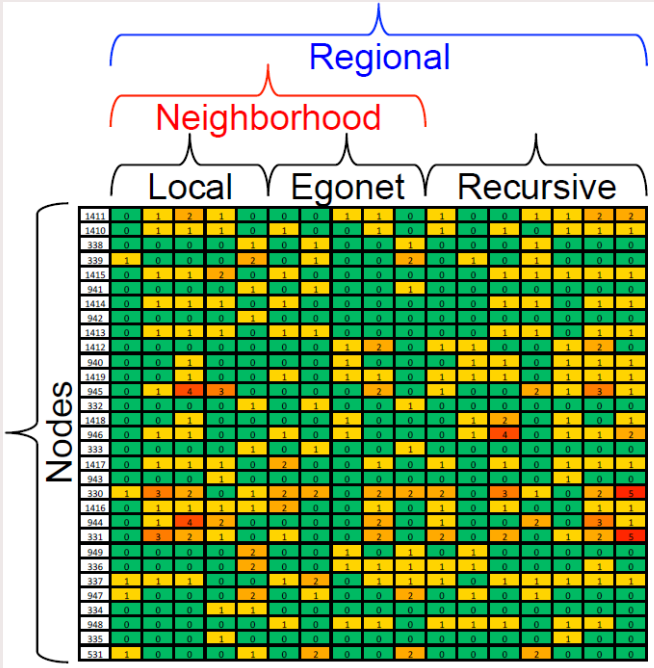
$$\min_{\mathbf{H},\mathbf{M}} \left|\left|\mathbf{F}_{ReFeX} - \mathbf{HM}\right|\right|_F^2, \ s.t.\ \mathbf{H},\mathbf{M} \geq 0$$

TU/e

Tianjin University

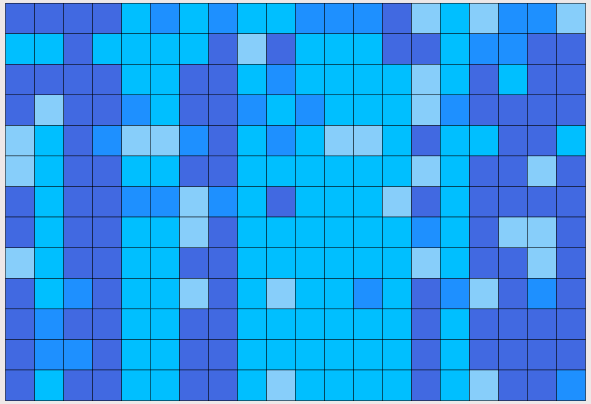
GLRD: (Guided Learning for Role Discovery) [7]:

Structural Feature Matrix Factorization



Structural Features

NMF



Role-oriented Embeddings

$$\min_{\mathbf{H},\mathbf{M}} \left\|\mathbf{F}_{ReFeX} - \mathbf{HM}\right\|_F^2, \; s.t.\; \mathbf{H},\mathbf{M} \geq 0$$

+

Optional Constraints in GLRD.

Constraint	Formula
Sparsity	$\forall i \;\; \|\mathbf{H}_{\cdot i}\|_1 \leq \epsilon_{\mathbf{H}}$ $\forall i \;\; \|\mathbf{M}_{i\cdot}\|_1 \leq \epsilon_{\mathbf{M}}$
Diversity	$\forall i,j \;\; \mathbf{H}_{\cdot i}^{\top}\mathbf{H}_{\cdot j} \leq \epsilon_{\mathbf{H}} \;\; i \neq j$ $\forall i,j \;\; \mathbf{M}_{i\cdot}\mathbf{M}_{j\cdot}^{\top} \leq \epsilon_{\mathbf{M}} \;\; i \neq j$
Alternativeness	$\forall i,j \;\; \mathbf{H}_{\cdot i}^{*\top}\mathbf{H}_{\cdot j} \leq \epsilon_{\mathbf{H}} \;\; i \neq j$ $\forall i,j \;\; \mathbf{M}_{i\cdot}^{*}\mathbf{M}_{j\cdot}^{\top} \leq \epsilon_{\mathbf{M}} \;\; i \neq j$

GLRD: (Guided Learning for Role Discovery) [7]:

Structural Feature Matrix Factorization

$$\min_{\mathbf{H},\mathbf{M}} \left\| \mathbf{F}_{ReFeX} - \mathbf{HM} \right\|_F^2, \quad s.t. \ \mathbf{H},\mathbf{M} \geq 0$$

+

Optional Constraints in GLRD.

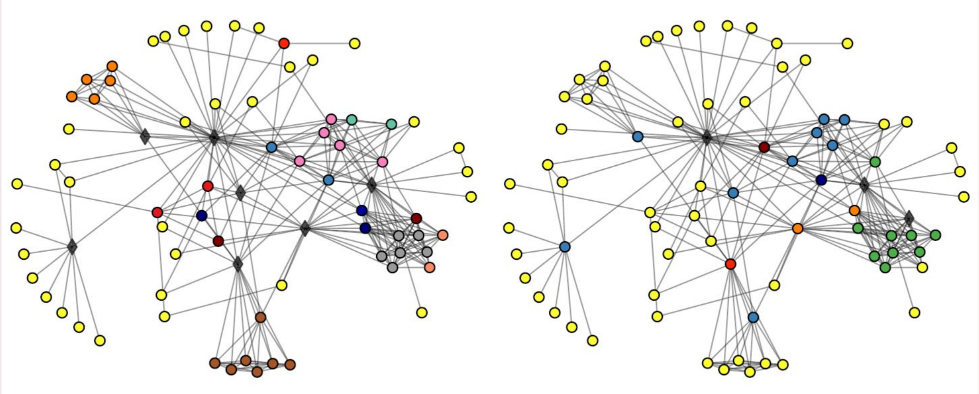
Constraint	Formula
Sparsity	$\forall i \quad \|\mathbf{H}_{\cdot i}\|_1 \leq \epsilon_{\mathbf{H}}$ $\forall i \quad \|\mathbf{M}_{i\cdot}\|_1 \leq \epsilon_{\mathbf{M}}$
Diversity	$\forall i,j \quad \mathbf{H}_{\cdot i}^\top \mathbf{H}_{\cdot j} \leq \epsilon_{\mathbf{H}} \quad i \neq j$ $\forall i,j \quad \mathbf{M}_{i\cdot}\mathbf{M}_{j\cdot}^\top \leq \epsilon_{\mathbf{M}} \quad i \neq j$
Alternativeness	$\forall i,j \quad \mathbf{H}_{\cdot i}^{*\top} \mathbf{H}_{\cdot j} \leq \epsilon_{\mathbf{H}} \quad i \neq j$ $\forall i,j \quad \mathbf{M}_{i\cdot}^{*}\mathbf{M}_{j\cdot}^\top \leq \epsilon_{\mathbf{M}} \quad i \neq j$

Types	On Role Membership Matrix (G)	On Role-Feature Association Matrix (F)
Sparsity	Encourages role assignments to be more definitive; Reduces number of nodes that have minority membership in role.	Increases ability to interpret role by using feature most strongly correlated with role; Decreases likelihood that features with small explanatory benefit be included.
Diversity	Roles cannot have memberships that are too similar; Limits amount of allowable overlap in assignments.	Roles cannot have definitions that are too similar; Roles must be explained with completely different sets of features.
Alternativ e	Find a role that lends itself to a different role assignment than a provided one; Decreases the allowable similarity between two sets of role assignments	Learn a role definition matrix that is significantly different than a provided role definition; Ensures that the definitions must be very dissimilar.

Low-rank matrix factorization based methods :

Structural Feature Matrix Factorization

RID$\mathcal{E}$Rs: ((Role Identification and Discovery using ε-equitable Refinement) [8]:



Les Mis´erables Network: Roles discovered by εER for ε = 2 and ε = 6 respectively.

- Partition nodes into different cells based on ε-equitable refinement:

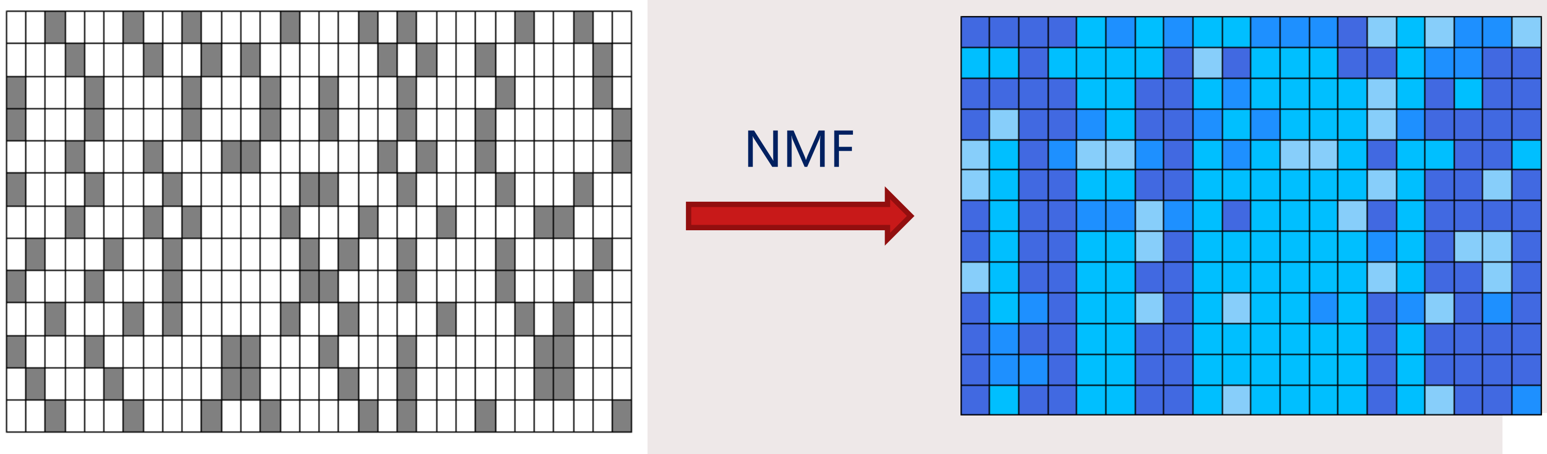
$$\deg(u,\mathcal{C}_j) = |\{u|(u,v) \in E \wedge v \in \mathcal{C}_j\}|$$

$$|\deg(u,\mathcal{C}_j) - \deg(v,\mathcal{C}_j)| \le \varepsilon, \forall u,v \in \mathcal{C}_j, \forall 1 \le i,j \le K$$

- Compute global features :

$$(\mathbf{F}^{\varepsilon}_{\varepsilon ER})_{ij} = |\mathcal{N}_i \cap \mathcal{C}_j|$$

- Prune and Bin.



Structural Features

Role-oriented Embeddings

Low-rank matrix factorization based methods：

天津大学 Tianjin University

GraphWave [9]:

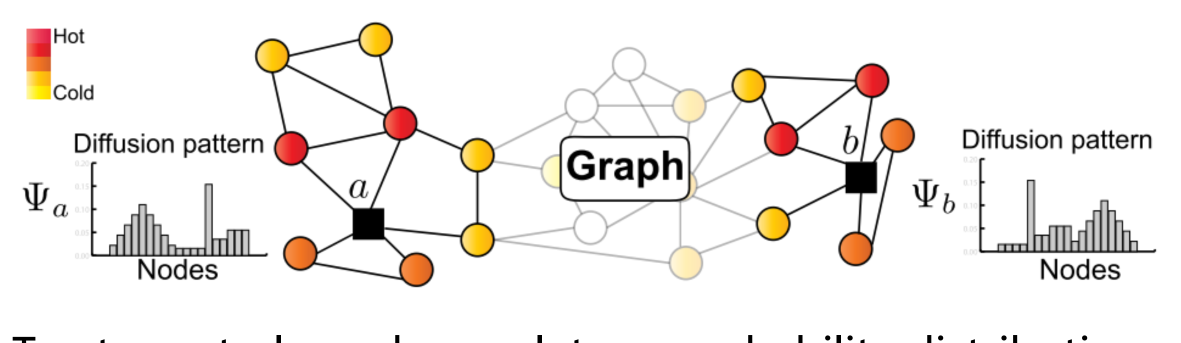
Structural Feature Matrix Factorization

- Spectral graph wavelets:

$$\mathbf{L} = \mathbf{D} - \mathbf{A}$$

$$\mathbf{L} = \mathbf{U}\Lambda\mathbf{U}^\top \quad \Lambda = \mathrm{Diag}(\lambda_1, \dots, \lambda_n)$$

$$\mathbf{\Psi} = \mathcal{I}\mathbf{U}\mathrm{Diag}(g_\varsigma(\lambda_1), \dots, g_\varsigma(\lambda_n))\mathbf{U}^\top$$



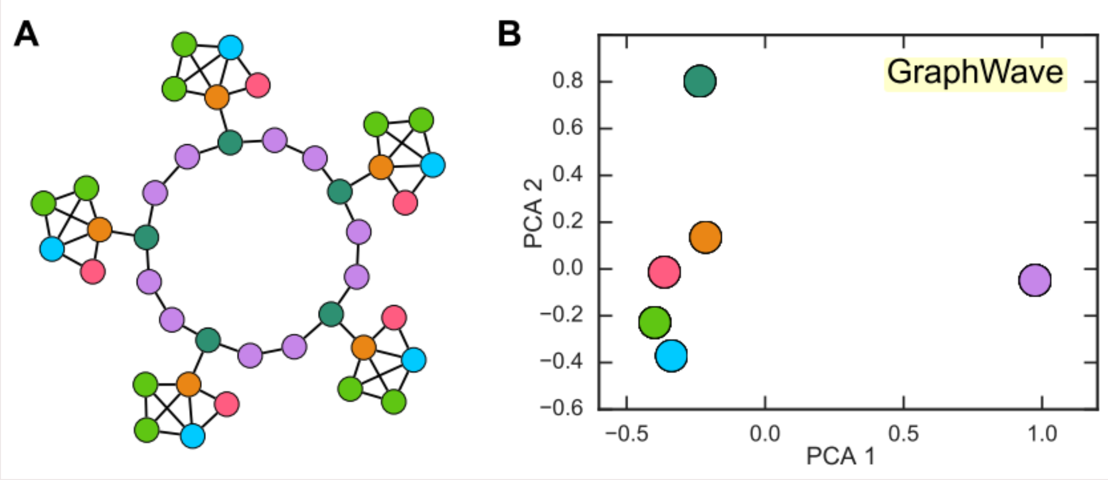
Treat spectral graph wavelets as probability distributions.

- Empirical characteristic function:

$$\varphi_i(t) = \frac{1}{n}\sum_{j=1}^{n} e^{it\mathbf{\Psi}_{ij}}$$

- Embedding:

$$\mathbf{H}_i = [\mathrm{Re}(\varphi_i(t)), \mathrm{Im}(\varphi_i(t))]$$



2D PCA projection of GraphWave’ s embeddings

TU/e

Tianjin University

HONE (Higher-Order Network Embeddings) [10]:

Structural Feature Matrix Factorization

- For each motif, generate k-step embeddings:

$$\underset{\mathbf{H}^{(k)}_{\mathcal{M}_m}, \mathbf{M}^{(k)}_{\mathcal{M}_m}}{\arg\min} \ \mathbb{D}_{Breg}(\mathbf{F}^{(k)}_m | \Psi(\mathbf{H}^{(k)}_{\mathcal{M}_m} \mathbf{M}^{(k)}_{\mathcal{M}_m}))$$

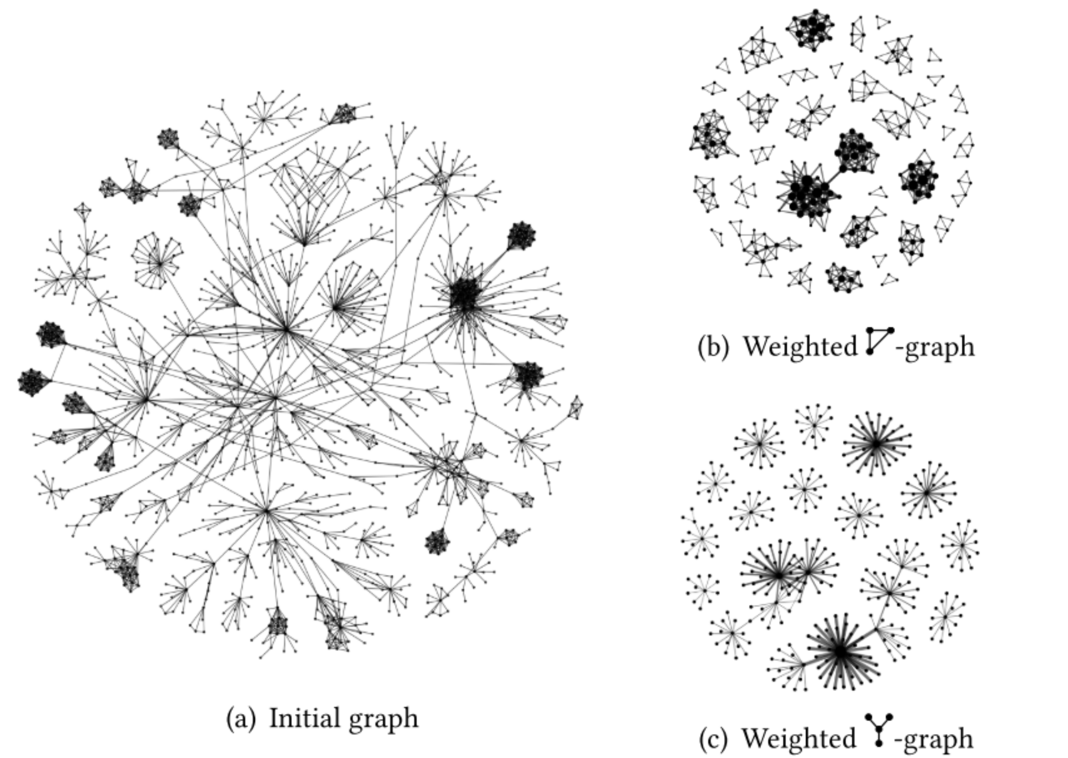
$$\mathbf{P} = \mathbf{D}^{-1}\mathbf{A} \quad \cdots \quad \mathbf{L} = \mathbf{D} - \mathbf{A}$$

Feature matrix transformed from the k-step weighted motif adjacency matrix.

- Global embeddings:

$$\min_{\mathbf{H},\mathbf{M}} \left\|\mathbf{F}_{HONE} - \mathbf{HM}\right\|_F^2$$

Concatenated $\mathbf{H}^{(k)}_{\mathcal{M}_m}$ with all k and m.



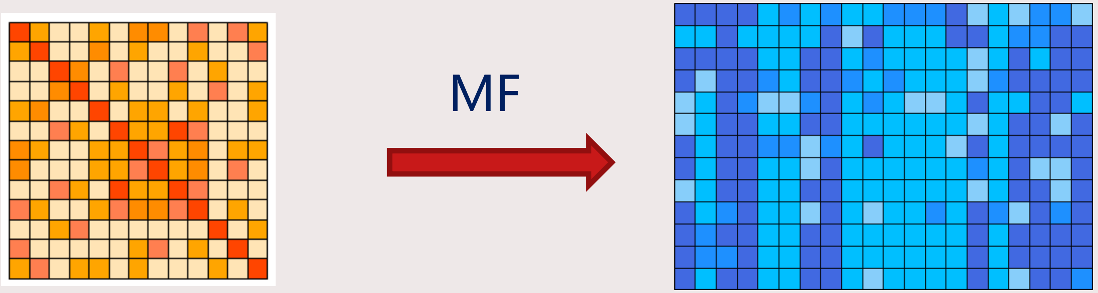
Weighted Motif Graphs

TU/e

Low-rank matrix factorization based methods :

xNetMF (Cross-Network Matrix Factorization) [11]:

Structural Similarity
Matrix Factorization



Structural Similarities

Role-oriented Embeddings

Nyström method

$$\mathbf{S}_{ij} = \exp(-\gamma_s \mathrm{dist}_s(v_i, v_j) - \gamma_a \mathrm{dist}_a(v_i, v_j))$$

On features   On attributes

$$\mathbf{F}^k_{ic} = |\mathcal{D}^k_{i,c}| = |\{v_j \in \mathcal{N}^k_i \,|\, \lfloor \log_2 d_j \rfloor = c\}|$$

$$\mathbf{F}_i = \sum_{k=1}^{K} \delta^k \mathbf{F}^k_i$$

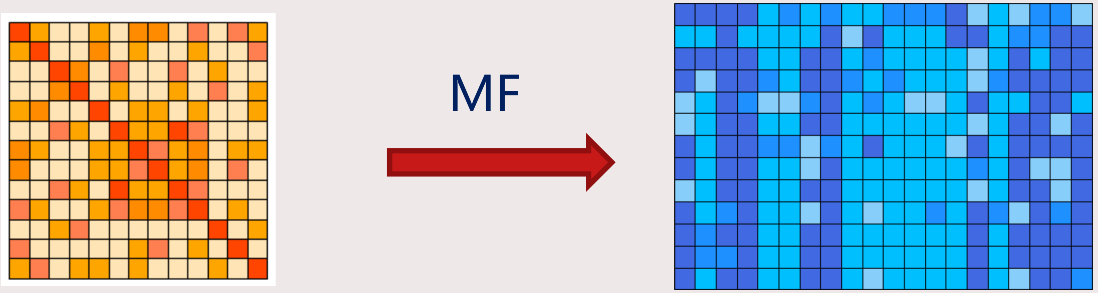
1) Select $r \ll n$ nodes as landmarks randomly or based on node centralities.
2) Compute a node-to-landmark similarity matrix $\mathbf{C} \in \mathbb{R}^{n \times r}$ and extract a landmark-to-landmark similarity matrix $\mathbf{B} \in \mathbb{R}^{r \times r}$ from $\mathbf{C}$.
3) Apply Singular Value Decomposition on the pseudoinverse of $\mathbf{B}$ so that $\mathbf{B}^{\dagger} = \mathbf{V}\mathbf{\Sigma}\mathbf{Y}^{\top}$.
4) Obtain embedding matrix $\mathbf{H}$ by computing and normailize $\mathbf{C}\mathbf{V}\mathbf{\Sigma}^{-\frac{1}{2}}$.

Low-rank matrix factorization based methods :

天津大学 Tianjin University

EMBER (EMBedding Email-based Roles) [13]:

Structural Similarity
Matrix Factorization



Structural Similarities

Role-oriented Embeddings

$$\mathbf{S}_{ij} = \exp(-\|\mathbf{F}_i - \mathbf{F}_j\|^2)$$

Nyström method is usd.

$$\mathbf{F}_{EMBER} = [\mathbf{F}^+, \mathbf{F}^-]$$

$$\mathbf{F}_{ic}^{k+} = \sum_{v_j \in \mathcal{D}_{i,c}^{k+}} \mathrm{pw}(\mathcal{P}_{v_i \to v_j}^{k+})$$

The product of all edge weights in a k-step shortest outgoing path

$$\mathbf{F}_i^+ = \sum_{k=1}^{K} \delta^k \mathbf{F}_i^{k+}$$

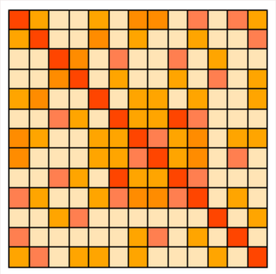
TU/e

Low-rank matrix factorization based methods :

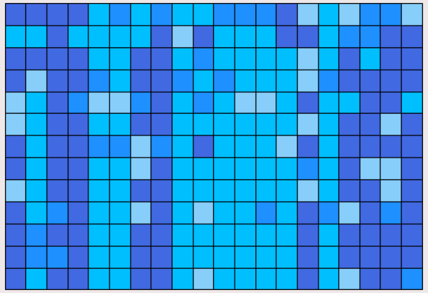
天津大学 Tianjin University

Structural Similarity Matrix Factorization

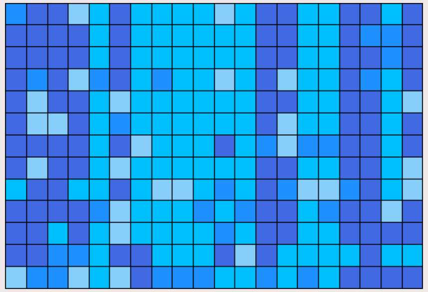
SPaE (hybrid network embedding method that unifies both structural proximity and equivalence (SPaE)) [14]:



MF



+



Structural Similaritie s

Role-oriented Embeddings

Community-oriented Embeddings

$$\max_{\mathbf{H}_R} \mathcal{J}_R = \mathrm{Tr}(\mathbf{H}_R^\top \mathbf{L_S} \mathbf{H}_R), \; s.t. \; \mathbf{H}_R^\top \mathbf{H}_R = \mathbf{I}.$$

$$\max_{\mathbf{H}_C} \mathcal{J}_C = \mathrm{Tr}(\mathbf{H}_C^\top \mathbf{L_A} \mathbf{H}_C), \; s.t. \; \mathbf{H}_C^\top \mathbf{H}_C = \mathbf{I}.$$

Computed based on Graphlet Degree Vectors

$$\max_{\mathbf{H}_R,\mathbf{H}_C,\mathbf{H}_H} \quad \mathcal{J}_R + \mathrm{p}_R + \gamma(\mathcal{J}_C + \mathrm{p}_C),$$
$$s.t. \; \mathbf{H}_R^\top \mathbf{H}_R = \mathbf{I}, \mathbf{H}_C^\top \mathbf{H}_C = \mathbf{I}, \mathbf{H}_H^\top \mathbf{H}_H = \mathbf{I}.$$

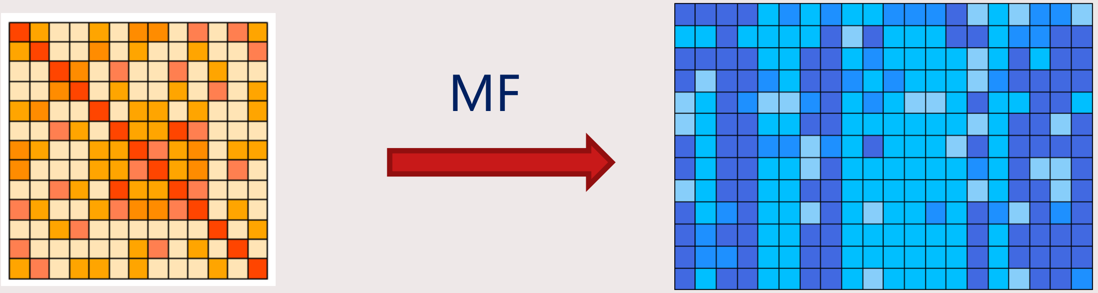
Computed based on adjacency matrix

$$\mathrm{p}_R = \mathrm{Tr}(\mathbf{H}_R^\top \mathbf{H}_H \mathbf{H}_H^\top \mathbf{H}_R) \qquad \mathrm{p}_C = \mathrm{Tr}(\mathbf{H}_C^\top \mathbf{H}_H \mathbf{H}_H^\top \mathbf{H}_C)$$

Low-rank matrix factorization based methods :

Structural Similarity Matrix Factorization

SEGK (Structural Embeddings using Graph Kernels) [5]:



Structural Similarities

Role-oriented Embeddings

$$\mathbf{S}_{ij} = \sum_{k=1}^{K} \hat{\mathcal{K}}(\mathcal{G}_i^k, \mathcal{G}_j^k)\hat{\mathcal{K}}(\mathcal{G}_i^{k-1}, \mathcal{G}_j^{k-1})$$

Initialization: $\hat{\mathcal{K}}(\mathcal{G}_i^0, \mathcal{G}_j^0) = 1$

Normalization: $\hat{\mathcal{K}}(\mathcal{G}, \mathcal{G}') = \dfrac{\mathcal{K}(\mathcal{G}, \mathcal{G}')}{\sqrt{\mathcal{K}(\mathcal{G}, \mathcal{G})\mathcal{K}(\mathcal{G}', \mathcal{G}')}}$

Nyström method is used:

$$\mathbf{H} = \mathbf{S}\mathbf{U}_{[r]}\mathbf{\Lambda}_{[r]}^{-\frac{1}{2}}$$

First r eigenvalues and eigenvectors.

Summary: Low-rank matrix factorization based methods

Tianjin University

Structural Feature Matrix

- Matrix Factorization (MF)
  - RolX, GLRD, RID$\mathcal{E}$Rs
  - Direct embeddings from MF
- Eigen-decomposition
  - GraphWave
- Motif factorization
  - HONE

Structural Similarity Matrix

- Similarity matrix calculation
  - Pair-wise calculation is time-consuming
- Nystrom method to improve the matrix factorization efficiency
  - xNetMF, EMBER, SEGK

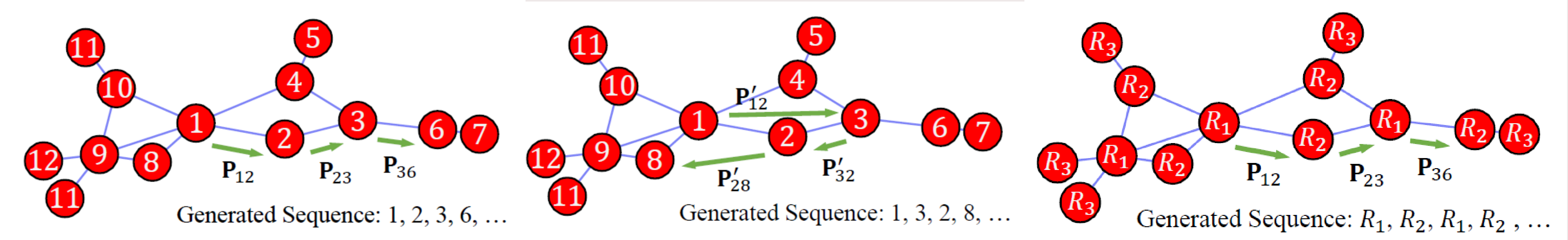
TU/e

The new two-level categorization：

Method	Embedding Mechanism		Vis	CLF/CLT	ER/NA/SS	LP	Year
			Conducted Tasks				
RolX	low-rank matrix factorization	on structural feature matrix	✓	✓	✗	✗	2012
GLRD			✗	✗	✓	✗	2013
RIDεRs			✓	✓	✓	✗	2017
GraphWave			✓	✓	✗	✗	2018
HONE			✓	✗	✓	✓	2020
xNetMF		on structural similarity matrix	✗	✗	✓	✗	2018
EMBER			✗	✓	✓	✗	2019
SEGK			✓	✓	✓	✗	2019
REACT			✗	✓	✗	✗	2019
SPaE			✓	✓	✗	✗	2019
struc2vec	random walk-based methods	on similarity-biased random walks	✓	✓	✗	✗	2017
SPINE			✗	✓	✗	✗	2019
struc2gauss			✓	✓	✗	✗	2020
Role2Vec		on feature-based random walks	✗	✗	✗	✓	2019
RiWalk			✗	✓	✗	✗	2019
NODE2BITS			✗	✗	✓	✗	2019
DRNE	deep learning	via structural information reconstruction/guidance	✓	✓	✗	✗	2018
GAS			✓	✓	✗	✗	2020
RESD			✓	✓	✓	✗	2021
GraLSP			✓	✓	✗	✓	2020
GCC			✗	✓	✓	✗	2020
RDAA			✓	✓	✗	✗	2021
CNESE			✓	✓	✓	✗	2021

Jiao, Pengfei, Xuan Guo, Ting Pan, Wang Zhang, and Yulong Pei. "A Survey on Role-Oriented Network Embedding." *arXiv preprint arXiv:2107.08379* (2021).

Random walk based methods：



(a) Normal Random Walks

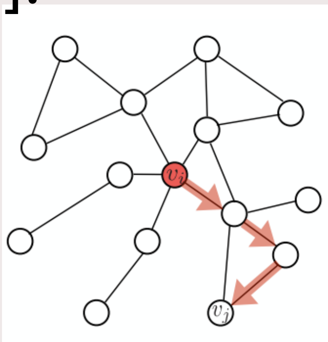
(b) Structural Similarity-biased Random Walks

(c) Structural Feature-based Random Walks

- Nodes in the same context have high proximity.
- Nodes in the same context have high structural similarity.
- Nodes have the similar labels have high structural similarity.

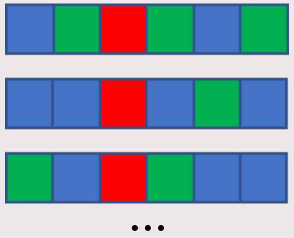
Random walk based methods：

struc2vec [4]:



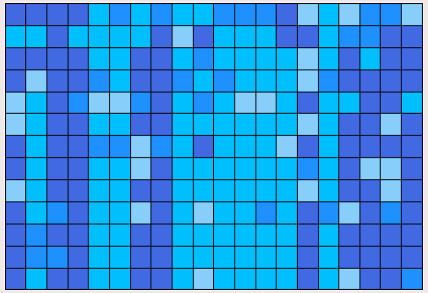
Input Network

Biased Random Walks



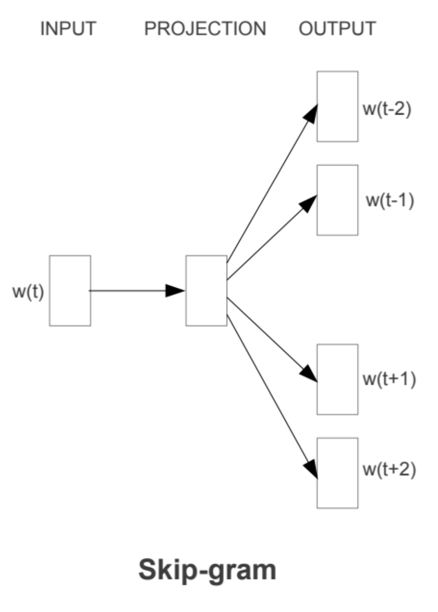
Sequences

Skip-Gram[15]



Role-oriented Embeddings

Structural Similarity-biased Random Walks



Compute structural distances:

$$\mathrm{dist}_d^k(v_i, v_j) = \mathrm{dist}_d^{k-1}(v_i, v_j) + \mathrm{DTW}(\mathcal{H}_i^k, \mathcal{H}_j^k),$$
$$0 \leq k \leq k^*$$

Build a multi-layer graph:

In each layer:

$$w_C^k(v_i^k, v_j^k) = \exp(-\mathrm{dist}_d^k(v_i^k, v_j^k)), k = 0, ..., k^*$$

Between layers:

$$w_C(v_i^k, v_i^{k+1}) = \log(\Gamma(v_i^k) + \mathrm{e}), k = 0, ..., k^* - 1$$
$$w_C(v_i^k, v_i^{k-1}) = 1, k = 1, ..., k^*$$

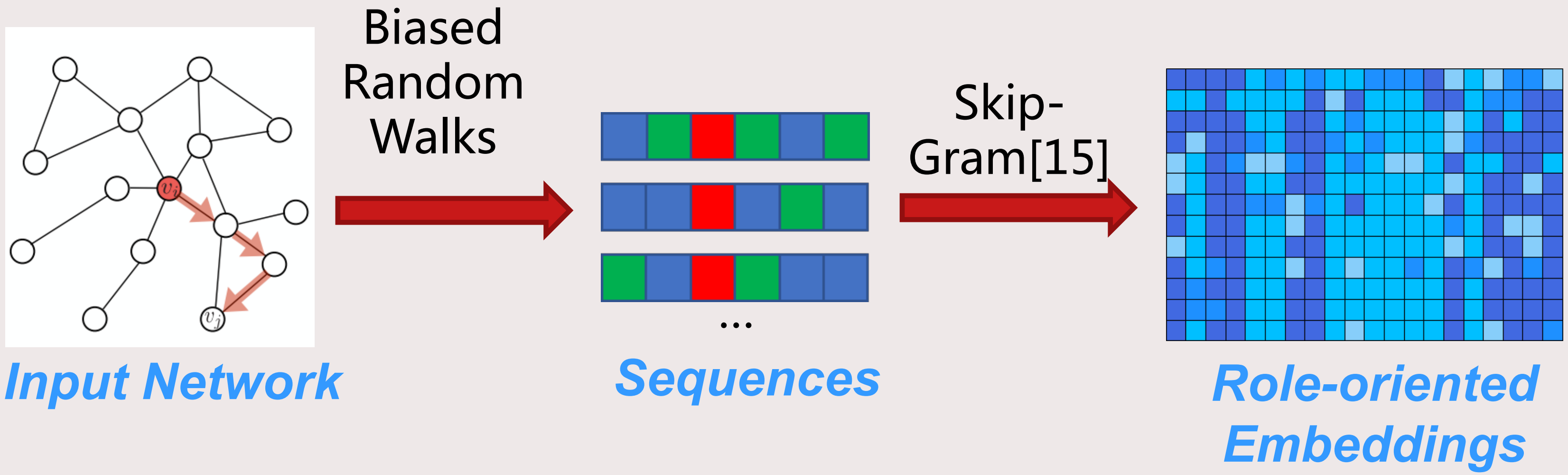
Walk probability:

$$(\mathbf{P}_{S2V}^k)_{ij} = \frac{w_C^k(v_i^k, v_j^k))}{\sum_{(v_i^k, v_{j'}^k) \in \mathcal{E}_C^k} w_C^k(v_i^k, v_{j'}^k))}$$

Random walk based methods：

Structural Similarity-biased Random Walks

SPINE (Structural Identity Preserved Inductive Network Embedding) [3]:



Structural features: largest values of Rooted PageRank Matrix $\mathbf{\Omega} = (1 - \beta_{RPR})(\mathbf{I} - \beta_{RPR}\mathbf{P})^{-1}$

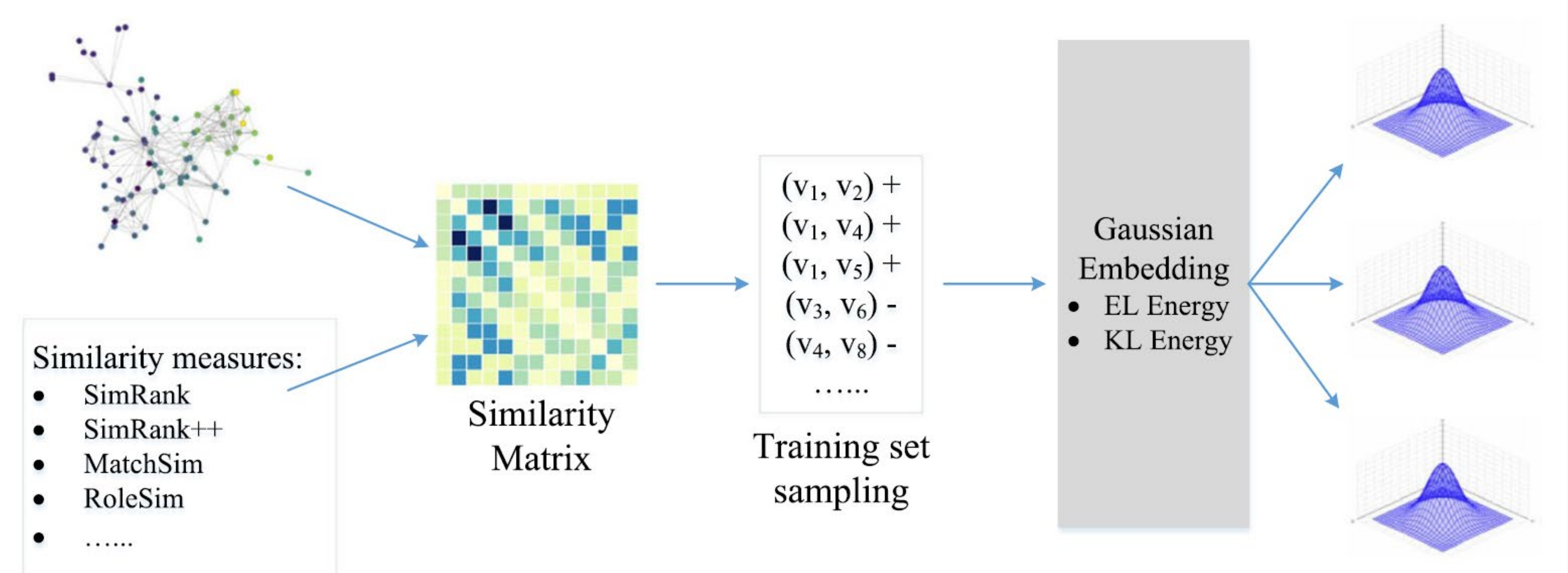
Structural similarities: DTW or other methods based on node features.

Walk probability:

$$(\mathbf{P}^k_{S2V})_{ij} = \frac{w^k_C(v^k_i, v^k_j))}{\sum_{(v^k_i, v^k_{j'}) \in \mathcal{E}^k_C} w^k_C(v^k_i, v^k_{j'}))}$$

struc2gauss [16]:

Structural Similarity-biased Random Walks



RoleSim:

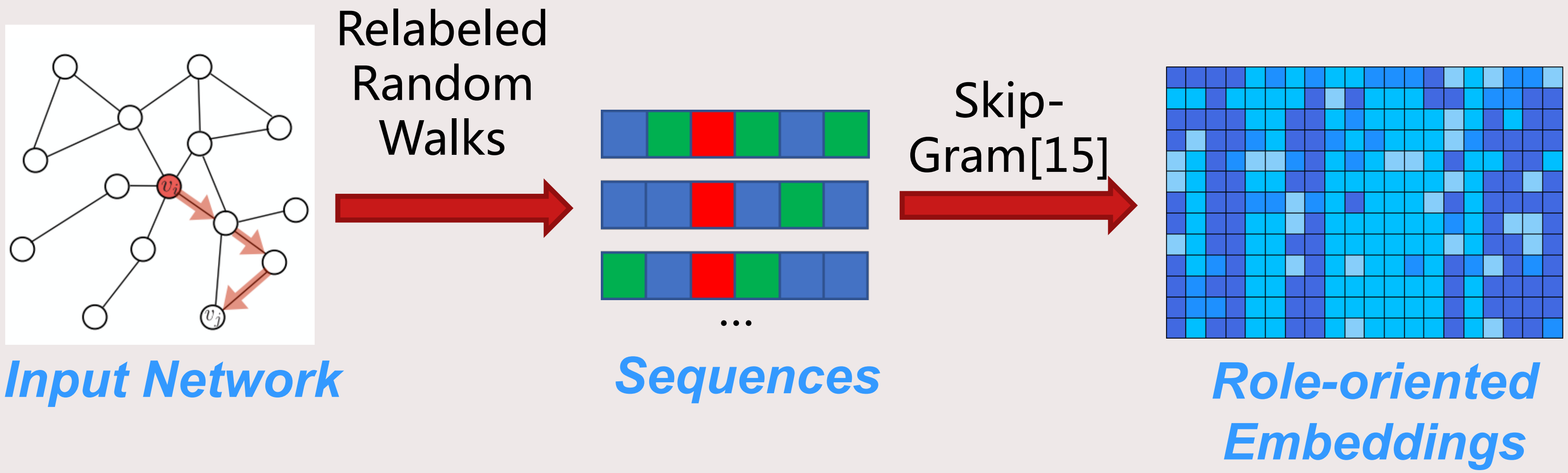
$$RoleSim(u,v) = (1-\beta)\max_{M(u,v)} \frac{\sum_{(x,y)\in M(u,v)} RoleSim(x,y)}{|N(u)|+|N(v)|-|M(u,v)|} + \beta$$

Energy function:

$$\mathcal{L} = \sum_{(v,u)\in\Gamma_+}\ \sum_{(v',u')\in\Gamma_-} \max(0, m - \mathcal{E}(z_v, z_u) + \mathcal{E}(z_{v'}, z_{u'}))$$

RiWalk (Role identification walk) [18]:

Structural Feature-based Random Walks



Indicator approximating shortest path kernel:

$$\phi_{SP}^{i}(v_j) = \mathrm{b}(d_i) \circ \mathrm{b}(d_j) \circ s_{ij}, v_j \in \mathcal{N}_i^k$$

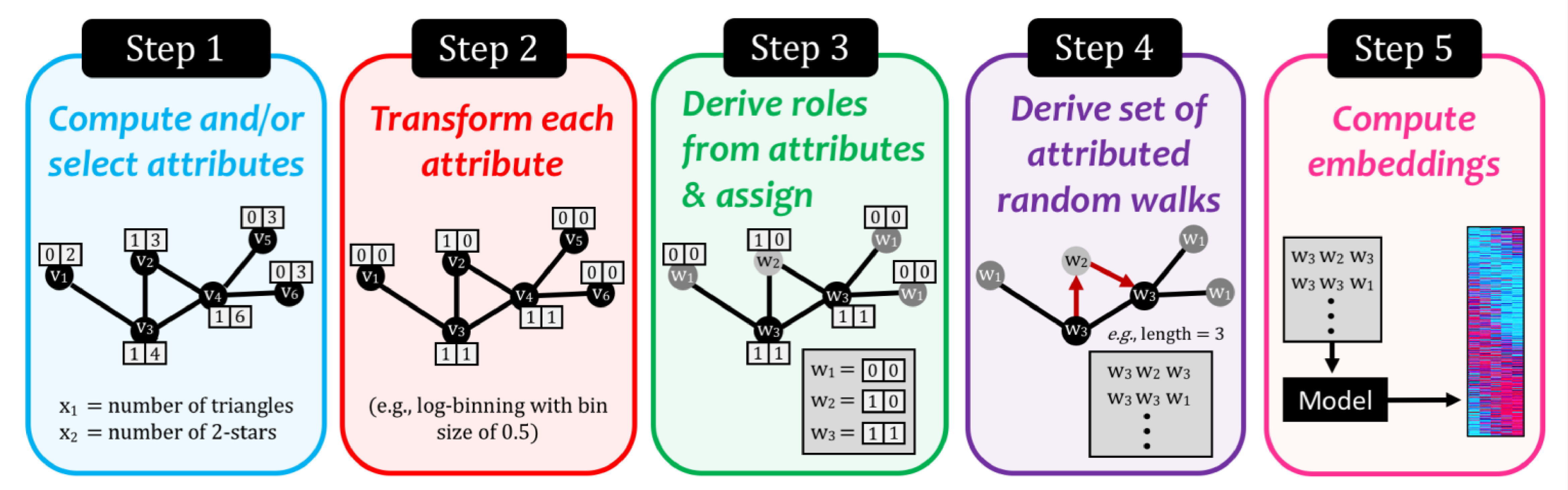
Indicator approximating Weisfeiler-Lehman sub-tree kernel:

$$\phi_{WL}^{i}(v_j) = \mathrm{b}(\mathbf{l}^{<i,i>}) \circ \mathrm{b}(\mathbf{l}^{<i,j>}) \circ s_{ij}, v_j \in \mathcal{N}_i^k$$

Random walk based methods：

role2vec [17]:

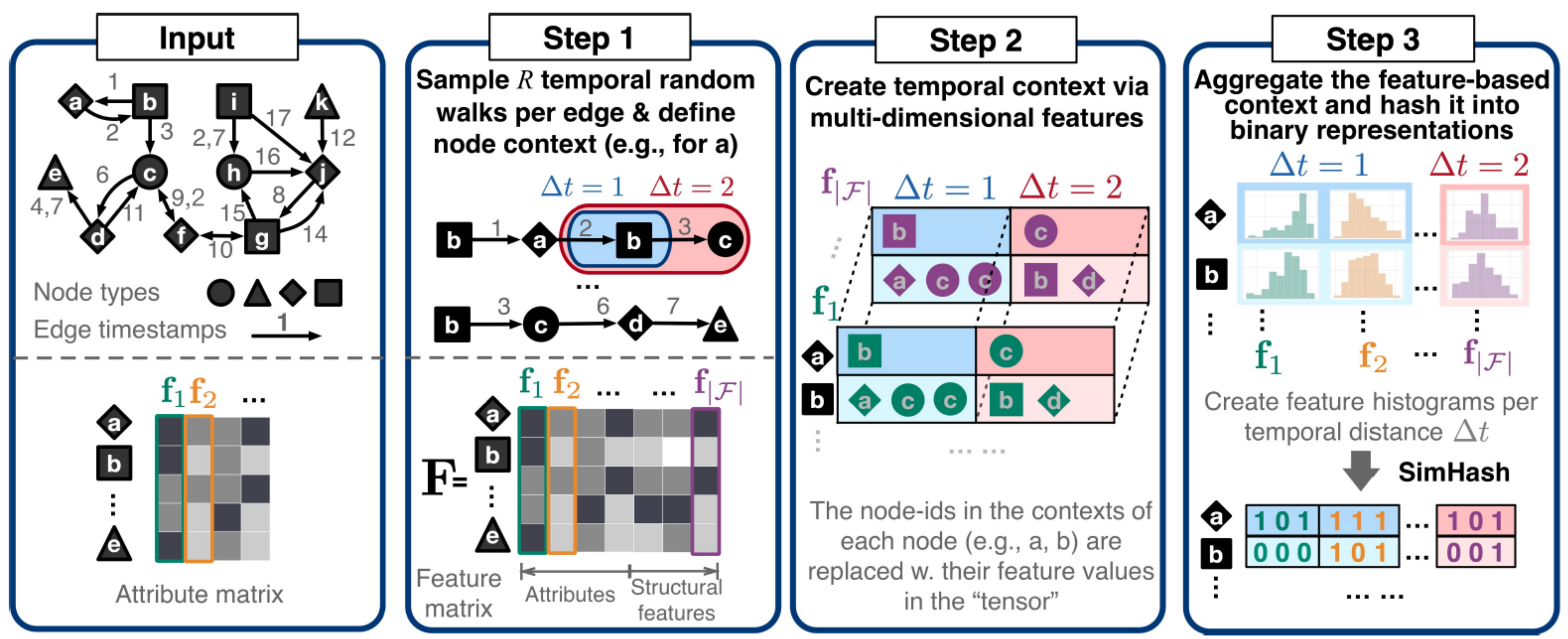
Structural Feature-based Random Walks



Random walk based methods：

NODE2BITS [19]:

Structural Feature-based Random Walks



Summary: Random walk based methods

Structural Similarity-based RW

Calculating similarity

- Strength: Random walk on constructed graph that can better capture role information
- Weakness: time-consuming for similarity calculation and graph construction

Structural Feature based RW

- No consistent frameworks
  - Graph kernels: RiWalk
  - Simhash: NODE2BITS
  - Graphlets: Role2Vec

The new two-level categorization :

天津大学 Tianjin University

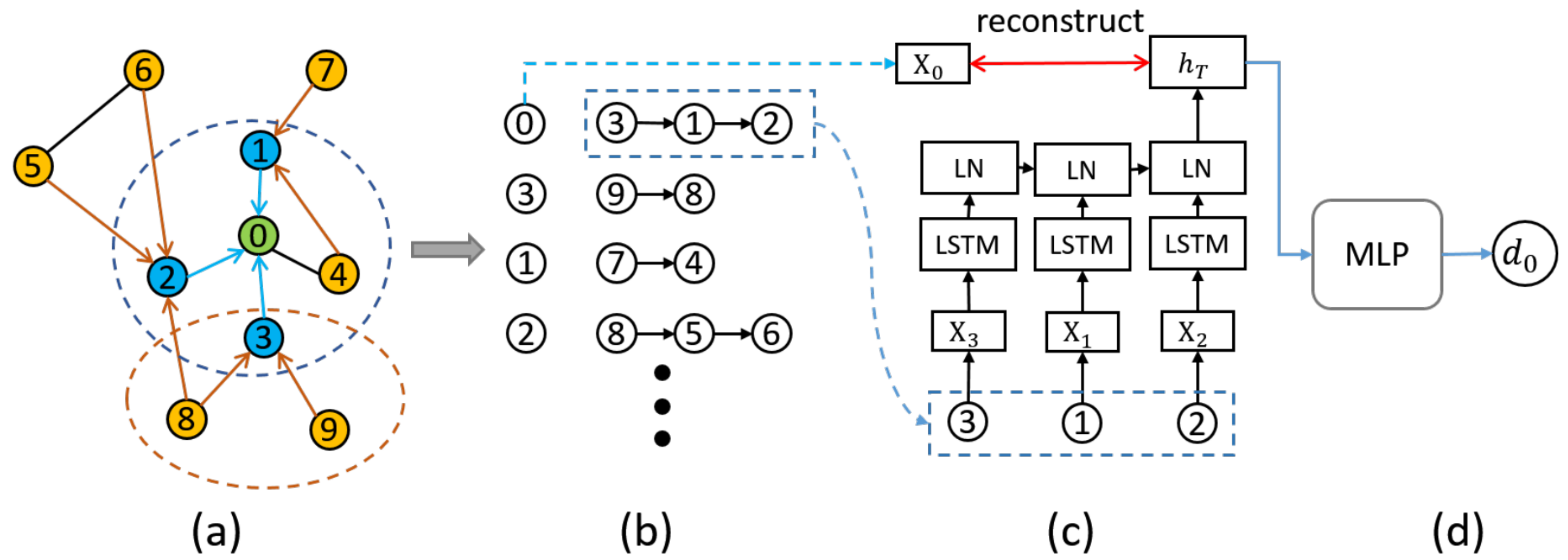
Method	Embedding Mechanism		Vis	CLF/CLT	ER/NA/SS	LP	Year
			Conducted Tasks				
RolX	low-rank matrix factorization	on structural feature matrix	✔	✔	✖	✖	2012
GLRD			✖	✖	✔	✖	2013
RIDεRs			✔	✔	✔	✖	2017
GraphWave			✔	✔	✖	✖	2018
HONE			✔	✖	✔	✔	2020
xNetMF		on structural similarity matrix	✖	✖	✔	✖	2018
EMBER			✖	✔	✔	✖	2019
SEGK			✔	✔	✔	✖	2019
REACT			✖	✔	✖	✖	2019
SPaE			✔	✔	✖	✖	2019
struc2vec	random walk-based methods	on similarity-biased random walks	✔	✔	✖	✖	2017
SPINE			✖	✔	✖	✖	2019
struc2gauss			✔	✔	✖	✖	2020
Role2Vec		on feature-based random walks	✖	✖	✖	✔	2019
RiWalk			✖	✔	✖	✖	2019
NODE2BITS			✖	✖	✔	✖	2019
DRNE	deep learning	via structural information reconstruction/guidance	✔	✔	✖	✖	2018
GAS			✔	✔	✖	✖	2020
RESD			✔	✔	✔	✖	2021
GraLSP			✔	✔	✖	✔	2020
GCC			✖	✔	✔	✖	2020
RDAA			✔	✔	✖	✖	2021
CNESE			✔	✔	✔	✖	2021

Jiao, Pengfei, Xuan Guo, Ting Pan, Wang Zhang, and Yulong Pei. "A Survey on Role-Oriented Network Embedding." *arXiv preprint arXiv:2107.08379* (2021).

TU/e

DRNE (Deep recursive network embedding) [2]:

Structural Information Reconstruction/Guidance



Loss for capturing regular equivalence:

$$\mathcal{L}_{equiv} = \sum_{v_i \in \mathcal{V}} \left\| \mathbf{H}_i - \breve{\mathbf{H}}_i \right\|_2^2$$

Embedding of node v_i' s neighbor

$$\breve{\mathbf{H}}_{(t)} = \mathrm{LNLSTM}(\mathbf{H}_{(t)}, \breve{\mathbf{H}}_{(t-1)})$$

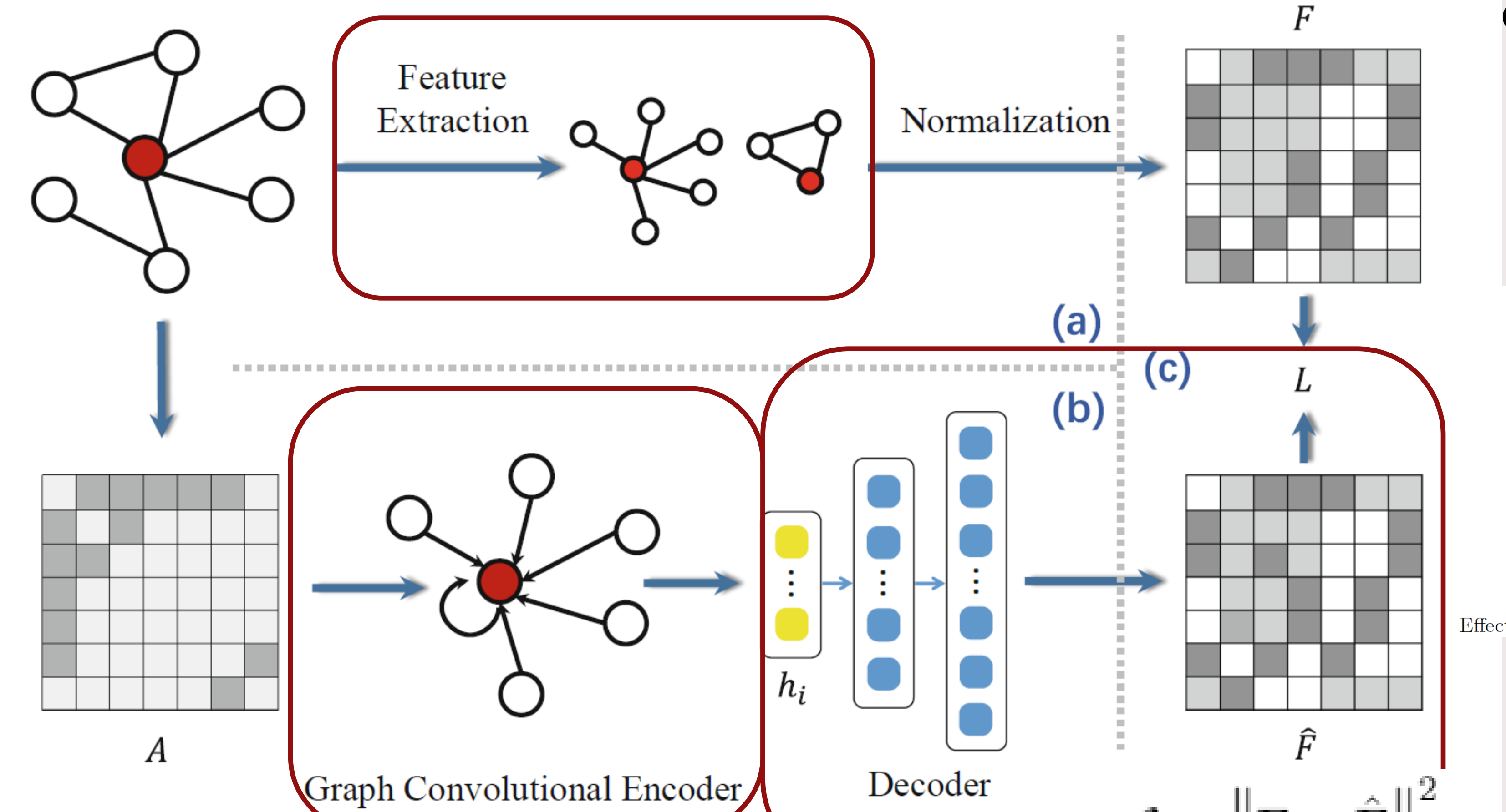
$$\breve{\mathbf{H}}_i = \breve{\mathbf{H}}_{(T)}$$

Loss for degree-guided regularizer:

$$\mathcal{L}_{deg} = \sum_{v_i \in \mathcal{V}} (\log(d_i + 1) - \mathrm{MLP}_{deg}(\breve{\mathbf{H}}_i))^2$$

GAS (Graph Auto-encoder Guided by Structural Information) [20]:

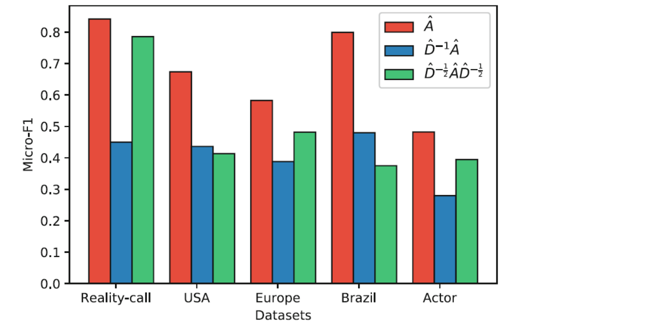
Structural Information Reconstruction/Guidance



$$\mathcal{L} = \left\| \mathbf{F} - \hat{\mathbf{F}} \right\|_F^2$$

Graph convolutional layer:

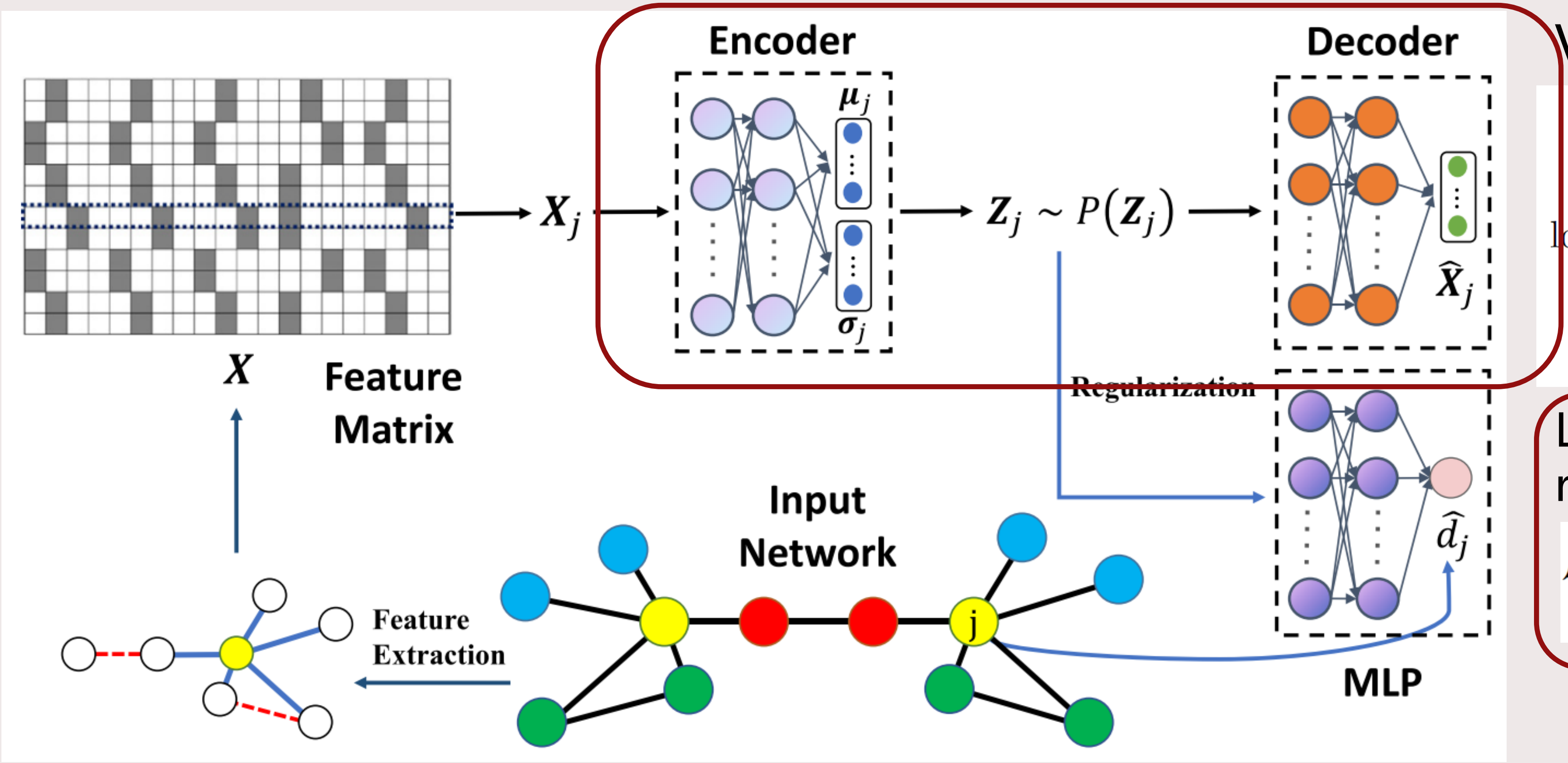
$$\mathbf{H}^{(l)} = \sigma(\tilde{\mathbf{A}}\mathbf{H}^{(l-1)}\Theta^{(l-1)})$$
$$\tilde{\mathbf{A}} = \mathbf{A} + \mathbf{I}$$



Effectiveness w.r.t the propagation rules of graph convolutional encoder.

RESD (Role-based network Embedding via Structural features reconstruction with Degree-regularized constraint) [21]:

Structural Information Reconstruction/Guidance



Variational encoder:

$$\begin{aligned}
\mathbf{Z}_i &= \mathrm{MLP}_{enc}(\mathbf{F}_i) \\
\boldsymbol{\mu}_i &= \mathbf{W}_{\boldsymbol{\mu}}\mathbf{Z}_i + \mathbf{b}_{\boldsymbol{\mu}} \\
\log(\boldsymbol{\sigma}_i) &= \mathbf{W}_{\boldsymbol{\sigma}}\mathbf{Z}_i + \mathbf{b}_{\boldsymbol{\sigma}} \\
\mathbf{H}_i &= \boldsymbol{\mu}_i + \boldsymbol{\sigma}_i \odot \boldsymbol{\epsilon}, \boldsymbol{\epsilon} \sim \mathrm{Gaussian}(\mathbf{0}, \mathbf{I}) \\
\hat{\mathbf{F}}_i &= \mathrm{MLP}_{dec}(\mathbf{H}_i)
\end{aligned}$$

Loss for degree-guided regularizer:

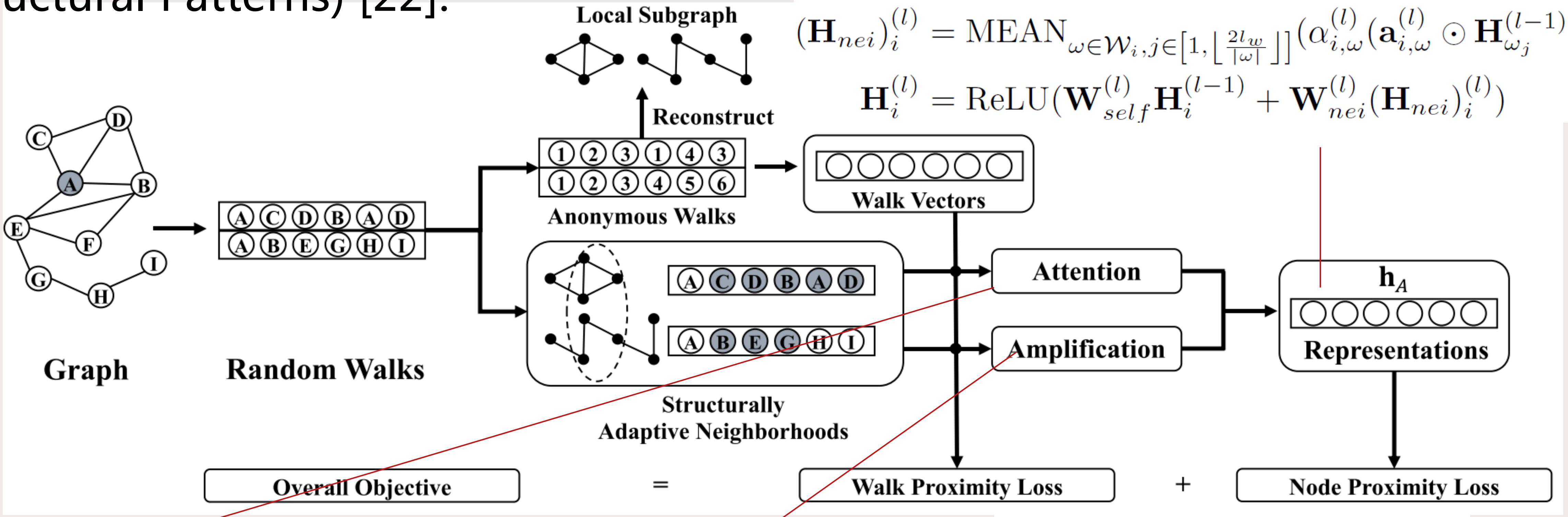
$$\mathcal{L}_{deg} = \sum_{v_i \in \mathcal{V}} (\log(d_i + 1) - \mathrm{MLP}_{deg}(\breve{\mathbf{H}}_i))^2$$

GraLSP (Graph Neural Networks with Local Structural Patterns) [22]:

Structural Information Reconstruction/Guidance

$$(\mathbf{H}_{nei})_i^{(l)} = \mathrm{MEAN}_{\omega \in \mathcal{W}_i, j \in [1, \lfloor \frac{2l_w}{|\omega|} \rfloor]} (\alpha_{i,\omega}^{(l)} (\mathbf{a}_{i,\omega}^{(l)} \odot \mathbf{H}_{\omega_j}^{(l-1)}))$$

$$\mathbf{H}_i^{(l)} = \mathrm{ReLU}(\mathbf{W}_{self}^{(l)} \mathbf{H}_i^{(l-1)} + \mathbf{W}_{nei}^{(l)} (\mathbf{H}_{nei})_i^{(l)})$$



$$\alpha_{i,\omega}^{(l)} = \frac{\exp(\mathrm{SLP}_{att}(\mathbf{u}_{\mathrm{aw}(\omega)}))}{\sum_{\omega' \in \mathcal{W}_i} \exp(\mathrm{SLP}_{att}(\mathbf{u}_{\mathrm{aw}(\omega')}))}$$

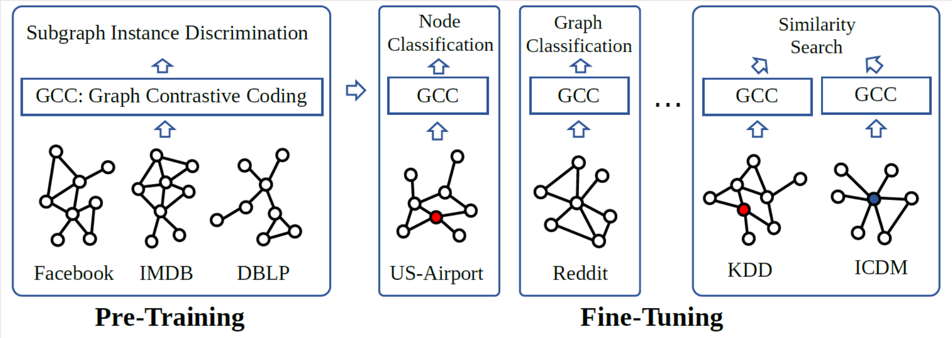
$$\mathbf{a}_{i,\omega}^{(l)} = \mathrm{SLP}_{amp}(\mathbf{u}_{\mathrm{aw}(\omega)})$$

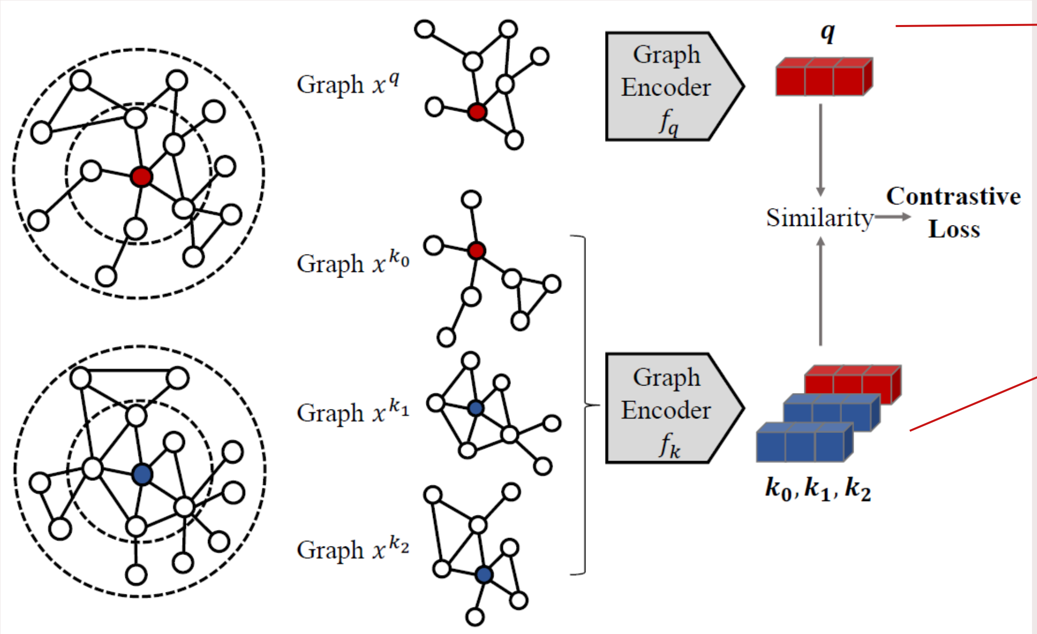
$$\mathcal{L}_{prox} = -\sum_{v_i \in \mathcal{V}} \sum_{v_j \in \mathcal{N}_i} (\log \sigma(\mathbf{H}_i \mathbf{H}_j^\top) - \gamma_{neg} \mathbb{E}_{v_k \sim P_n(v)} [\log \sigma(\mathbf{H}_i \mathbf{H}_k^\top)])$$

TU/e

GCC (Graph Contrastive Coding) [23]:

Structural Information Reconstruction/Guidance





Graph Isomorphic Network [24] encoder:

$$\mathbf{H}^{(l)} = \mathrm{MLP}_{GIN}((\mathbf{A} + (1+\epsilon)\cdot \mathbf{I})\mathbf{H}^{(l-1)})$$

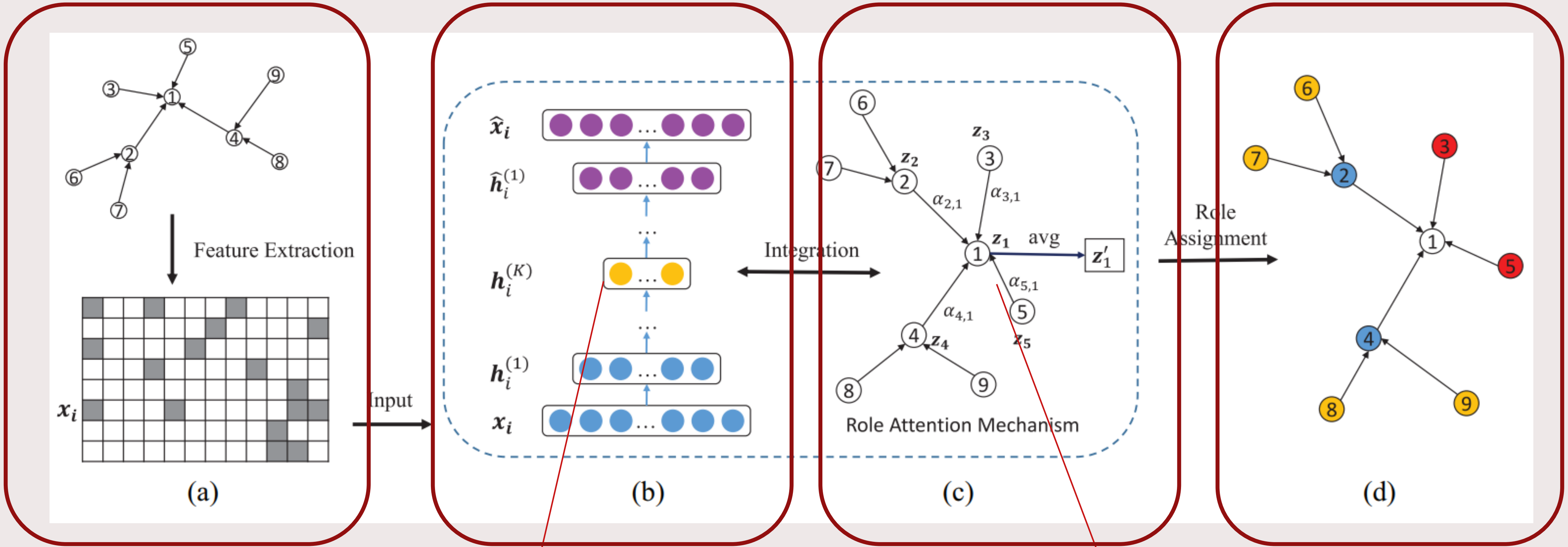
Contrastive learning loss (InfoNCE[25]):

$$\mathcal{L} = \sum_{v_i \in \mathcal{V}} -\log \frac{\exp(\mathbf{H}_i \mathbf{x}^+/\iota)}{\sum_{j=0}^{K} \exp(\mathbf{H}_i \mathbf{x}_j/\iota)}$$

Deep learning methods :

Structural Information Reconstruction/Guidance

RDAA (Role Discovery-Guided Network Embedding Based on Autoencoder and Attention Mechanism) [26]:



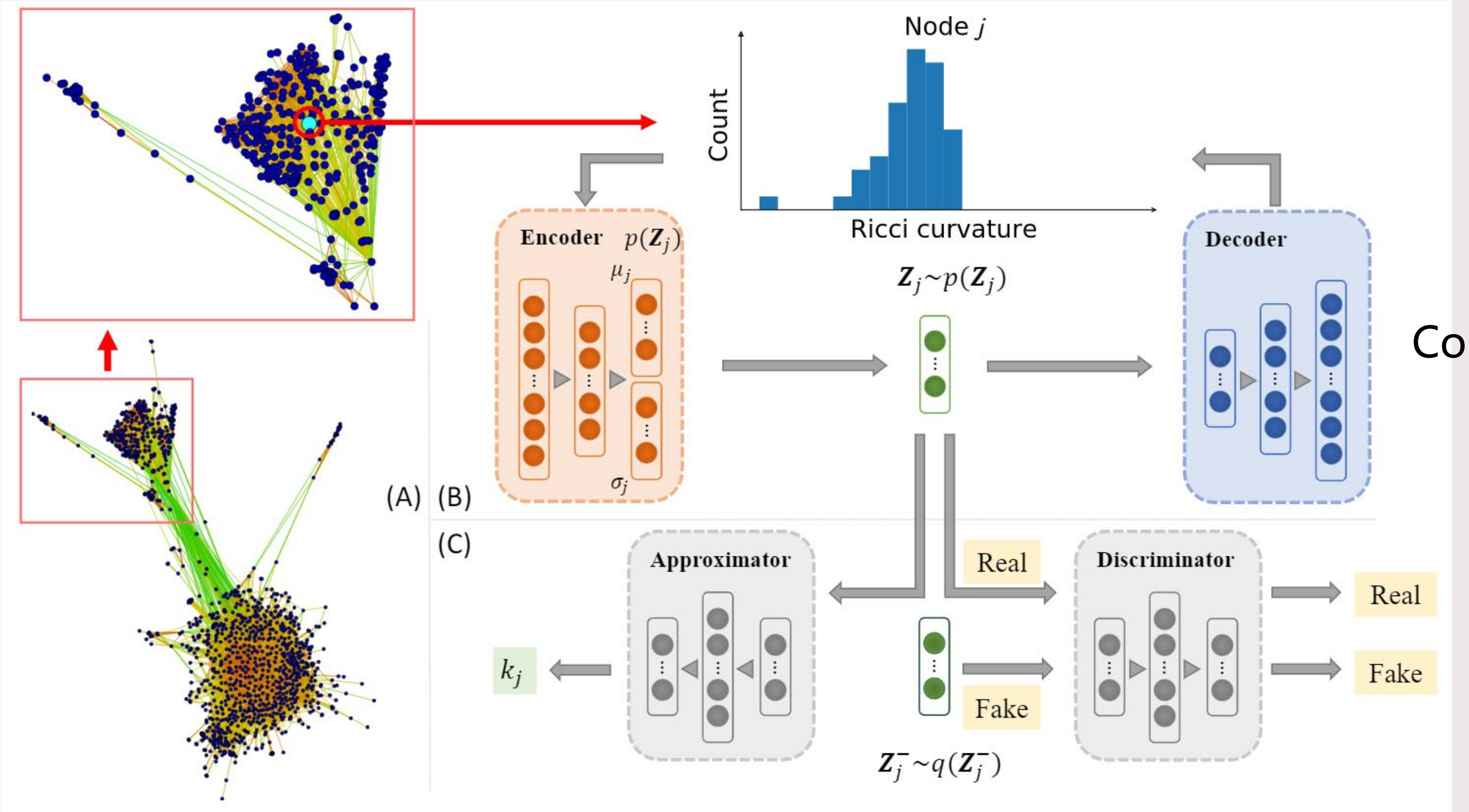
$$\mathcal{L}_{AE} = \sum_{i=1}^{n} \left\| (\mathbf{x}_i - \hat{\mathbf{x}}_i) \odot \boldsymbol{\beta}_i \right\|_2^2$$

$$\mathcal{L}_{\text{role}} = \sum_{i=1}^{n} \left(\left\| \mathbf{z}_i - \mathcal{G}(\{\mathbf{z}_j | j \in \mathcal{N}(i)\}) \right\|_2^2 \right)$$

Deep learning methods :

CNESE (Learning Stochastic Equivalence based on Discrete Ricci Curvature) [27]:

Structural Information Reconstruction/Guidance



Olivier`s Ricci Curvature:

$$\kappa(u,v) = 1 - \frac{W(m_u, m_v)}{d(u,v)}$$

$$W(m_u, m_v) = \inf_{A} \sum_{x,y \in V} A(x,y) d(x,y)$$

Contrastive Learning Regularizer:

$$\mathcal{L}_{con} = \frac{1}{2n}\Big(\sum_{i=1}^{n} \mathbb{E}_{\boldsymbol{Z}^-} log(\mathcal{D}(\boldsymbol{Z}_i^-)) + \sum_{j=1}^{n} \mathbb{E}_{\boldsymbol{H}} log(1 - \mathcal{D}(\mathcal{G}(\boldsymbol{H}_j)))\Big).$$

Summary: Deep learning methods

Deep learning architecture + X

- LSTM + regular equivalence = DRNE
- GNN + ReFeX features = GAS / RESD
- GIN + contrastive learning + subgraph patterns = GCC
- Autoencoder + Attention + regular equivalence = RDAA
- Ricci Curvature + contrastive learning = CNESE

References

[1] Henderson, Keith, et al. "Rolx: structural role extraction & mining in large graphs." In *KDD*, 2012.
[2] Tu, Ke, et al. "Deep recursive network embedding with regular equivalence." In *KDD*, 2018.
[3] Guo, Junliang, et al. "Spine: structural identity preserved inductive network embedding." In *IJCAI*, 2018.
[4] Ribeiro, Leonardo FR, et al. "struc2vec: Learning node representations from structural identity." In *KDD*, 2017.
[5] Nikolentzos, Giannis, and Michalis Vazirgiannis. "Learning structural node representations using graph kernels." *IEEE Transactions on Knowledge and Data Engineering* (2019).
[6] Henderson, Keith, et al. "It's who you know: graph mining using recursive structural features." In *SIGKDD*, 2011.
[7] Gilpin, Sean, et al. "Guided learning for role discovery (GLRD) framework, algorithms, and applications." In *KDD*, 2013.
[8] Gupte, Pratik Vinay, et al. "Role discovery in graphs using global features: Algorithms, applications and a novel evaluation strategy." In ICDE, 2017.
[9] Donnat, Claire, et al. "Learning structural node embeddings via diffusion wavelets." In *SIGKDD*, 2018.
[10] Rossi, Ryan A, et al. "A structural graph representation learning framework." In *WSDM*, 2020.
[11] Heimann, Mark, et al. "Regal: Representation learning-based graph alignment." In *CIKM*, 2018.
[12] Drineas, Petros, et al. "On the Nyström Method for Approximating a Gram Matrix for Improved Kernel-Based Learning." *Journal of Machine Learning Research* (2005).
[13] Jin, Di, et al. "Smart roles: Inferring professional roles in email networks." In *SIGKDD,* 2019.
[14] Shi, Benyun, et al. "Unifying structural proximity and equivalence for network embedding." *IEEE Access* (2019).
[15] Mikolov, Tomas, et al. "Efficient estimation of word representations in vector space." arXiv preprint arXiv:1301.3781 (2013).
[16] Pei, Yulong, et al. "struc2gauss: Structure preserving network embedding via gaussian embedding." *Data Mining and Knowledge Discovery* (2020).
[17] Ahmed, Nesreen, et al. "Role-based graph embeddings." *IEEE Transactions on Knowledge and Data Engineering* (2020).
[18] Ma, Xuewei, et al. "RiWalk: Fast structural node embedding via role identification." In *ICDM*, 2019.
[19] Jin, Di, et al. "Node2bits: Compact time-and attribute-aware node representations for user stitching." In *ECML PKDD*, 2019.
[20] Guo, Xuan, et al. "Role-Oriented Graph Auto-encoder Guided by Structural Information." In *DASFAA*, 2020.
[21] Zhang, Wang, et al. "Role-based network embedding via structural features reconstruction with degree-regularized constraint." *Knowledge-Based Systems* (2021).
[22] Jin, Yilun, et al. "GraLSP: Graph neural networks with local structural patterns." In *AAAI*, 2020.
[23] Qiu, Jiezhong, et al. "Gcc: Graph contrastive coding for graph neural network pre-training." In *KDD*, 2020.
[24] Xu, Keyulu, et al. "How powerful are graph neural networks?." In *ICLR*, 2019.
[25] Oord, Aaron van den, et al. "Representation learning with contrastive predictive coding." arXiv preprint arXiv:1807.03748 (2018).
[26] Jiao, Pengfei, et al. "Role Discovery-Guided Network Embedding Based on Autoencoder and Attention Mechanism." *IEEE Transactions on Cybernetics* (2021).
[27] Guo, Xuan, et al. "Learning Stochastic Equivalence based on Discrete Ricci Curvature." In *IJCAI*, 2021.

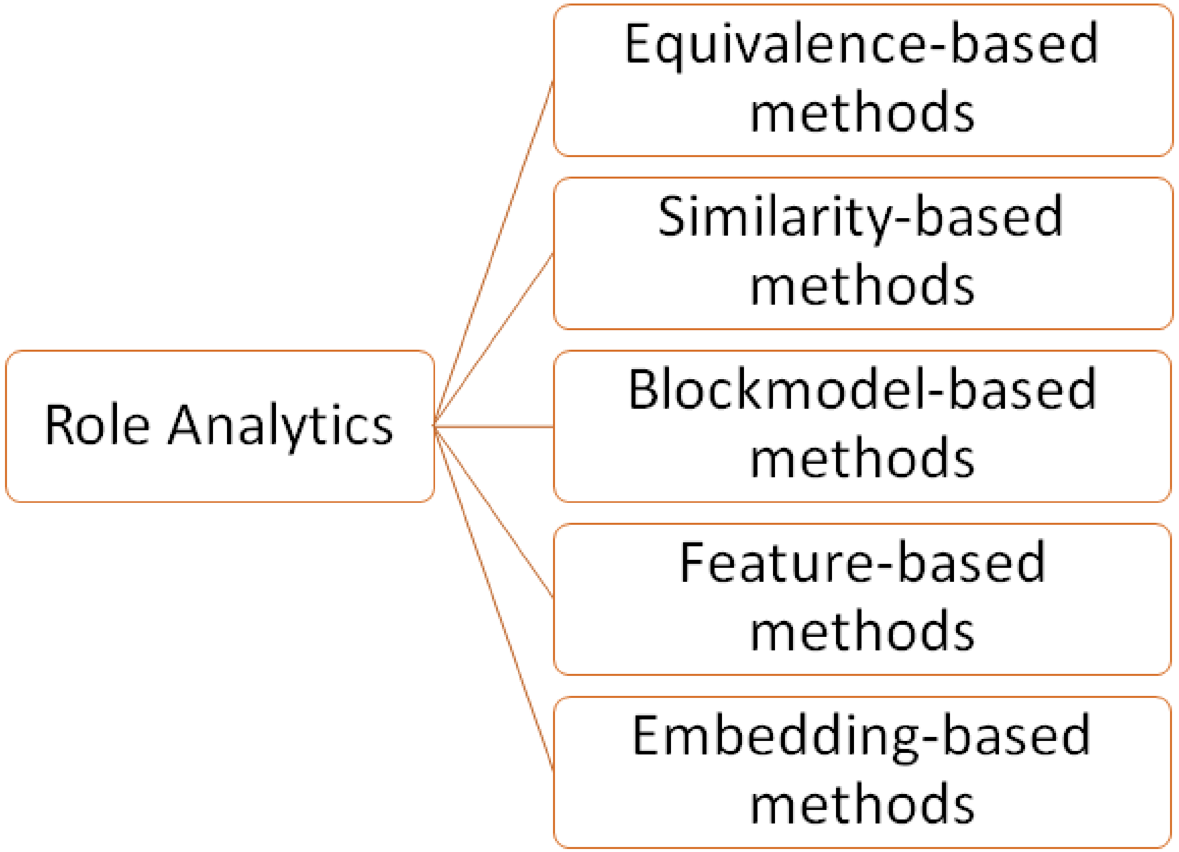
A Survey on Role-Oriented Network Embedding

P Jiao, X Guo, T Pan, W Zhang, Y Pei

Roles in Networks - Foundations, Methods and Applications

Coffee/Tea Break

Role Analytics Methods: Summary



- Relations
- Combinations

Challenges in Role Analytics

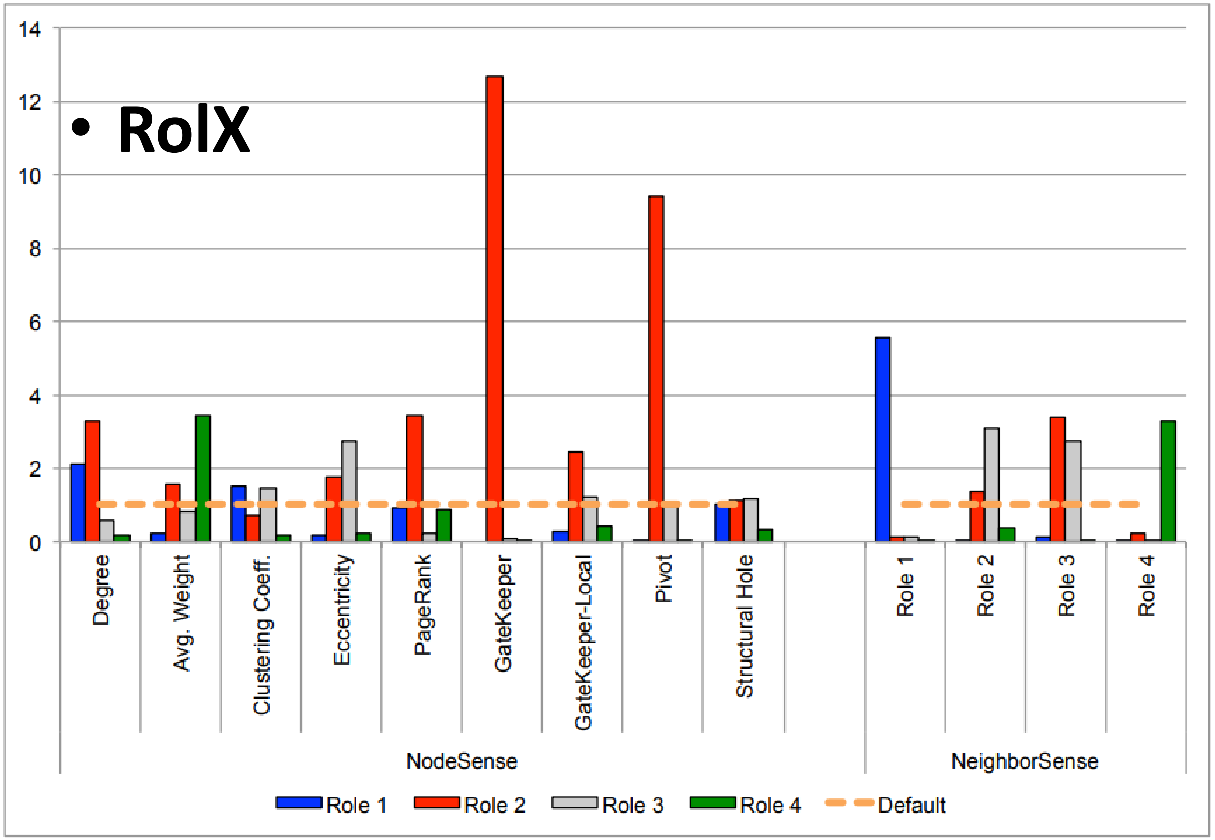
- Interpretable Role Analytics
- Role Analytics in Dynamic Networks
- Role Analytics Evaluation Framework
- Joint Role and Community Detection
- Other types of Embedding Spaces

Interpretable Role Analytics

- Roles often correspond to social identifications in social science
- Real-world networks:
  - the network data is often of a massive scale
  - human labeling is very costly and time-consuming

What are the meaninig of roles?

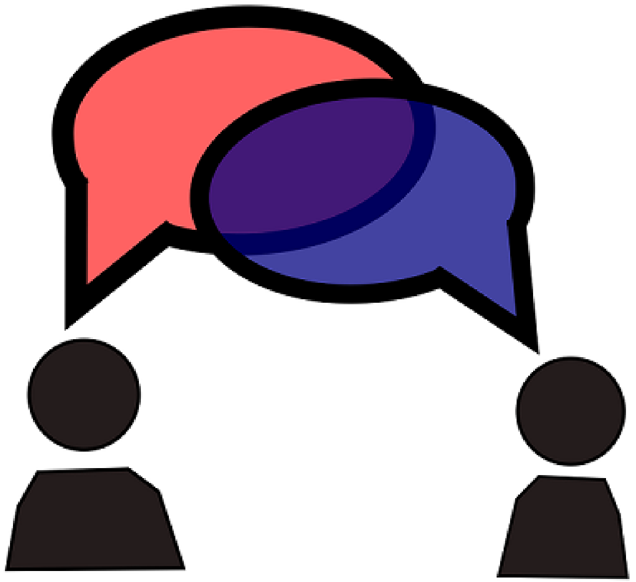
Interpretable Role Analytics



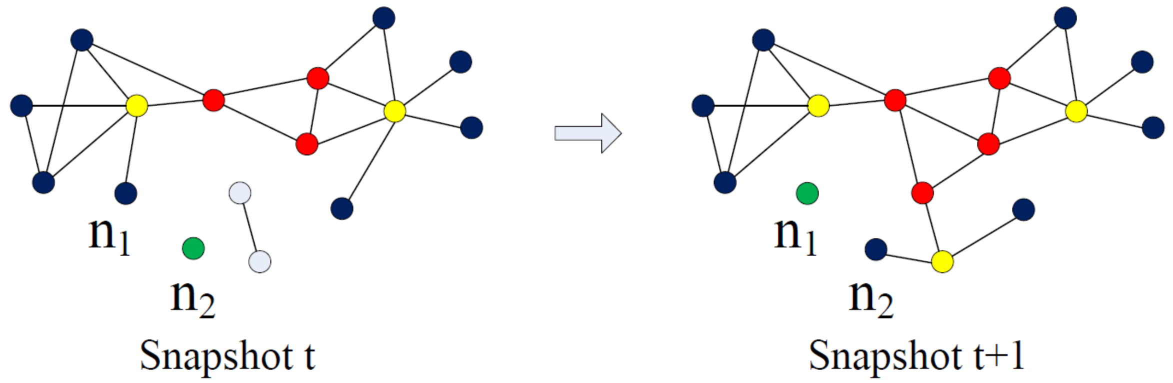
- Using graph measures to interpret roles
- Using neighbor information to interpret roles
- Using nodes' attributes to interpret roles

Interpretable Role Analytics: Challenges

- How to interpret roles using graph measures to interpret roles? If the measures cannot distinguish different roles?
- How to make use of other sources of data to help interpret roles, e.g., meta data of nodes in networks.
- It is possible to interpret structural roles by
- Incorporating other roles, e.g., social roles?



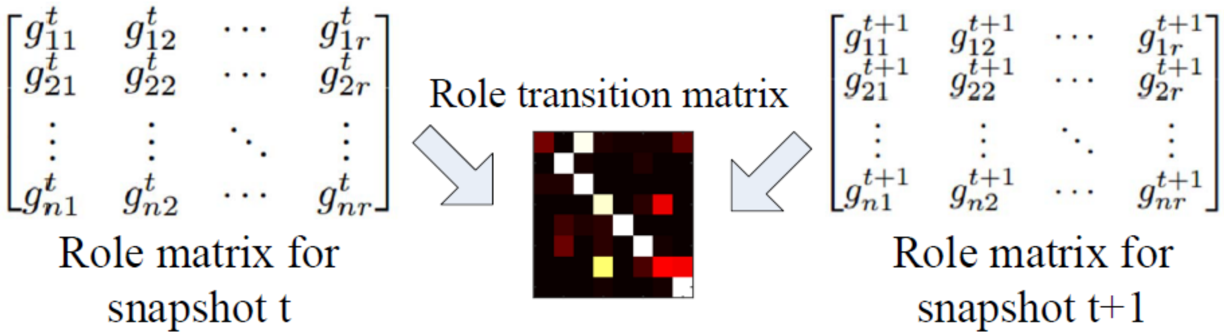
Role Analytics in Dynamic Networks



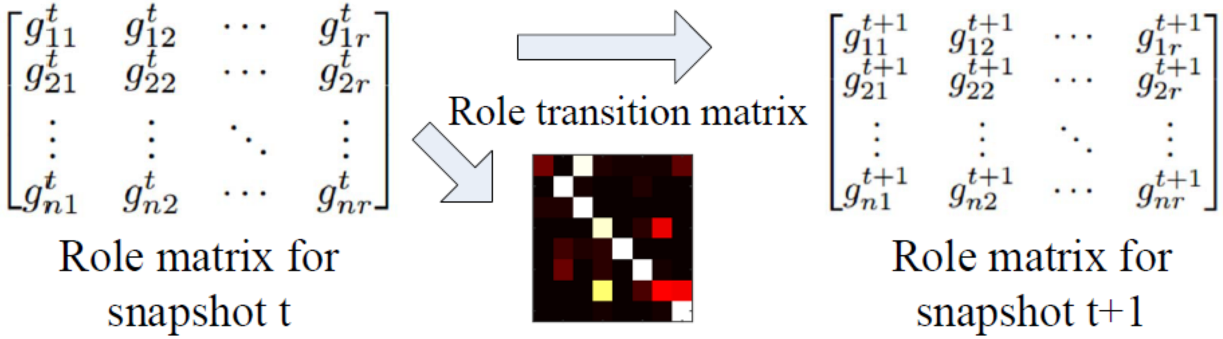
Real-world networks evolve with nodes/edges changed/added/deleted

- Different methods to analyze roles in dynamic networks
- Analyze roles in each graph snapshot and then analyze the role transition, e.g., DBMM
- Analyze roles and role transition simultaneously using a unified model, e.g., DyNMF and dynamic blockmodels

Role Analytics in Dynamic Networks

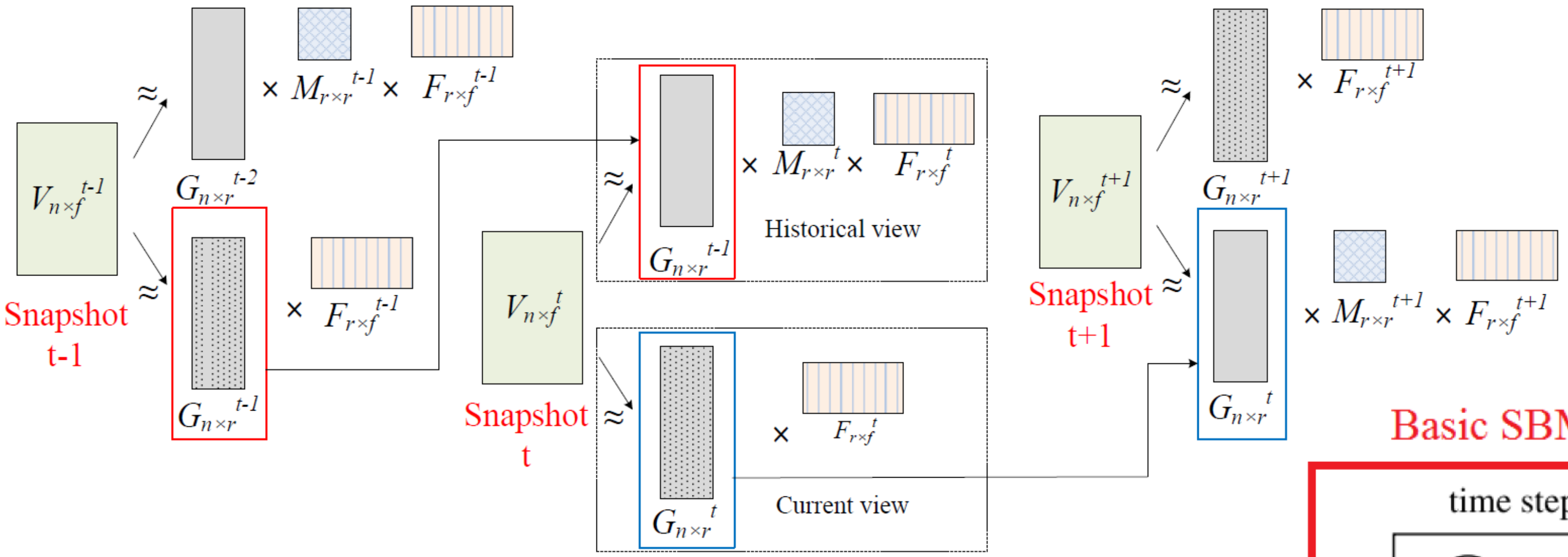


First analyze roles in each graph snapshot and then analyze the role transition



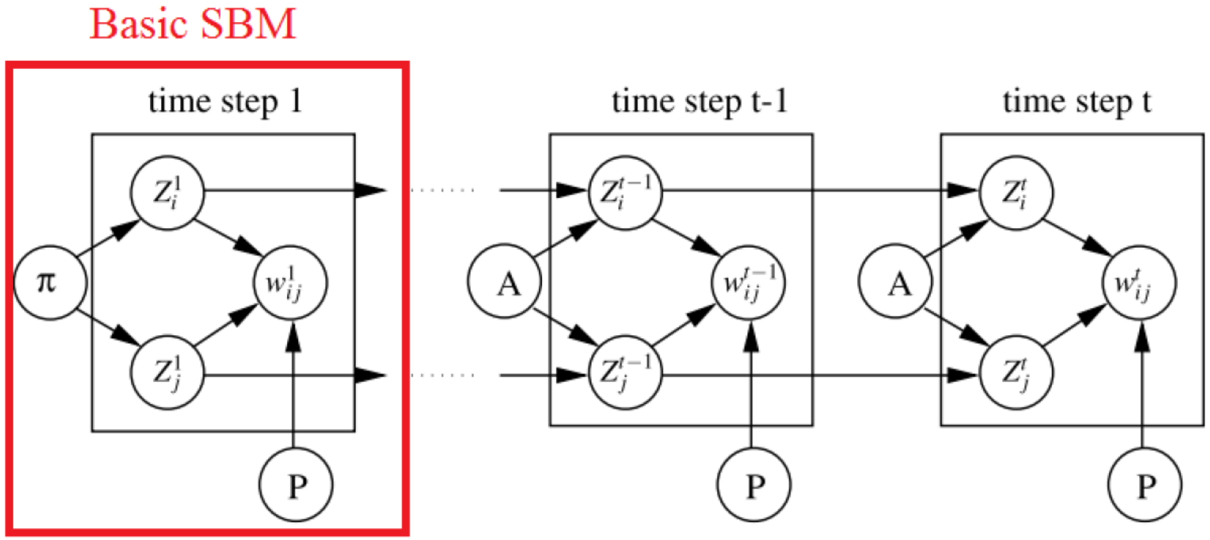
Analyze roles and role transition simultaneously using a unified model

Role Analytics in Dynamic Networks



Dynamic NMF for Role Analytics

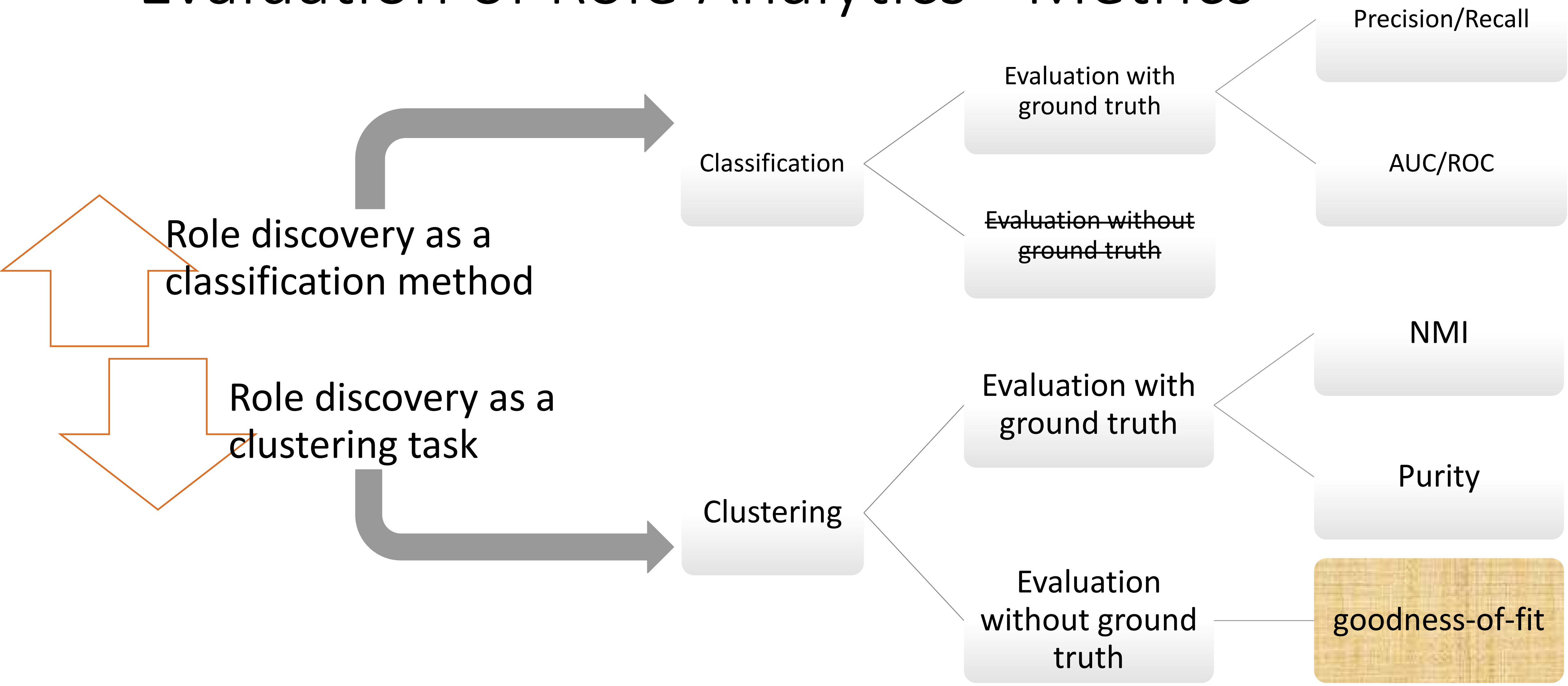
Dynamic SBM for Role Analytics



Role Analytics in Dynamic Networks: Challenges

- Streaming networks
  - Nodes/edges can be added/deleted
- Efficiency
  - Role discovery for evolving nodes
- New patterns
  - Nodes with new patterns which reflect new roles

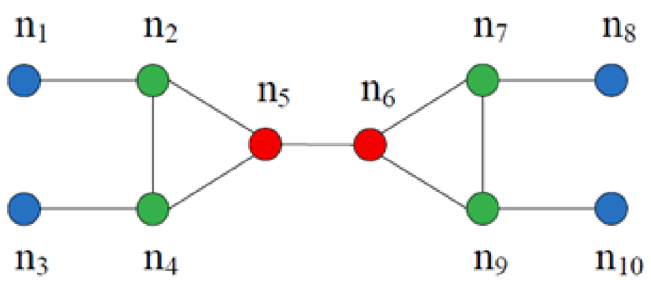
Evaluation of Role Analytics - Metrics



Goodness-of-fit

- In *goodness-of-fit* index, it is assumed that the output of a role discovery method is an optimal model, and nodes belonging to the same role are predicted to be perfectly structurally equivalent
- goodness-of-fit index can measure how well the representation of roles and the relations among these roles fit a given network
- Components
  - density matrix
  - criteria for constructing block matrix
    - Zeroblock
    - Oneblock
    - α-criteria
  - block matrix

Goodness-of-fit



$$
\begin{array}{c}
n_1\\ n_2\\ n_3\\ n_4\\ n_5\\ n_6\\ n_7\\ n_8\\ n_9\\ n_{10}
\end{array}
\begin{pmatrix}
0&1&0&0&0&0&0&0&0&0\\
1&0&0&1&1&0&0&0&0&0\\
0&0&0&1&0&0&0&0&0&0\\
0&1&1&0&1&0&0&0&0&0\\
0&1&0&1&0&1&0&0&0&0\\
0&0&0&0&1&0&1&0&1&0\\
0&0&0&0&0&1&0&1&1&0\\
0&0&0&0&0&0&1&0&0&0\\
0&0&0&0&0&1&1&0&0&1\\
0&0&0&0&0&0&0&0&1&0
\end{pmatrix}
$$

$$
\begin{array}{c}
n_5\\ n_6\\ n_2\\ n_4\\ n_7\\ n_9\\ n_1\\ n_3\\ n_8\\ n_{10}
\end{array}
\begin{pmatrix}
0&1&0&1&0&1&0&0&0&0\\
0&0&0&0&1&0&1&0&1&0\\
1&0&0&1&1&0&0&0&0&0\\
0&1&1&0&1&0&0&0&0&0\\
0&0&0&0&0&1&0&1&1&0\\
0&0&0&0&0&1&1&0&0&1\\
0&1&0&0&0&0&0&0&0&0\\
0&0&0&1&0&0&0&0&0&0\\
0&0&0&0&0&0&1&0&0&0\\
0&0&0&0&0&0&0&0&1&0
\end{pmatrix}
\begin{array}{l}
\text{Role 1}\\ \\ \text{Role 2}\\ \\ \\ \\ \text{Role 3}\\ \\ \\ \\
\end{array}
$$

Discovered roles

Role 1 = $\{n_5, n_6\}$

Role 2 = $\{n_2, n_4, n_7, n_9\}$

Role 3 = $\{n_1, n_3, n_8, n_{10}\}$

$$\alpha = \sum_{1 \le i, j \le n} A_{ij} / (n \cdot (n-1))$$

$$\Delta_{ij} = \begin{cases} \sum_{v_m \in R_i, v_n \in R_j} A_{mn} / (|R_i| \cdot |R_j|), \text{if } i \ne j \\ \sum_{v_m \in R_i, v_n \in R_j} A_{mn} / (|R_i| \cdot (|R_j| - 1)), \text{if } i = j \end{cases}$$

$$B_{ij} = \begin{cases} 1, \text{if } \Delta_{ij} \ge \alpha \\ 0, \text{if } \Delta_{ij} < \alpha \end{cases}$$

Structural equivalence

$$\text{Density matrix } \Delta = \begin{pmatrix} 1/2 & 1/2 & 0 \\ 1/2 & 1/6 & 1/4 \\ 0 & 1/4 & 0 \end{pmatrix} \longrightarrow \text{Block matrix B} = \begin{pmatrix} 1 & 1 & 0 \\ 1 & & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

Goodness-of-fit index

$$e = \sum_{1 \le i,j \le 3} |B_{ij} - \Delta_{ij}|$$

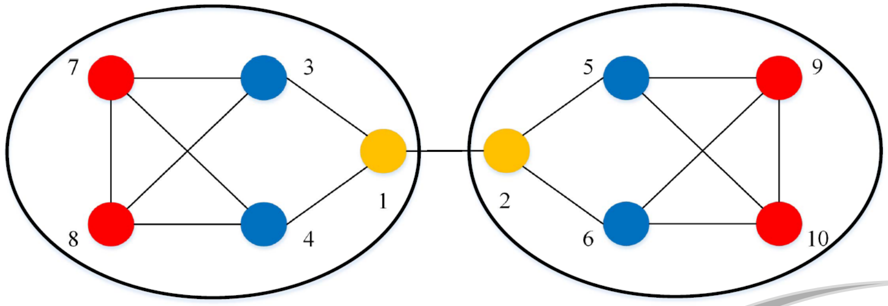
Evaluation of Role Analytics - Benckmark

- All the methods for role oriented network embedding are evaluated on relatively small-scale networks data with thousands of
- Real-world networks are often of a massive scale, e.g., there are billions of users in social networks.
- Constructing larger-scale benchmark datasets is very important to evaluate existing approaches in effectiveness, efficiency and robustness, and also beneficial for researchers to develop new models.

Evaluation: Challenges

- Evaluation with ground-truth labels
  - Benchmark datasets
- Evaluation without ground-truth labels
  - How to capture other equivalence relations, e.g. regular equivalence
  - Generalized modularity
- Evaluation with large-scale benchmarks
  - Constructing benchmarks

Joint Role and Community Detection



Roles VS Communities:

- Roles shown in different colors
  - E.g., yellow nodes are bridges
- Communities shown inside the ellipses
  - Denser internal connections inside each community

Global structure. It reflects the topological properties of graphs through the *unbounded* observation of the input graph as an entirety

Local structure. It captures the topological properties of graphs by observing a *bounded* part of the input graph

RC-Joint [Ruan and Parthasarathy, COSN 2014]

$\mathbf{C^0} \leftarrow \texttt{InitComm}(G, N_c)$
$\mathbf{R^0} \leftarrow \texttt{InitRole}(G, N_r)$

$$\max_{\mathbf{C}} \left(\texttt{Likelihood}(G, \mathbf{C})\right)$$
$$\text{subject to } \mathbf{c}_{\bullet i} \cdot \mathbf{r}_{\bullet j} < \epsilon_{ij}, \forall i \in 1 \cdots N_c, j \in 1 \cdots N_r$$

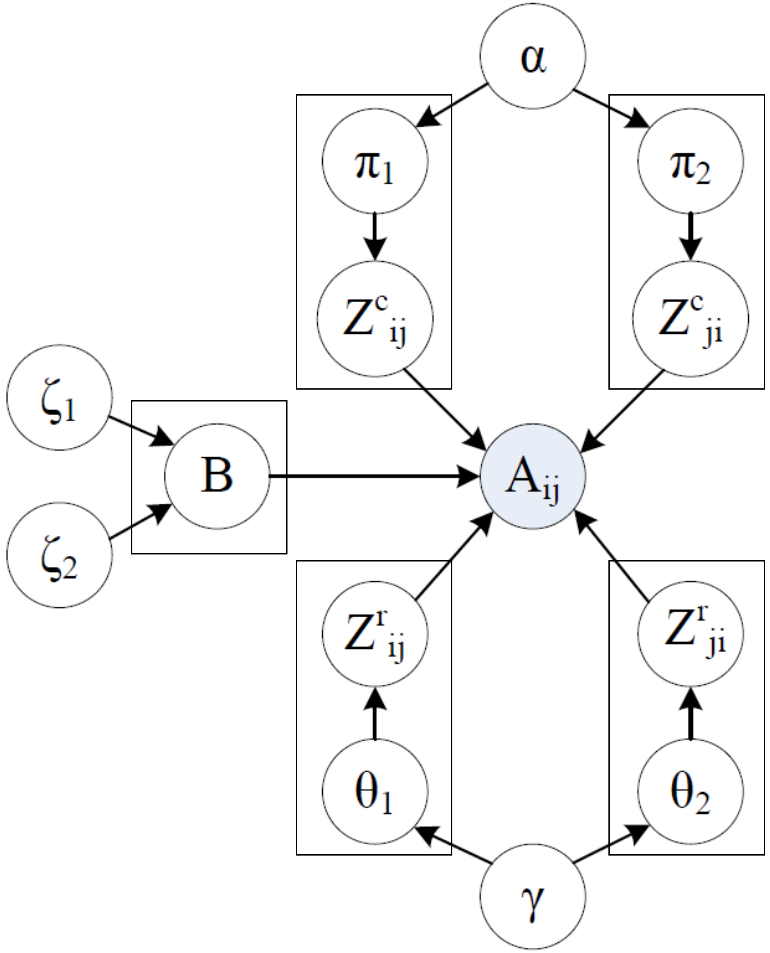
Diversity

$\mathbf{C^i} = \texttt{UpdateComm}(G, \mathbf{C^{i-1}}, \mathbf{R^{i-1}}, N_c)$
if $\frac{\texttt{Likelihood}(G,\mathbf{C^i}) - \texttt{Likelihood}(G,\mathbf{C^{i-1}})}{\texttt{Likelihood}(G,\mathbf{C^{i-1}})} < \delta_{comm}$ **then**
  $conv_{comm} \leftarrow$ **true** $\quad \triangleright$ Communities converge
end if

$\mathbf{R^i} = \texttt{UpdateComm}(G, \mathbf{R^{i-1}}, \mathbf{C^i}, N_r)$
if $||R^i - R^{i-1}||_{max} < \delta_{role}$ **then**
  $conv_{role} \leftarrow$ **true** $\quad \triangleright$ Roles converge
end if

$$\frac{|\{u \in \Gamma_v | \arg\max_{i'} (c_{ui'}) = \arg\max_{i'} (c_{vi'})\}|}{|\Gamma_v|}$$

Mixed Membership Community and Role [Chen et al., SDM 2016]



Community Modeling

For each entry (k, p, q) in B (k can take 0 here):

- Draw $B_{k,p,q} \sim \text{Beta}(\xi^1_{k,p,q}, \xi^2_{k,p,q})$

For each node i:

- Draw a community membership distribution vector $\pi_i \sim \text{Dirichlet}(\alpha^c)$
- Draw a role membership distribution vector $\theta_i \sim \text{Dirichlet}(\alpha^r)$

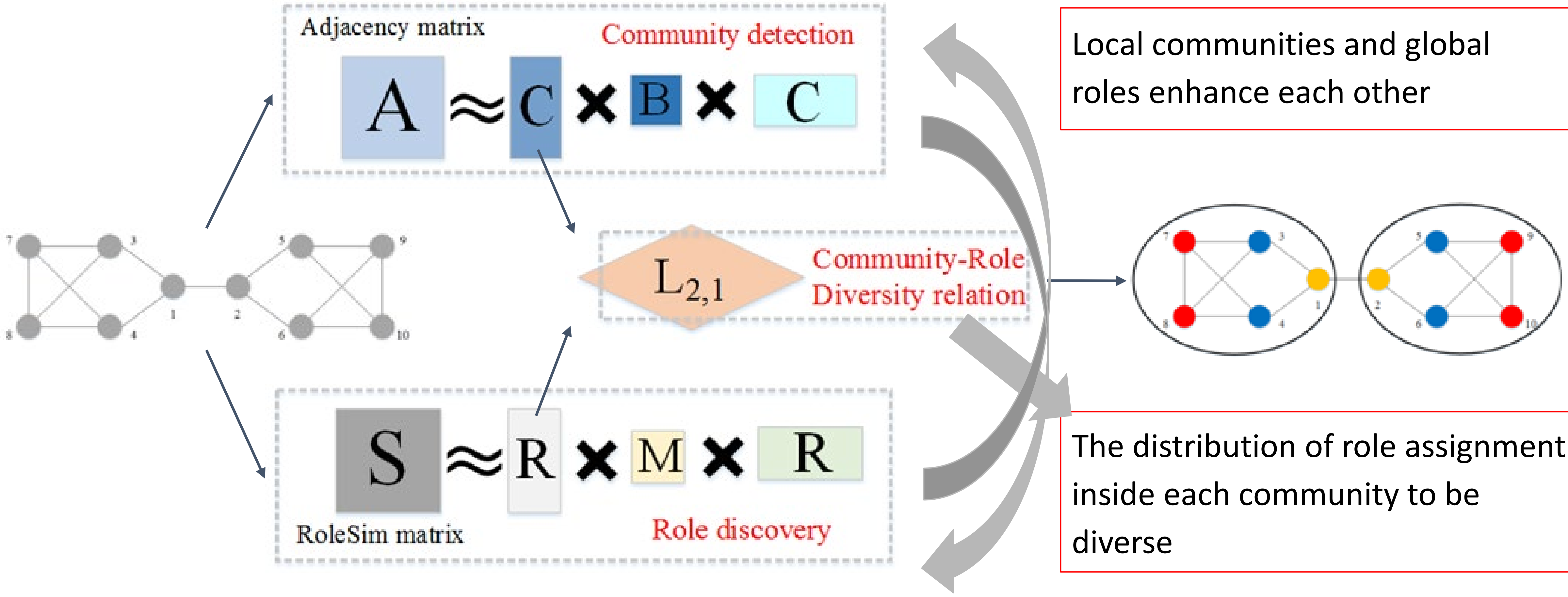
For each node pair (i, j):

- Draw node i's community $Z^c_{ij} \sim \text{Multinomial}(\pi_i)$
- Draw node j's community $Z^c_{ji} \sim \text{Multinomial}(\pi_j)$
- Draw node i's role $Z^r_{ij} \sim \text{Multinomial}(\theta_i)$
- Draw node j's role $Z^r_{ji} \sim \text{Multinomial}(\theta_j)$
- Draw link $E_{ij} \sim \text{Bernoulli}(B_{\delta(Z^c_{ij}, Z^c_{ji}), Z^r_{ij}, Z^r_{ji}})$

Role Modeling

REACT (RolE And Community deTection)

[Pei et al., ASONAM 2019]

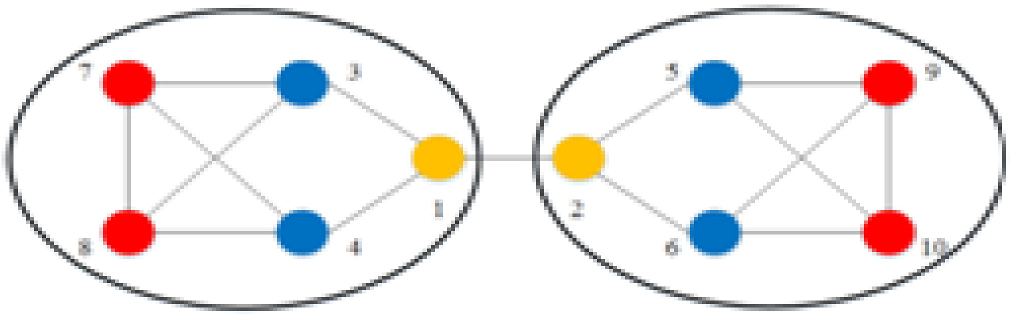


Local communities and global roles enhance each other

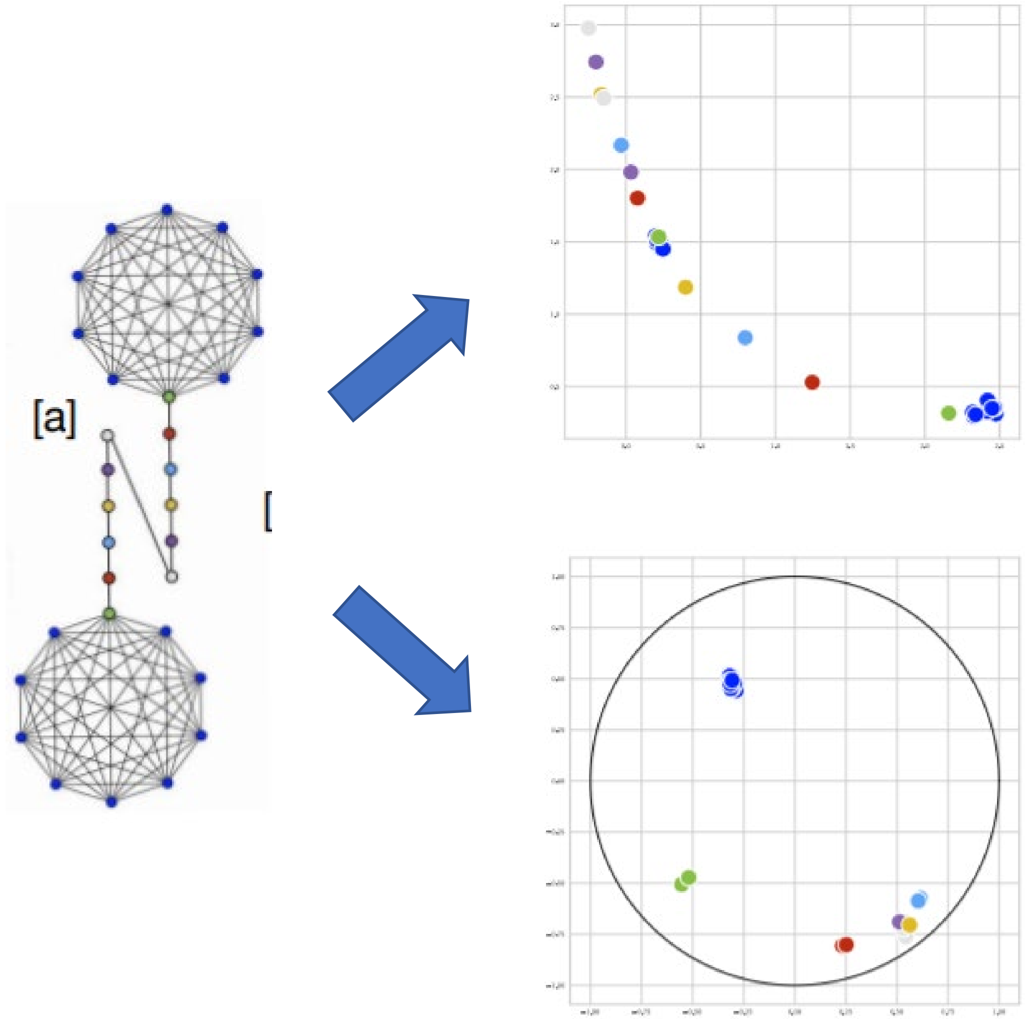
The distribution of role assignment inside each community to be diverse

Joint Role and Community Detection: Challenges

- How to formally define and model the relations between roles and communities?
  - Other relations except diveristy?
  - Unified model (MMCR, REACT) or iterative model (RC-Joint)?



Other Types of Embedding Spaces



Euclidean space

Hyperbolic space

Challenges in Role Analytics

- Interpretable Role Analytics
- Role Analytics in Dynamic Networks
- Role Analytics Evaluation Framework
- Joint Role and Community Detection
- Other types of Embedding Spaces

Conclusions and Future Directions

Conclusions

- Equivalence Relations
- Taxonomy of Role Analytics Methods
- Role-oriented network embedding
- Challenges in Role Analytics

Future Directions

- Solutions to These Challenges
- Bridging Roles with GNN
- Applying Roles in Practical Problems

Roles in Networks - Foundations, Methods and Applications

Thank you

Q & A

References [Equivalence Relations]

- Francois Lorrain and Harrison C White. Structural equivalence of individuals in social networks. The Journal of mathematical sociology, 1(1):49–80, 1971.
- Stephen P Borgatti and Martin G Everett. Notions of position in social network analysis. Sociological methodology, pages 1–35, 1992.
- Martin G Everett and Stephen P Borgatti. Regular equivalence: General theory. Journal of mathematical sociology, 19(1):29–52, 1994.

References [Equivalence-based Methods]

- Ronald L Breiger, Scott A Boorman, and Phipps Arabie. An algorithm for clustering relational data with applications to social network analysis and comparison with multidimensional scaling. Journal of mathematical psychology, 12(3):328–383, 1975.
- Ronald S Burt. Positions in networks. Social forces, 55(1):93–122, 1976.
- Zilong Bai, Peter Walker, Anna Tschiffely, Fei Wang, and Ian Davidson. Unsupervised network discovery for brain imaging data. In Proceedings of the 23rd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, pages 55–64. ACM, 2017.
- Zilong Bai, Buyue Qian, and Ian Davidson. Discovering models from structural and behavioral brain imaging data. In Proceedings of the 24th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining, pages 1128–1137. ACM, 2018.
- Jeffrey Chan, Wei Liu, Andrey Kan, Christopher Leckie, James Bailey, and Kotagiri Ramamohanarao. Discovering latent blockmodels in sparse and noisy graphs using non-negative matrix factorisation. In Proceedings of the 22nd ACM international conference on Information & Knowledge Management, pages 811–816. ACM, 2013.
- Mohadeseh Ganji, Jeffrey Chan, Peter J Stuckey, James Bailey, Christopher Leckie, Kotagiri Ramamohanarao, and Laurence Park. Semi-supervised blockmodelling with pairwise guidance. In Joint European Conference on Machine Learning and Knowledge Discovery in Databases, pages 158–174. Springer, 2018.
- Stanley Wasserman and Katherine Faust. Social network analysis: Methods and applications, volume 8. Cambridge university press, 1994.

References [Role Embedding Methods]

[1] Henderson, Keith, et al. "Rolx: structural role extraction & mining in large graphs." In KDD, 2012.
[2] Tu, Ke, et al. "Deep recursive network embedding with regular equivalence." In KDD, 2018.
[3] Guo, Junliang, et al. "Spine: structural identity preserved inductive network embedding." In IJCAI, 2018.
[4] Ribeiro, Leonardo FR, et al. "struc2vec: Learning node representations from structural identity." In KDD, 2017.
[5] Nikolentzos, Giannis, and Michalis Vazirgiannis. "Learning structural node representations using graph kernels." IEEE Transactions on Knowledge and Data Engineering (2019).
[6] Henderson, Keith, et al. "It's who you know: graph mining using recursive structural features." In SIGKDD, 2011.
[7] Gilpin, Sean, et al. "Guided learning for role discovery (GLRD) framework, algorithms, and applications." In KDD, 2013.
[8] Gupte, Pratik Vinay, et al. "Role discovery in graphs using global features: Algorithms, applications and a novel evaluation strategy." In ICDE, 2017.
[9] Donnat, Claire, et al. "Learning structural node embeddings via diffusion wavelets." In SIGKDD, 2018.
[10] Rossi, Ryan A, et al. "A structural graph representation learning framework." In WSDM, 2020.
[11] Heimann, Mark, et al. "Regal: Representation learning-based graph alignment." In CIKM, 2018.
[12] Drineas, Petros, et al. "On the Nyström Method for Approximating a Gram Matrix for Improved Kernel-Based Learning." Journal of Machine Learning Research (2005).
[13] Jin, Di, et al. "Smart roles: Inferring professional roles in email networks." In SIGKDD, 2019.
[14] Shi, Benyun, et al. "Unifying structural proximity and equivalence for network embedding." IEEE Access (2019).

References [Role Embedding Methods]

[15] Mikolov, Tomas, et al. "Efficient estimation of word representations in vector space." arXiv preprint arXiv:1301.3781 (2013).

[16] Pei, Yulong, et al. "struc2gauss: Structure preserving network embedding via gaussian embedding." Data Mining and Knowledge Discovery (2020).

[17] Ahmed, Nesreen, et al. "Role-based graph embeddings." IEEE Transactions on Knowledge and Data Engineering (2020).

[18] Ma, Xuewei, et al. "RiWalk: Fast structural node embedding via role identification." In ICDM, 2019.

[19] Jin, Di, et al. "Node2bits: Compact time-and attribute-aware node representations for user stitching." In ECML PKDD, 2019.

[20] Guo, Xuan, et al. "Role-Oriented Graph Auto-encoder Guided by Structural Information." In DASFAA, 2020.

[21] Zhang, Wang, et al. "Role-based network embedding via structural features reconstruction with degree-regularized constraint." Knowledge-Based Systems (2021).

[22] Jin, Yilun, et al. "GraLSP: Graph neural networks with local structural patterns." In AAAI, 2020.

[23] Qiu, Jiezhong, et al. "Gcc: Graph contrastive coding for graph neural network pre-training." In KDD, 2020.

[24] Xu, Keyulu, et al. "How powerful are graph neural networks?." In ICLR, 2019.

[25] Oord, Aaron van den, et al. "Representation learning with contrastive predictive coding." arXiv preprint arXiv:1807.03748 (2018).

[26] Jiao, Pengfei, et al. "Role Discovery-Guided Network Embedding Based on Autoencoder and Attention Mechanism." IEEE Transactions on Cybernetics (2021).

References [Challenges]

- D'Agostino R B. Goodness-of-fit-techniques. CRC press, 1986.
- Wasserman S, Faust K. Social network analysis: Methods and applications. Cambridge university press, 1994.
- Yiye Ruan and Srinivasan Parthasarathy. Simultaneous detection of communities and roles from large networks. In Proceedings of the second edition of the ACM conference on Online social networks, pages 203–214. ACM, 2014.
- Ting Chen, Lu-An Tang, Yizhou Sun, Zhengzhang Chen, Haifeng Chen, and Guofei Jiang. Integrating community and role detection in information networks. In Proceedings of the 2016 SIAM International Conference on Data Mining, pages 72–80. SIAM, 2016.
- Yulong Pei, George Fletcher, and Mykola Pechenizkiy. Joint role and community detection in networks via l2,1 norm regularized nonnegative matrix tri-factorization. In Proceedings of the 2019 IEEE/ACM International Conference on Advances in Social Networks Analysis and Mining. IEEE Press, 2019.
- Mehta N, Duke L C, Rai P. Stochastic Blockmodels meet Graph Neural Networks. International Conference on Machine Learning. 2019: 4466-4474.