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Carnegie Mellon University

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Rutgers

Node Similarity, Graph Similarity and Matching: Theory and Applications

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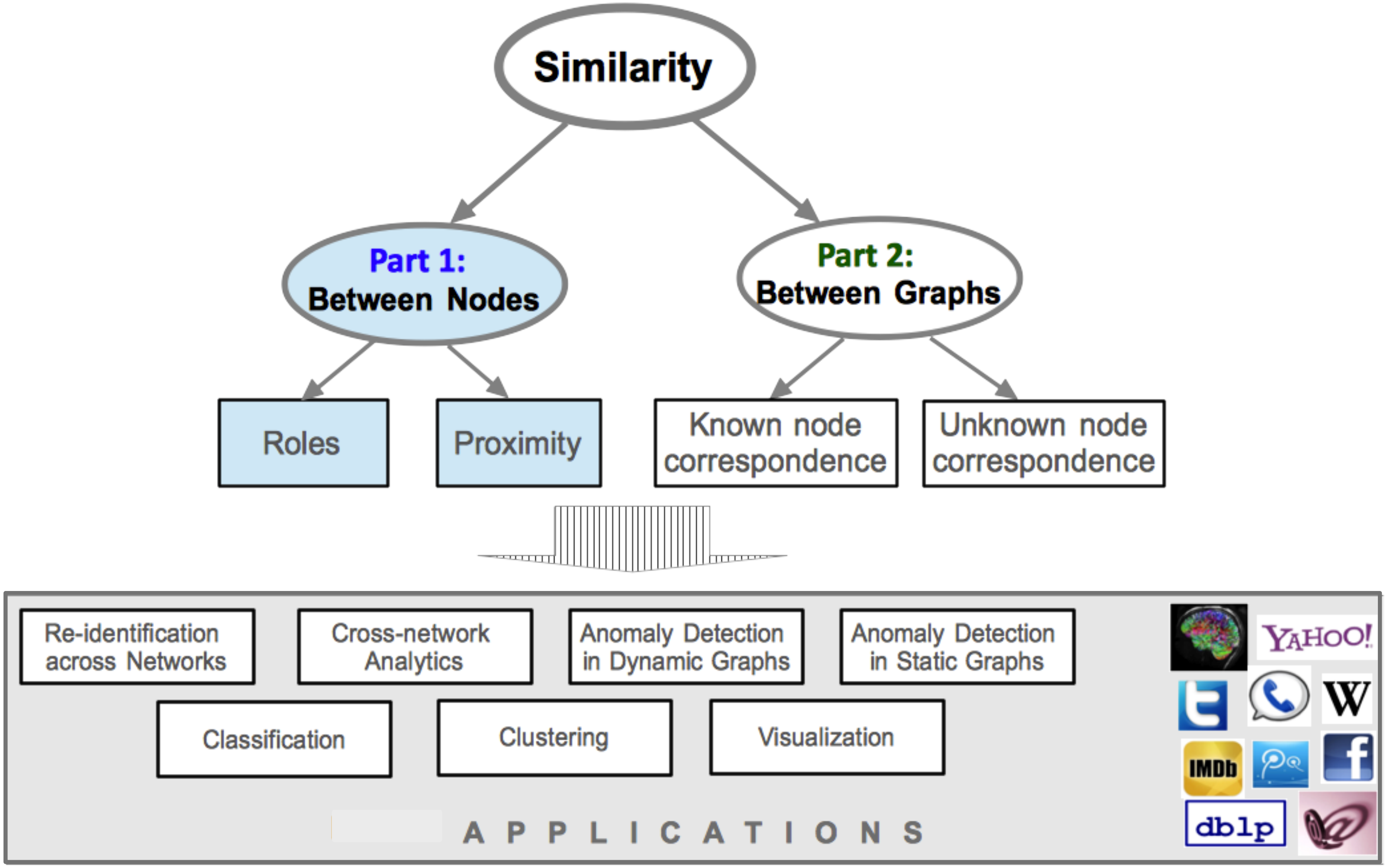
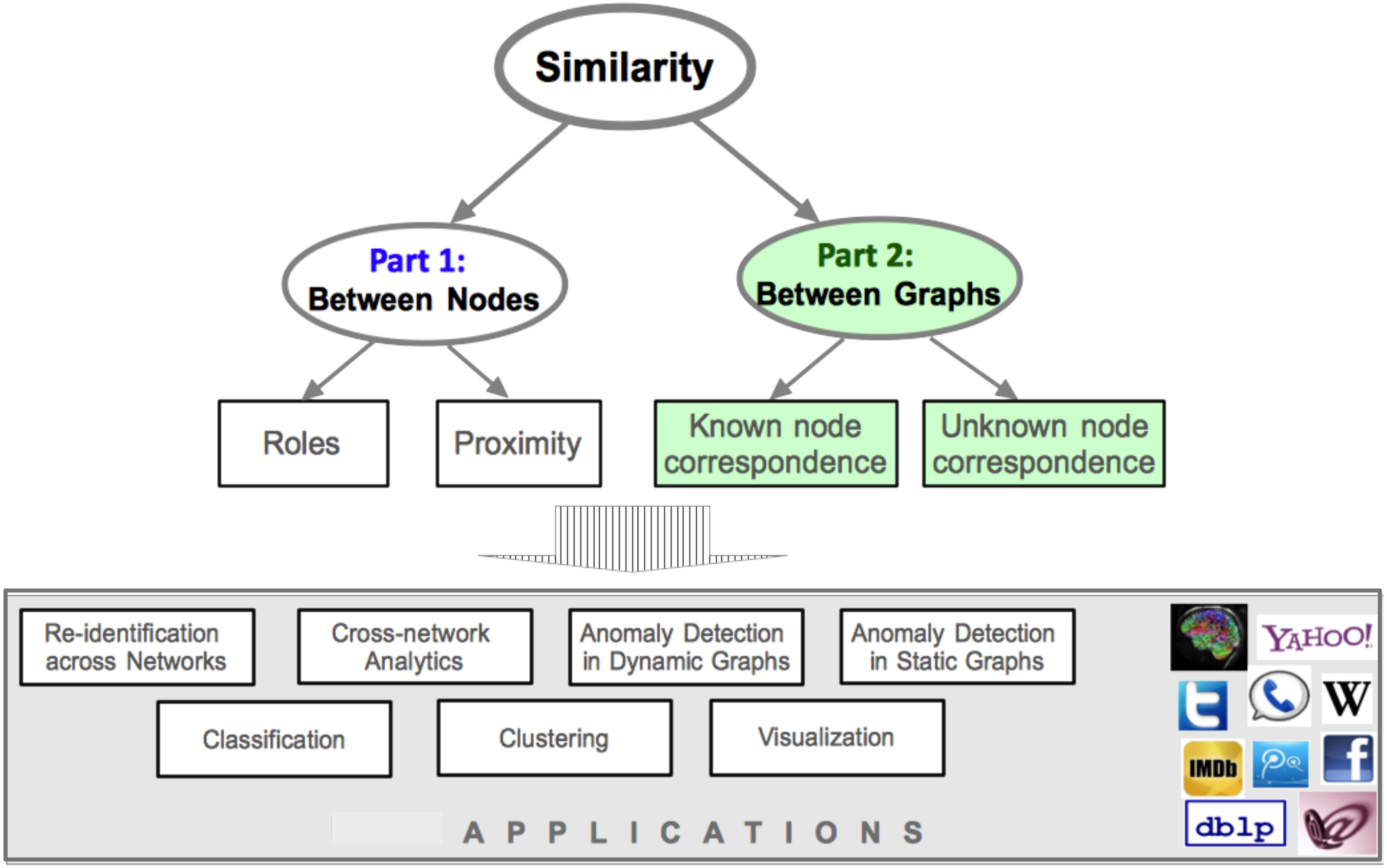
Who we are

- Danai Koutra, CMU
  - Node and graph similarity, summarization, pattern mining
  - http://www.cs.cmu.edu/~dkoutra/
- Tina Eliassi-Rad, Rutgers
  - Data mining, machine learning, big complex networks analysis
  - http://eliassi.org/
- Christos Faloutsos, CMU
  - Graph and stream mining, …
  - http://www.cs.cmu.edu/~christos

What we will cover



What we will cover



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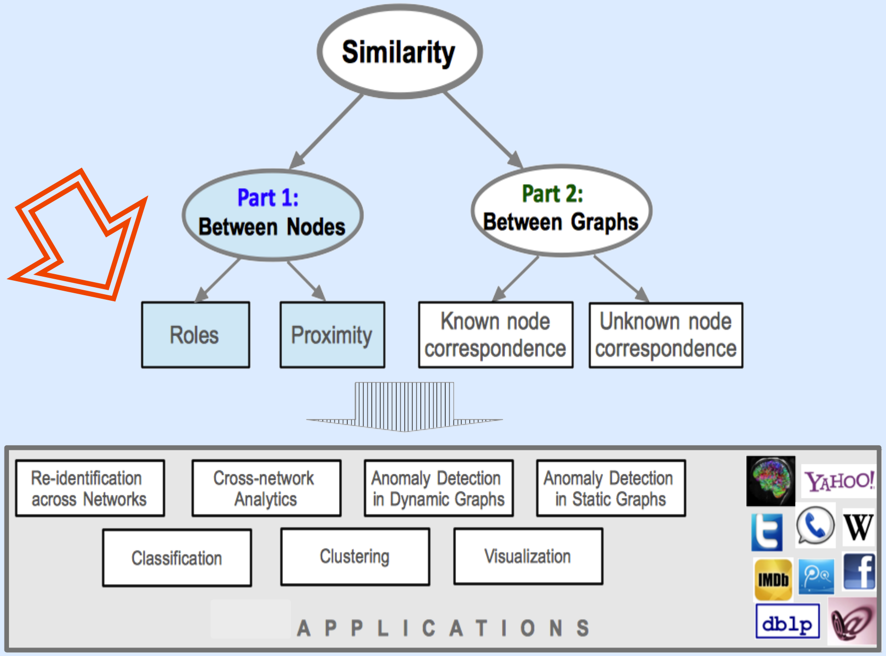
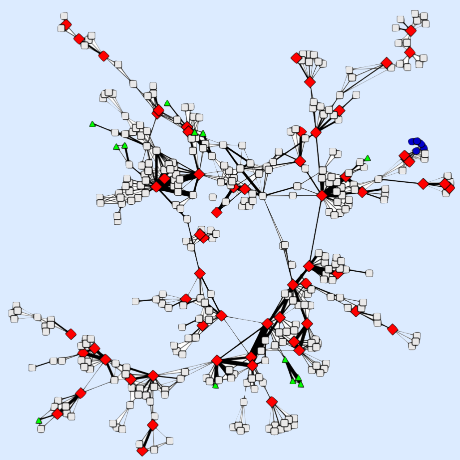
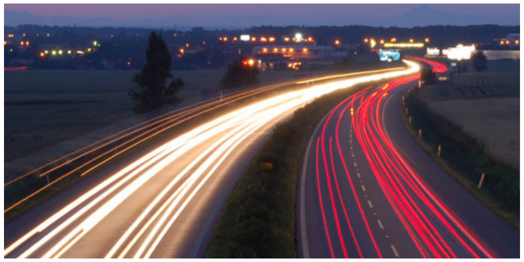
Part 1a
Similarity between Nodes: Roles





Roadmap

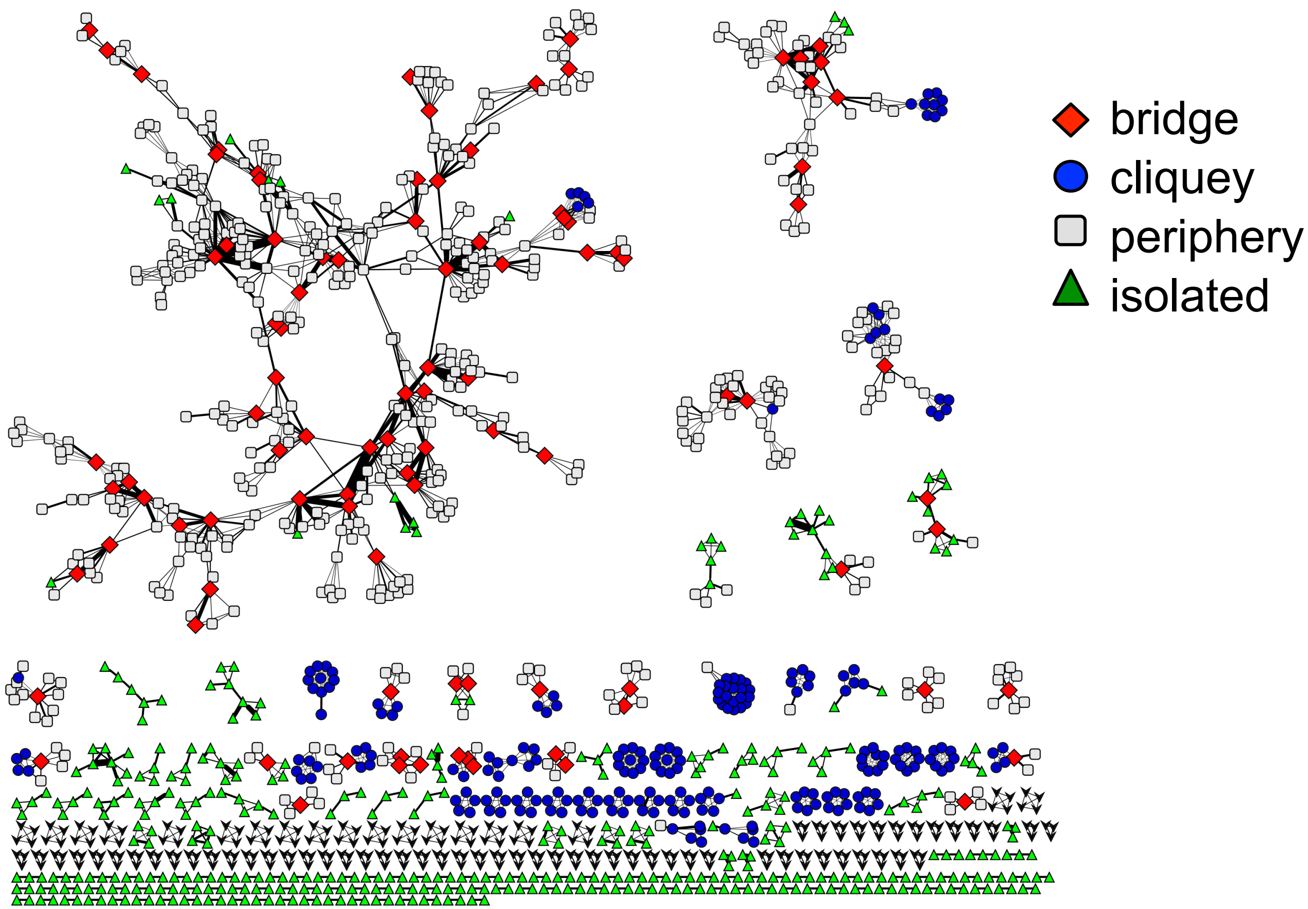
- Node Roles
  - What are roles
  - Roles and communities
  - Roles and equivalences (from sociology)
  - Roles (from data mining)
  - Summary
- Node Proximity



What are roles?

- "Functions" of nodes in the network
  - Similar to functional roles of species in ecosystems
- Measured by **structural behaviors**
- Examples
  - centers of stars
  - members of cliques
  - peripheral nodes
  - …

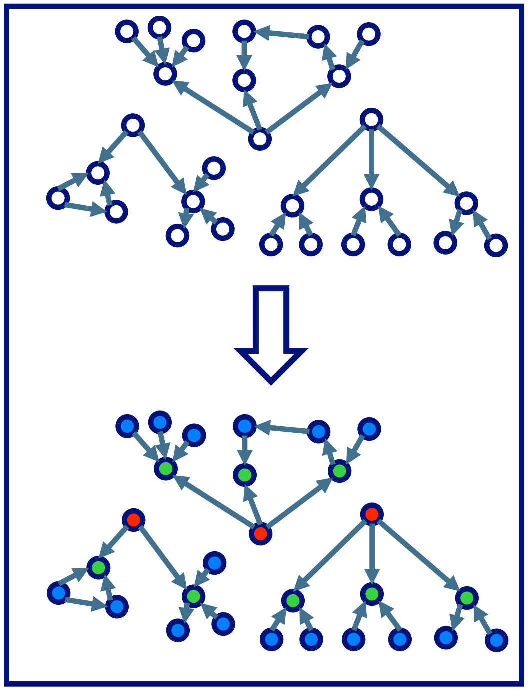
Example of Roles



Network Science Co-authorship Graph
[Newman 2006]

Why are the roles important?

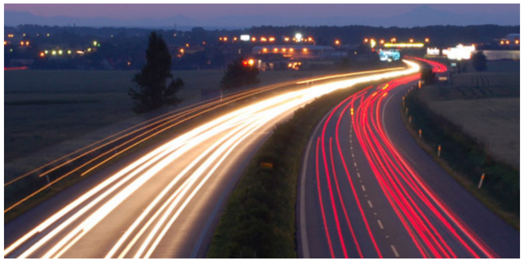
Role Discovery



- ✓ Automated discovery
- ✓ Behavioral roles
- ✓ Roles generalize

Task	Use Case
Role query	Identify individuals with similar behavior to a known target
Role outliers	Identify individuals with unusual behavior
Role dynamics	Identify unusual changes in behavior
Identity resolution	Identify known individuals in a new network
Role transfer	Use knowledge of one network to make predictions in another
Network comparison	Determine network compatibility for knowledge transfer

Roadmap



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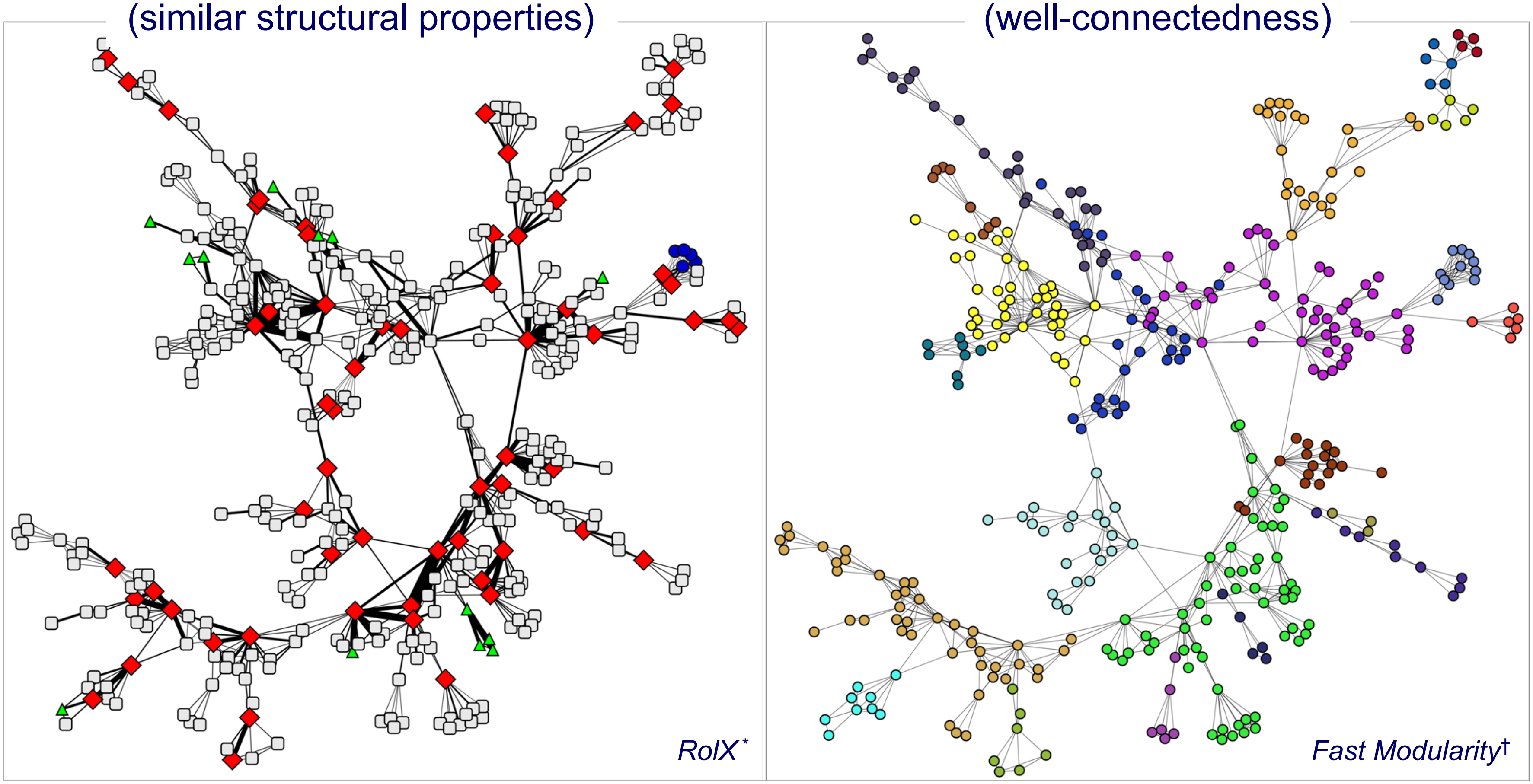
Roles and Communities are Complementary

<u>Roles</u>
(similar structural properties)

<u>Communities</u>
(well-connectedness)



* Henderson, et al. 2012; † Clauset, et al. 2004

Roles and Communities

Consider the social network of a CS dept

- Roles
  - Faculty
  - Staff
  - Students
  - …
- Communities
  - AI lab
  - Database lab
  - Architecture lab
  - …

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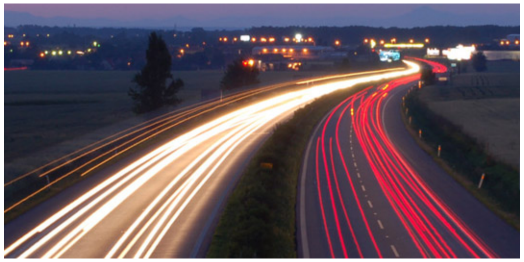


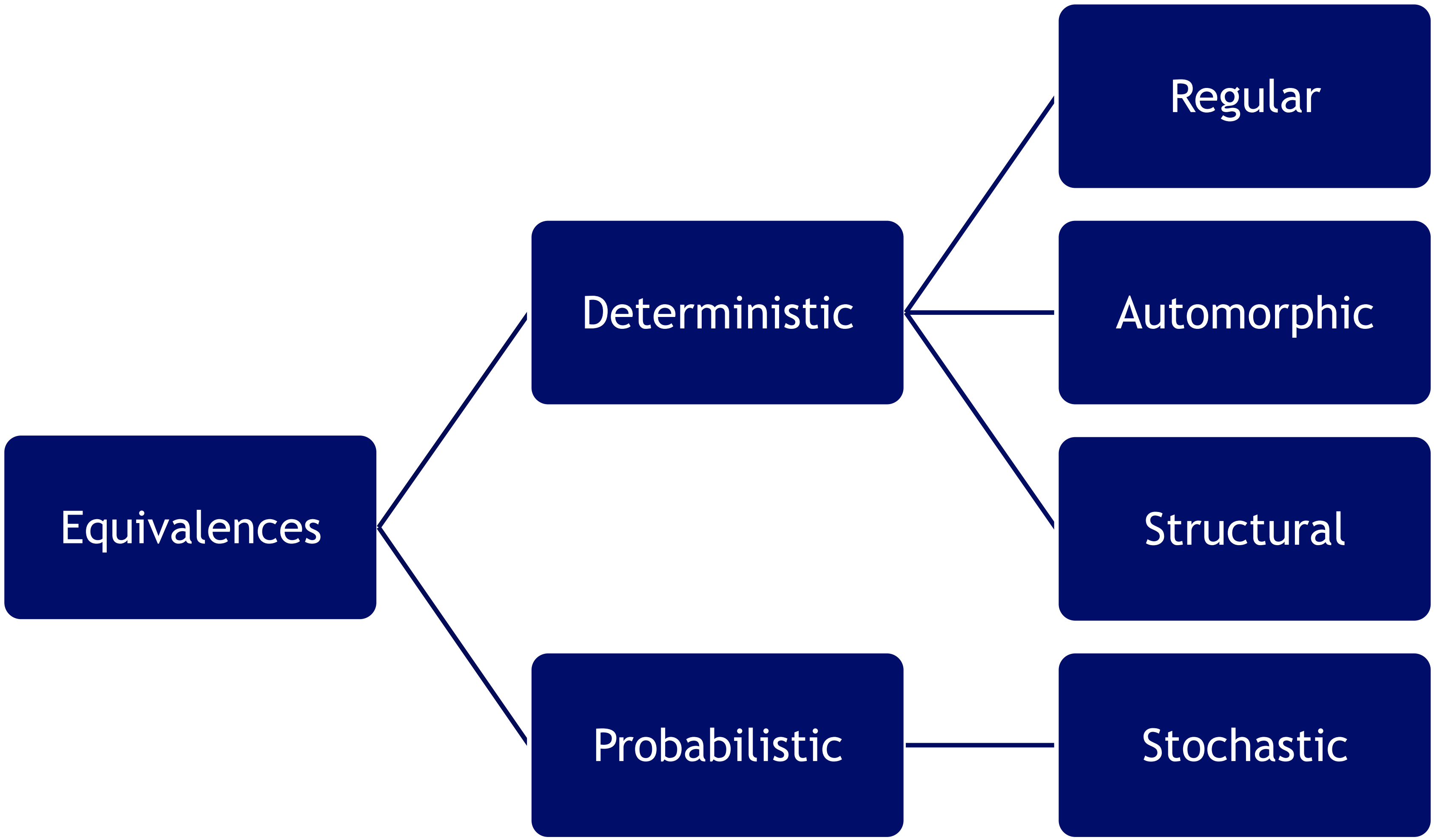
Equivalences

- Equivalence is any relation that satisfies these 3 conditions:

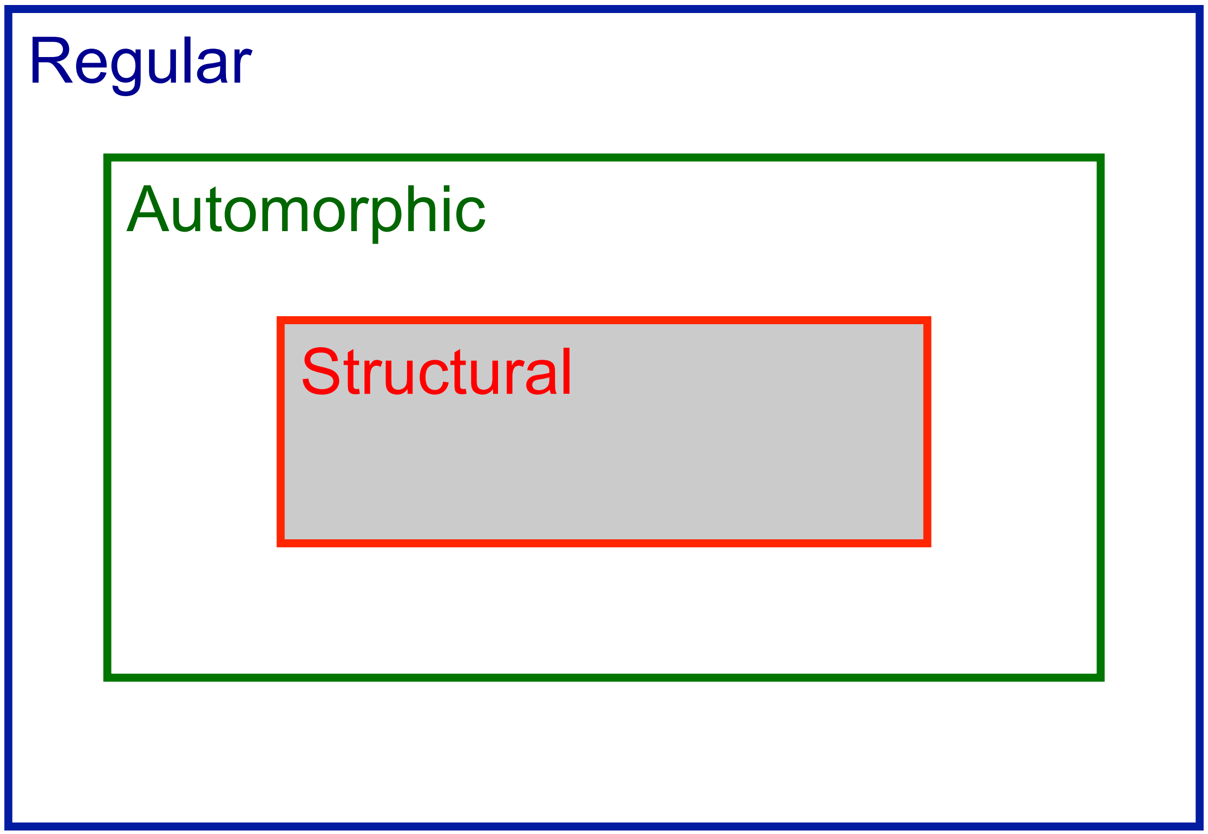
  1. *Transitivity*: $(a, b), (b, c) \in E \Rightarrow (a,c) \in E$
  2. *Symmetry*: $(a, b) \in E$ iff $(b, a) \in E$
  3. *Reflexivity*: $(a, a) \in E$

Roles are referred to as “positions” in sociology.

Equivalences

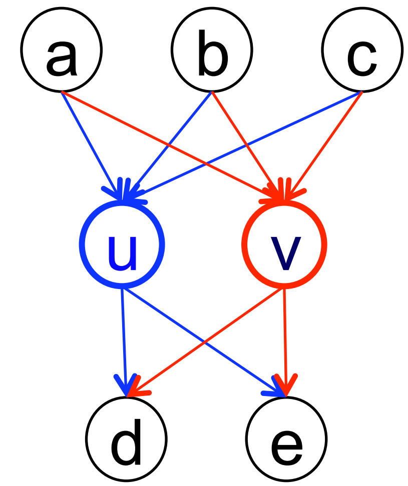


Deterministic Equivalences



Structural Equivalence

- [Lorrain & White, 1971]
- Two nodes u and v are structurally equivalent if they have the same relationships to all other nodes
- Hypothesis: Structurally equivalent nodes are likely to be similar in other ways – i.e., you are your friend
- Weights & timing issues are not considered
- Rarely appears in real-world networks



Structural Equivalence: Algorithms

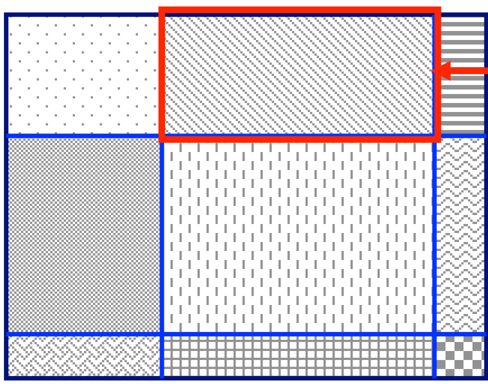
- CONCOR (CONvergence of iterated CORrelations) [Breiger et al. 1975]
- STRUCUTRE [Burt 1976]
- Combinatorial optimization approaches
  - Numerical optimization with tabu search [UCINET]
  - Local optimization [Pajek]
- Partition the sociomatrices into blocks based on a cost function that minimizes the sum of within block variances
  - Basically, minimize the sum of code cost within each block

Cross-Associations (XA)

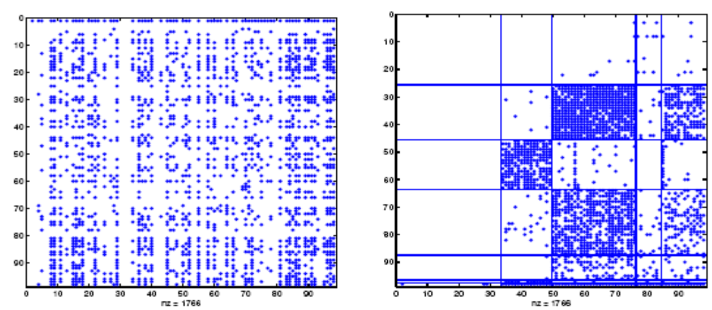
- [Chakrabarti+, KDD 2004]
- Minimize total encoding cost of the adjacency matrix

$$\overbrace{\sum_i \left((n_i^1+n_i^0)\times H(p_i^1)\right)}^{\text{Code Cost}} + \overbrace{\sum_i \left(\text{cost of describing } n_i^1, n_i^0 \text{ and groups}\right)}^{\text{Description Cost}}$$

Binary Matrix

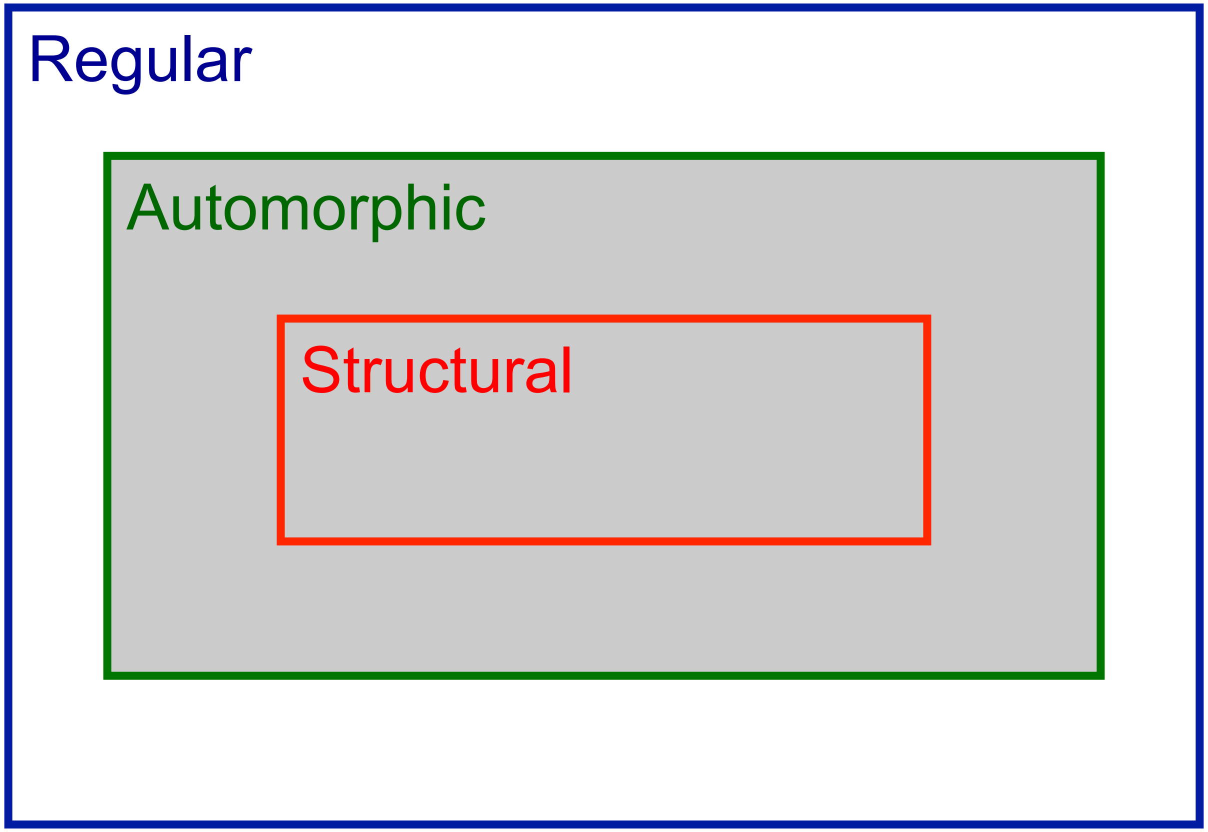


$p_i^1 = n_i^1 / (n_i^1 + n_i^0)$



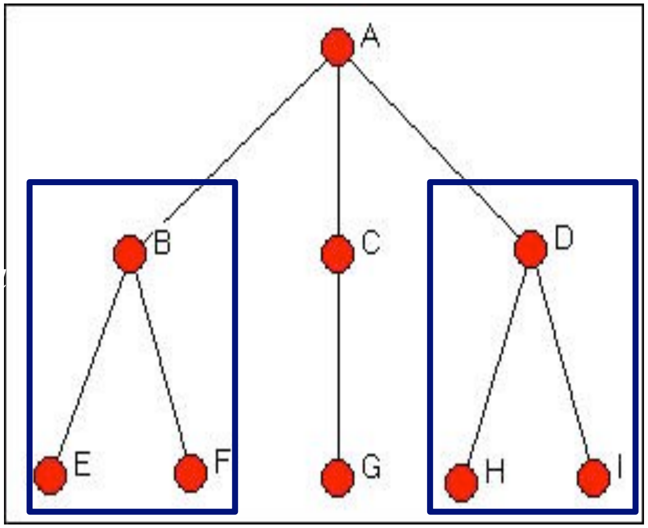
(a) before (b) after

Deterministic Equivalences



Automorphic Equivalence

- [Borgatti, et al. 1992; Sparrow 1993]
- Two nodes *u* and *v* are automorphically equivalent if all the nodes can be relabeled to form an isomorphic graph with the labels of *u* and *v* interchanged
  - Swapping *u* and *v* (possibly along with their neighbors) does not change graph distances
- Two nodes that are automorphically equivalent share exactly the same label-independent properties



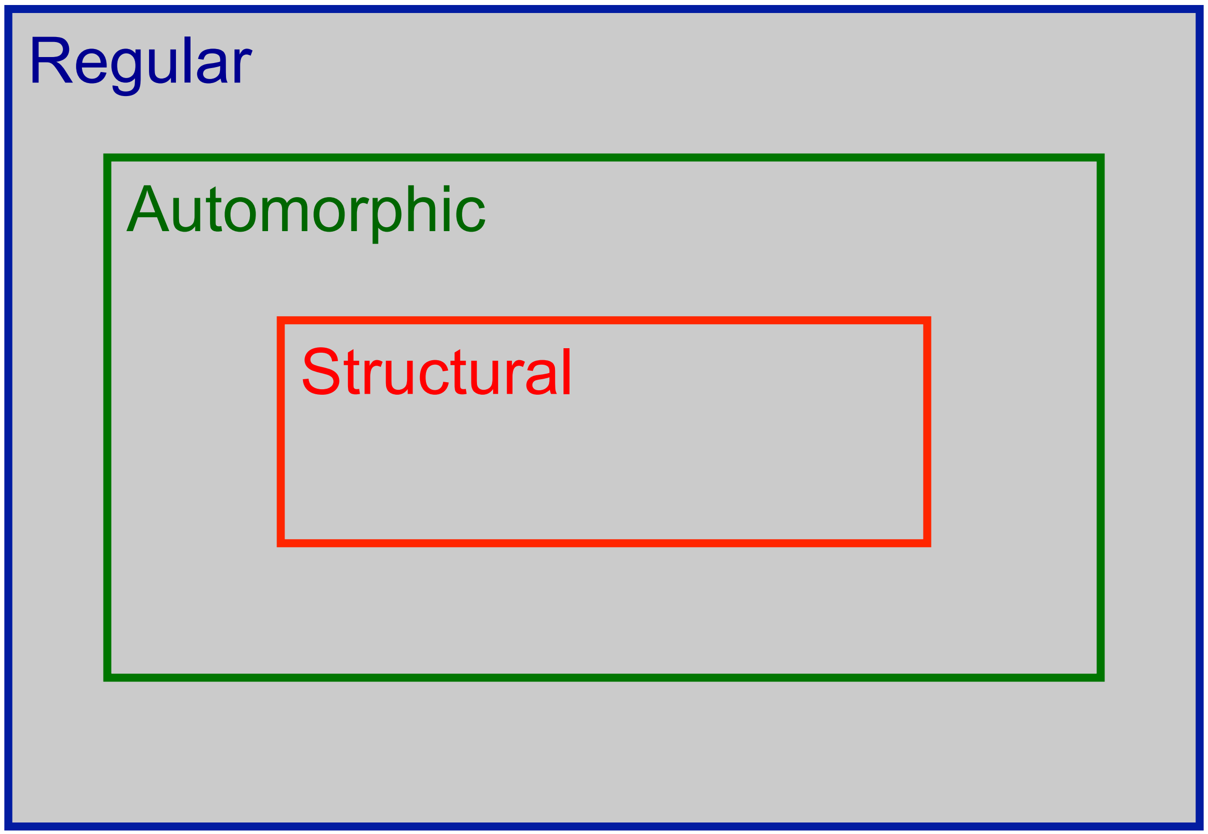
Automorphic Equivalence: Algorithms

- Sparrow (1993) proposed an algorithm that scales linearly to the number of edges
- Use numerical signatures on degree sequences of neighborhoods
- Numerical signatures use a unique transcendental number like π, which is independent of any permutation of nodes
- Suppose node i has the following degree sequence: 1, 1, 5, 6, and 9. Then its signature is

$$S_{i,1} = (1 + \pi)(1 + \pi)\ (5 + \pi)\ (6 + \pi)\ (9 + \pi)$$

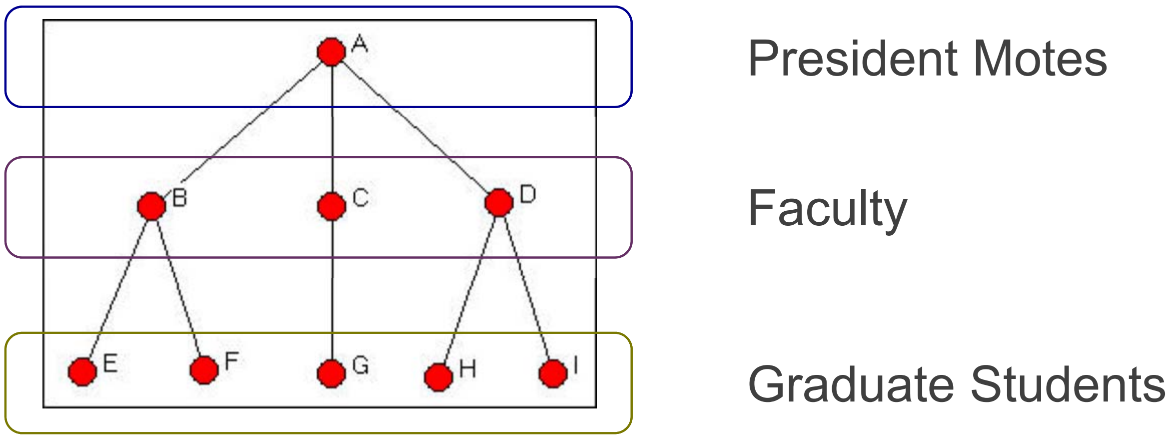
- The signature for node i at k+1 hops is $S_{i,(k+1)} = \Pi(S_{i,k} + \pi)$
- To find automorphic equivalence, simply compare numerical signatures of nodes

Deterministic Equivalences



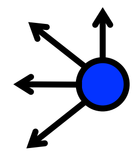
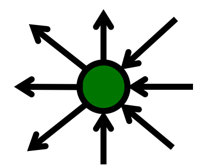
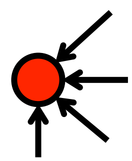
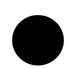
Regular Equivalence

- [Everett & Borgatti, 1992]
- Two nodes *u* and *v* are regularly equivalent if they are equally related to equivalent others



Hanneman, Robert A. and Mark Riddle. 2005. Introduction to social network methods. Riverside, CA: University of California, Riverside (published in digital form at http://faculty.ucr.edu/~hanneman/)

Regular Equivalence (cont'd)

- Basic roles of nodes
  - source 
  - repeater 
  - sink 
  - isolate 

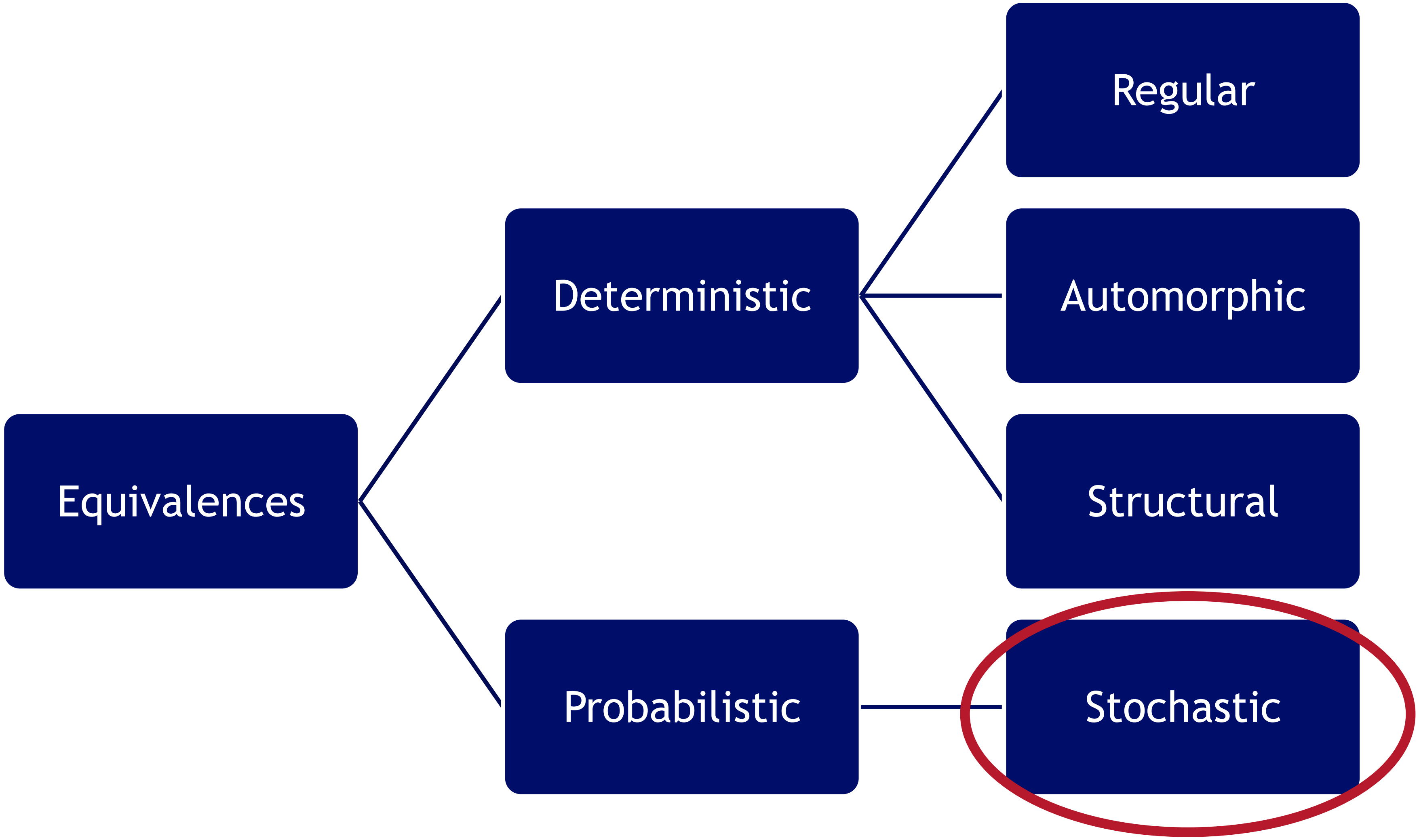
Regular Equivalence (cont'd)

- Based solely on the social roles of neighbors
- Interested in
  - Which nodes fall in which social roles?
  - How do social roles relate to each other?
- Hard partitioning of the graph into social roles
- A given graph can have more than one valid regular equivalence set
- Exact regular equivalences can be rare in large graphs

Regular Equivalence: Algorithms

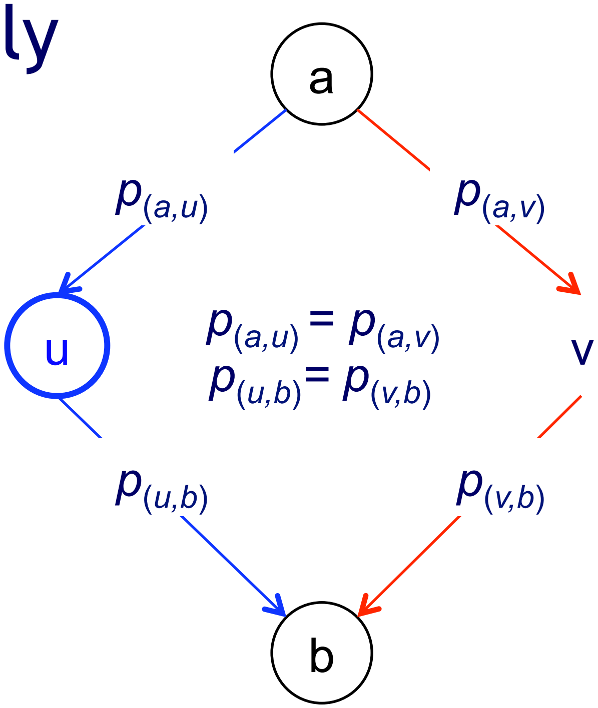
- Many algorithms exist here
  - Maximal Regular coloration [Everett & Borgatti, 1997] – a polynomial time alg
- Basic notion
  - Profile each node's neighborhood by the presence of nodes of other "types"
  - Nodes are regularly equivalent to the extent that they have similar "types" of other nodes at similar distances in their neighborhoods

Equivalences



Stochastic Equivalence

- [Holland, et al. 1983; Wasserman & Anderson, 1987]
- Two nodes are stochastically equivalent if they are "exchangeable" w.r.t. a probability distribution
- Similar to structural equivalence but probabilistic



Stochastic Equivalence: Algorithms

- Many algorithms exist here
- Most recent approaches are generative [Airoldi, et al 2008]
- Some choice points
  - Single [Kemp, et al 2006] vs. mixed-membership [Koutsourelakis & Eliassi-Rad, 2008] equivalences (a.k.a. "positions")
  - Parametric vs. non-parametric models

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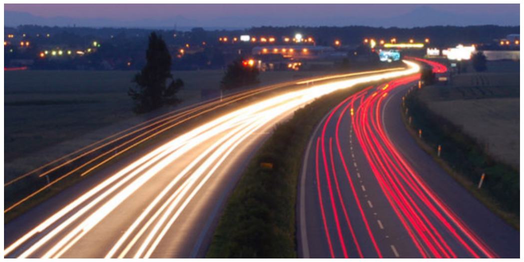
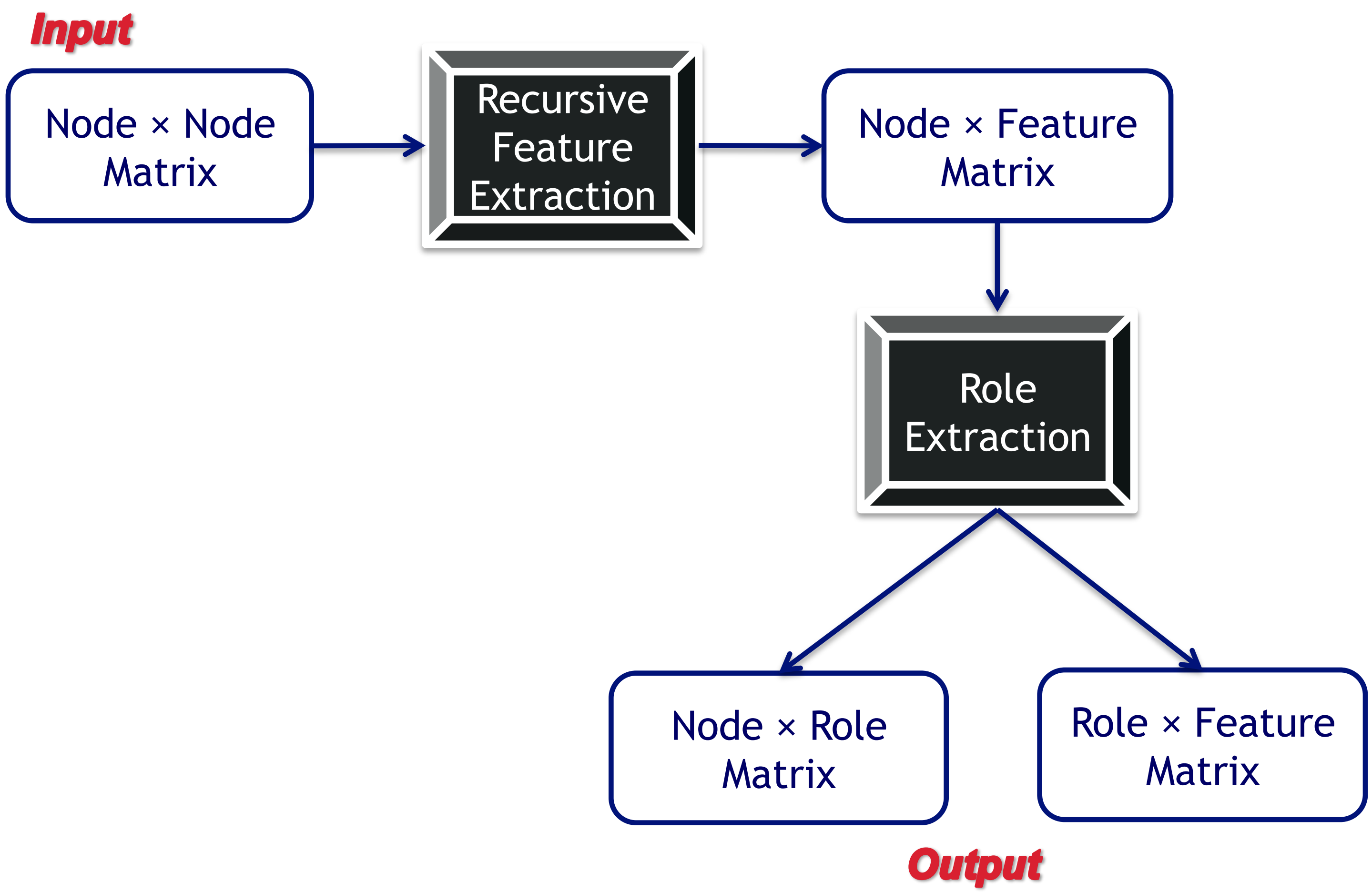


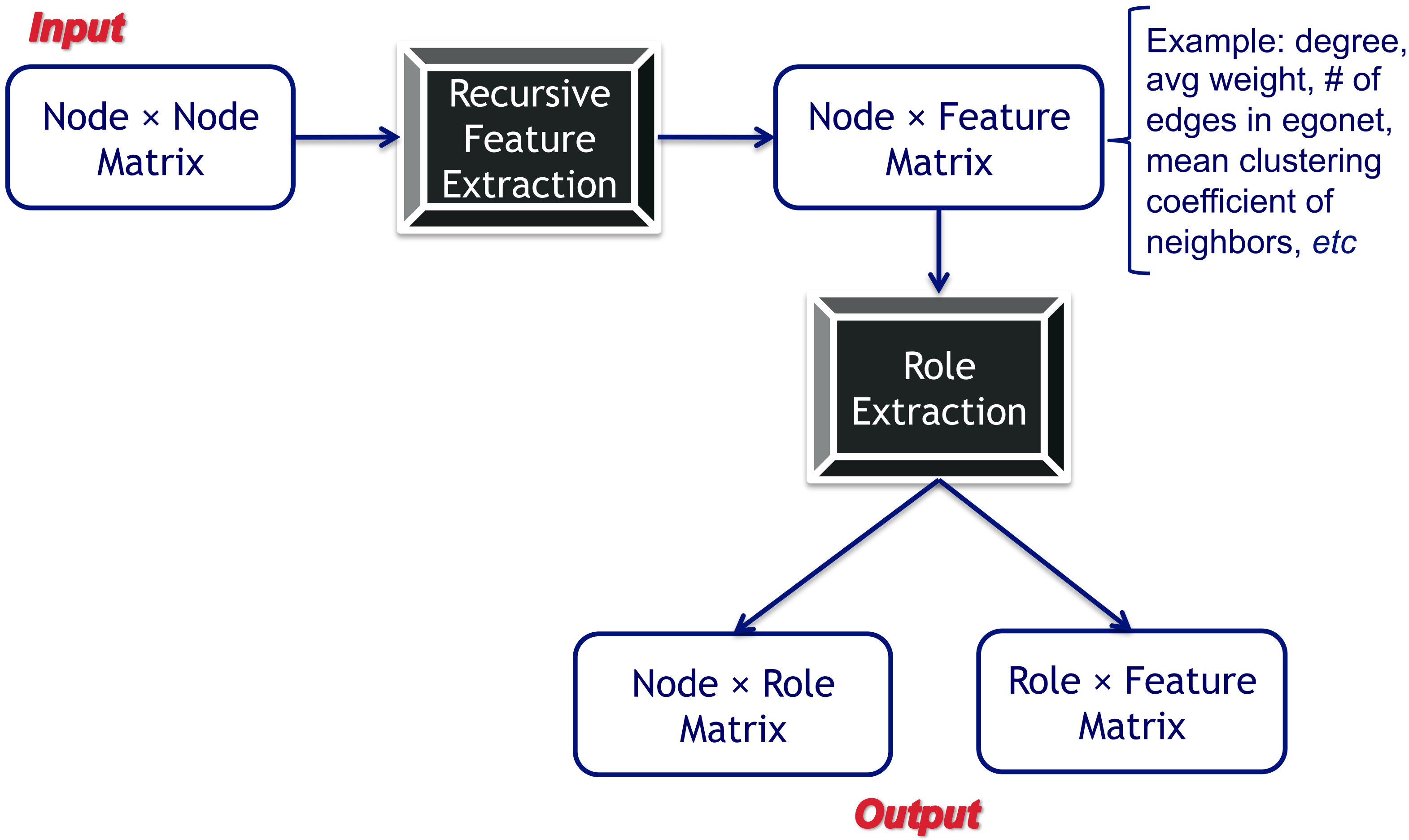
RolX: Role eXtraction

- Introduced by Henderson et al. KDD 2012
- Automatically extracts the underlying roles in a network
  - No prior knowledge required
- Determines the number of roles automatically
- Assigns a mixed-membership of roles to each node
- Scales linearly on the number of edges

RolX: Flowchart

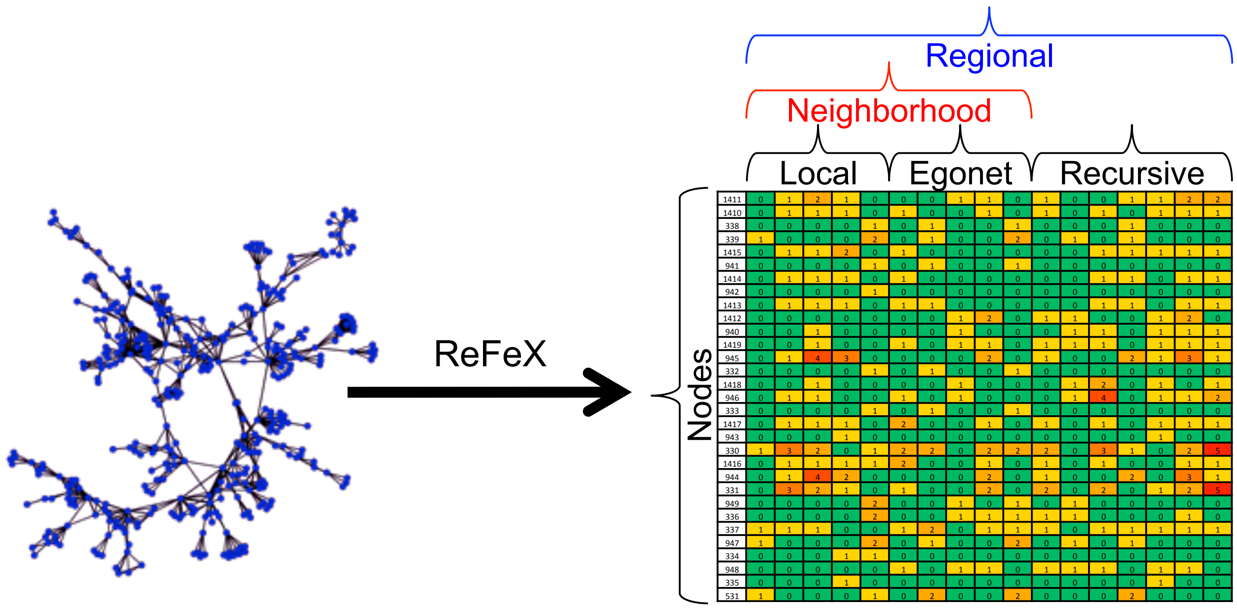


RolX: Flowchart



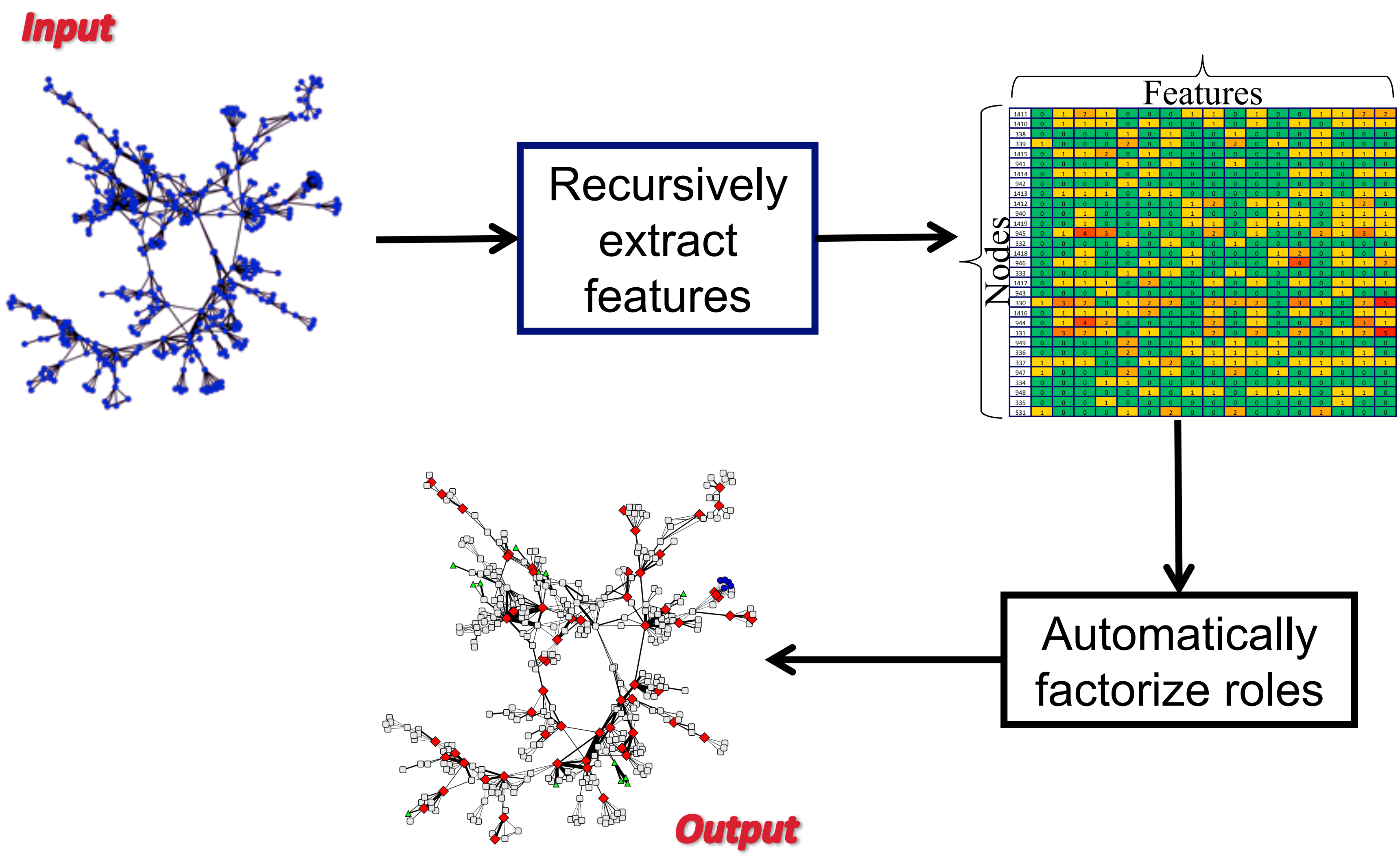
Recursive Feature Extraction

- ReFeX [Henderson, et al. 2011a] turns network connectivity into recursive structural features



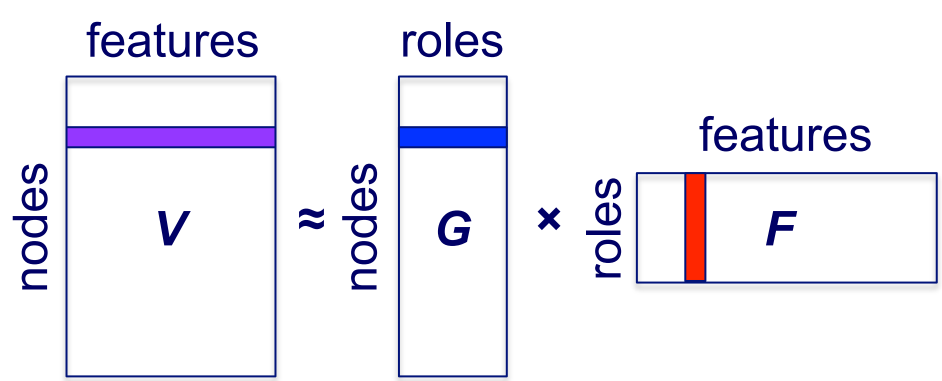
- Neighborhood features: What is your connectivity pattern?
- Recursive Features: To what kinds of nodes are you connected?

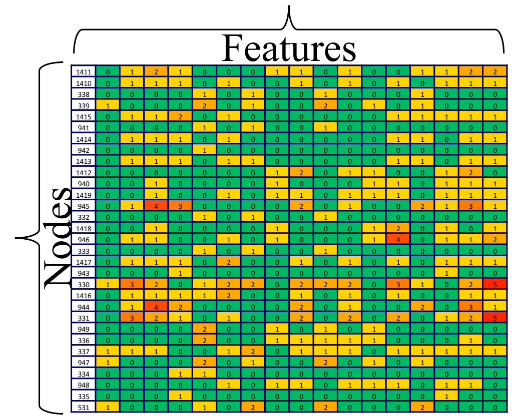
Role Extraction



Role Extraction: Feature Grouping

- Soft clustering in the structural feature space
  - Each node has a mixed-membership across roles
- Generate a rank *r* approximation of V ≈ GF





- RolX uses NMF for feature grouping
  - Computationally efficient
  - Non-negative factors simplify interpretation of roles and memberships

$$\boxed{\mathrm{argmin}_{G,F} \|V - GF\|_{fro}, \text{s.t. } G \geq 0,\ F \geq 0}$$

Role Extraction: Model Selection

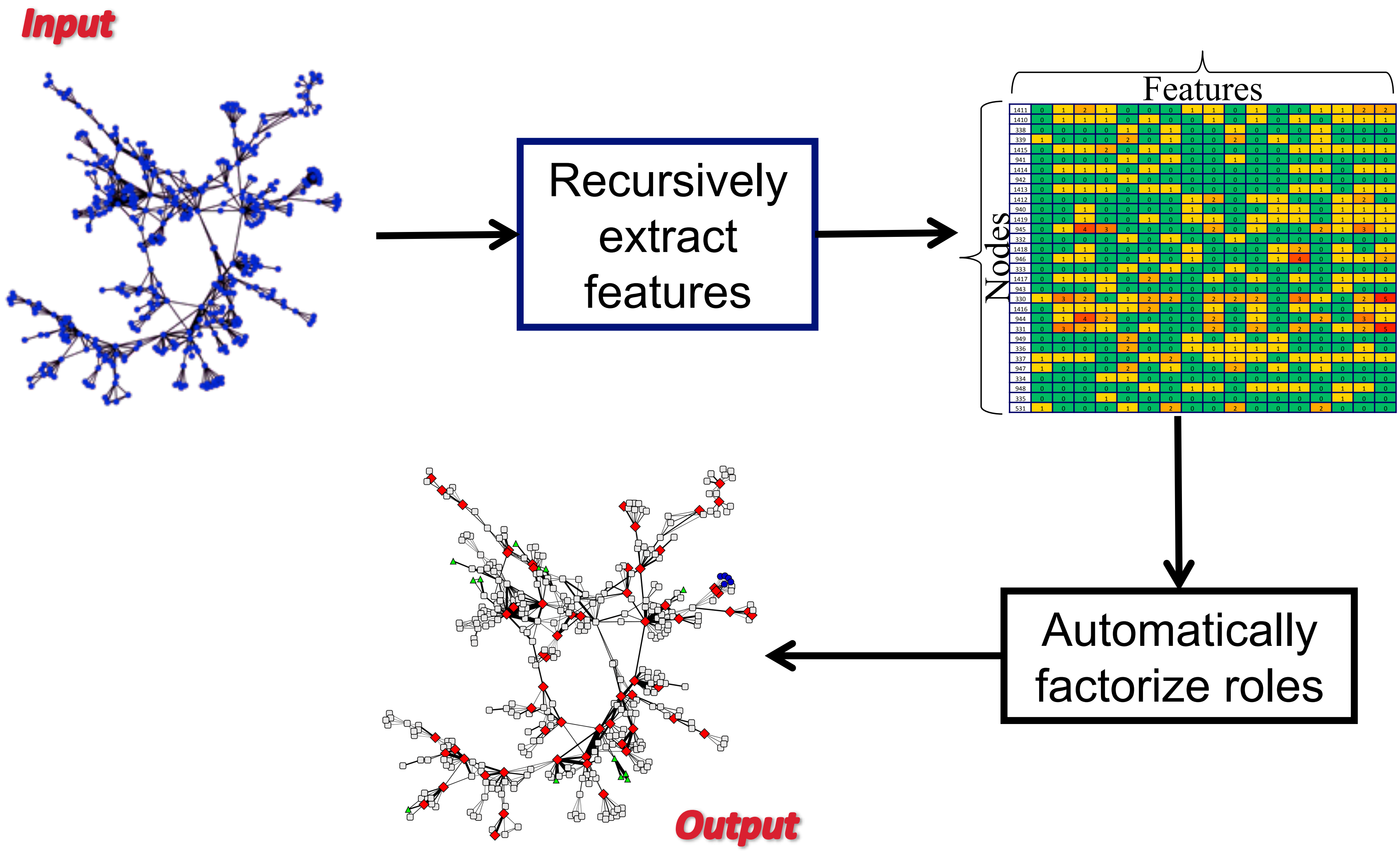
- Roles summarize behavior
  - Or, they compress the feature matrix, V
- Use MDL to select the model size *r* that results in the best compression
  - L: description length
  - M: # of bits required to describe the model
  - E: cost of describing the reconstruction errors in V – GF
  - Minimize L = M + E
    - To compress high-precision floating point values, RolX combines Llyod-Max quantization with Huffman codes

$$M = \bar{b}r(n+f)$$

    - Errors in V-GF are not distributed normally, RolX uses KL divergence to compute E

$$E = \sum_{i,j}\left(V_{i,j}\log\frac{V_{i,j}}{(GF)_{i,j}} - V_{i,j} + (GF)_{i,j}\right)$$

Role Extraction



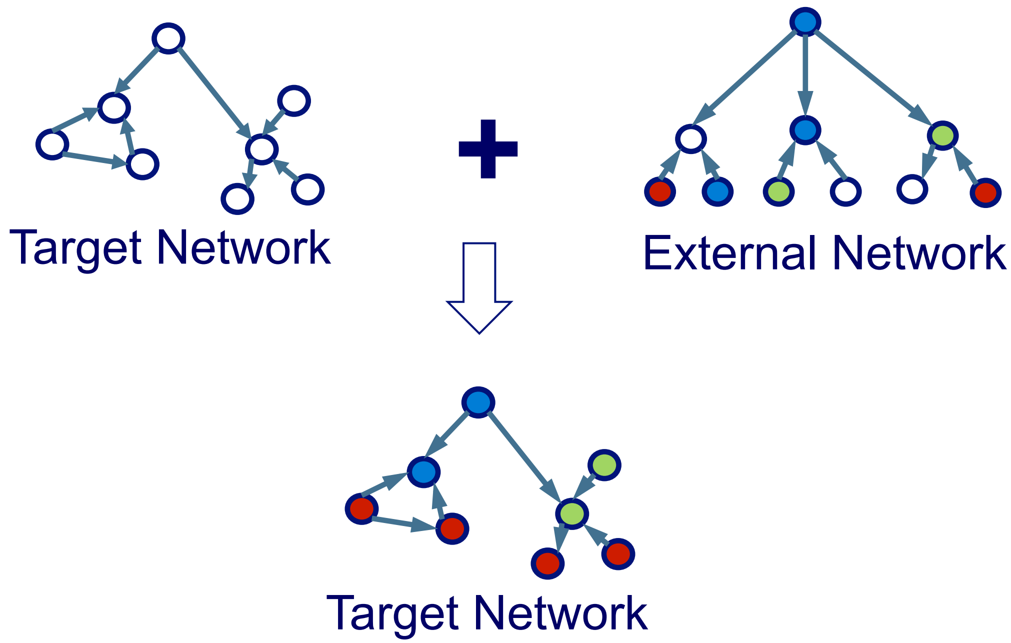
Experiments on Role Discovery

- Role transfer
- Role sense-making
- Role query
- Role mixed-memberships

Details in Henderson *et al.* KDD 2012

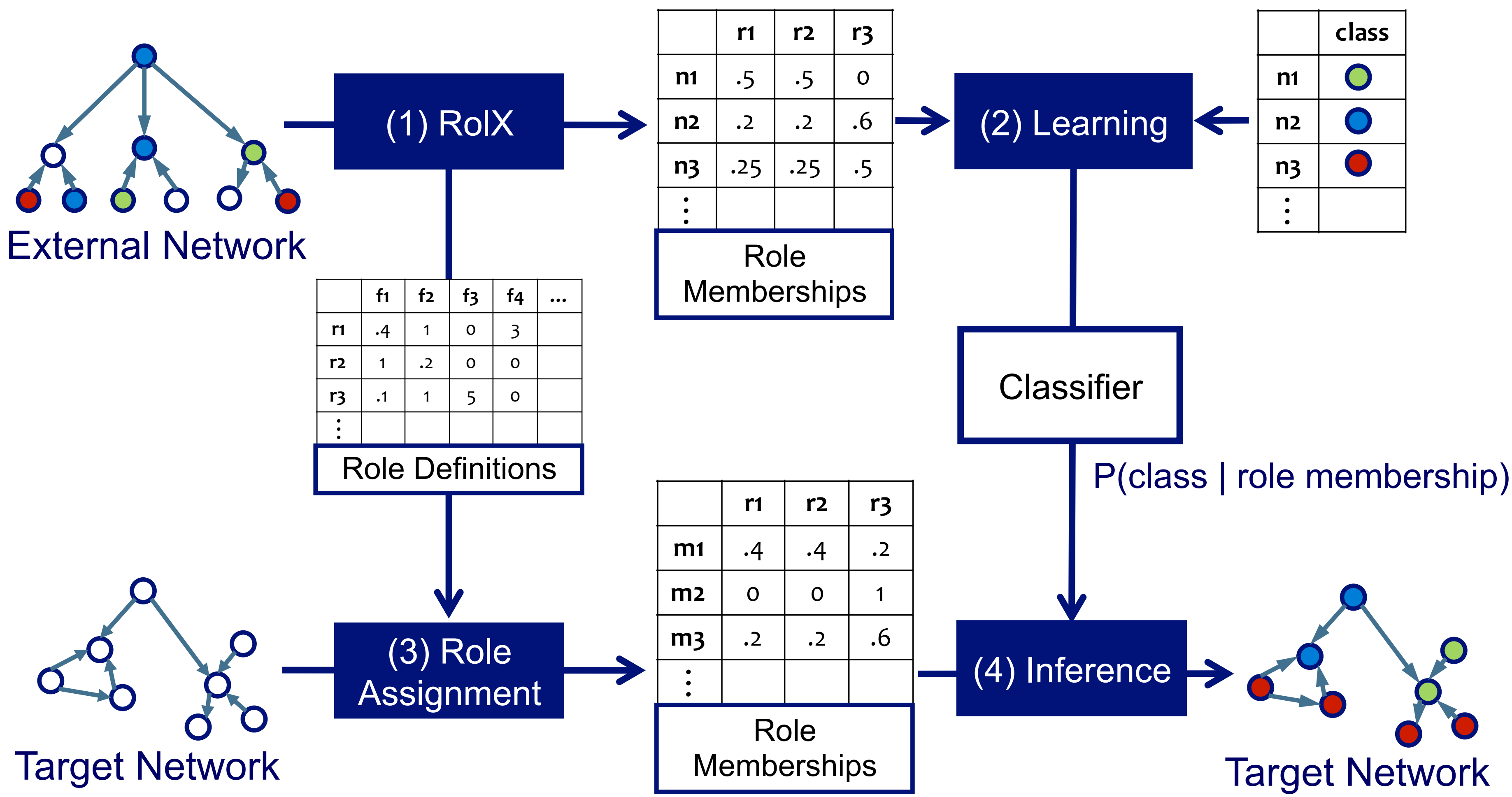
Role Transfer

- Question: How can we use labels from an external source to predict labels on a network with no labels?

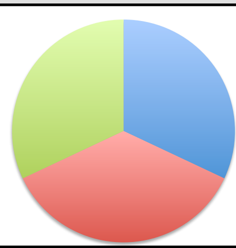
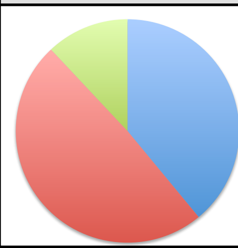
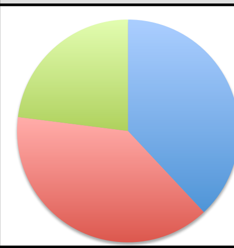
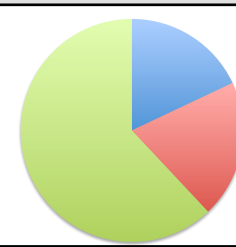
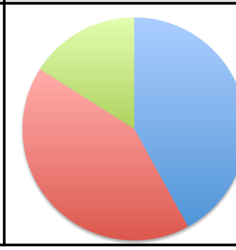


- Conjecture: Nodes with similar roles are likely to have similar labels

Role Transfer = RolX + SL

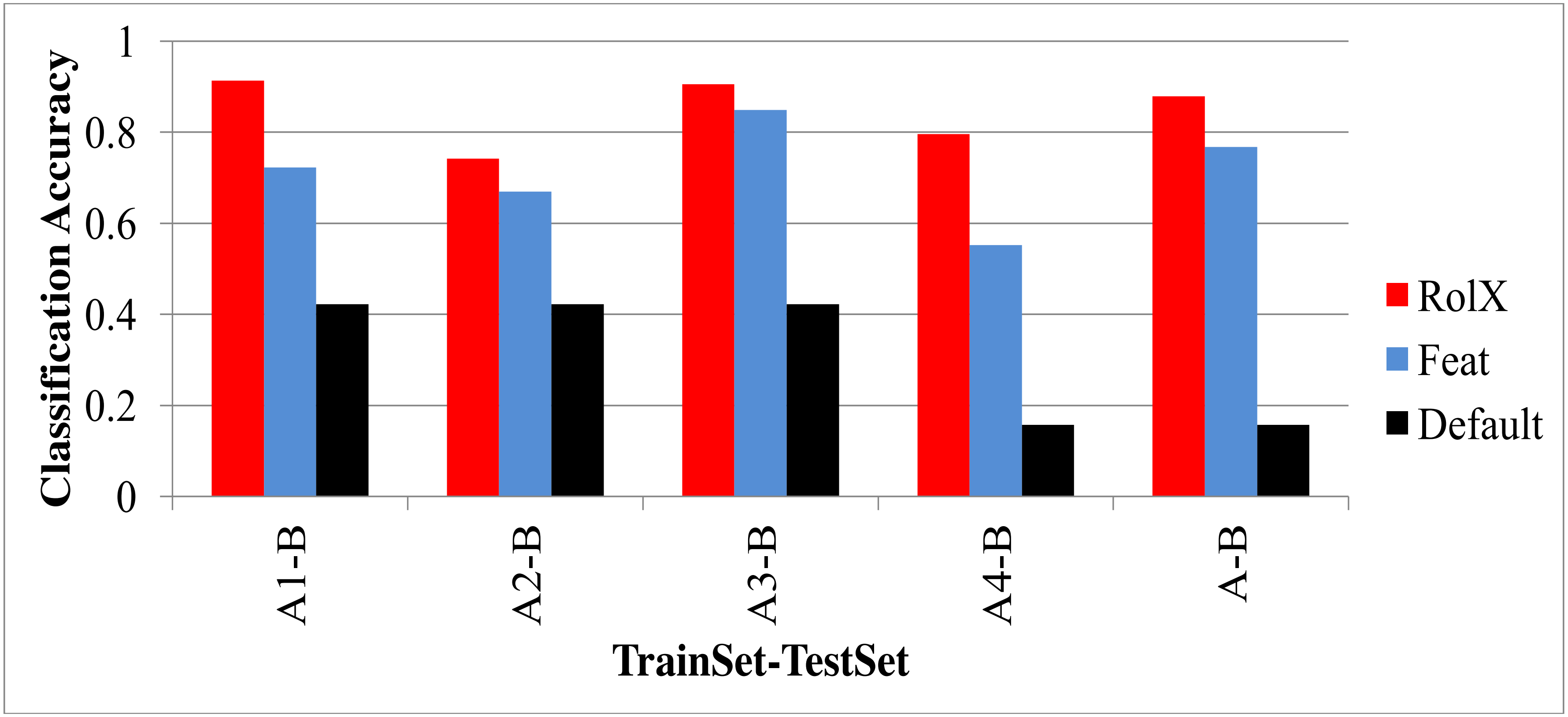


Data for Role Transfer

	IP-A1	IP-A2	IP-A3	IP-A4	IP-B
# Nodes	81,450	57,415	154,103	206,704	181,267
% labeled	36.7%	28.1%	20.1%	32.9%	15.3%
# Links	968,138	432,797	1,266,341	1,756,082	1,945,215
(# unique)	206,112	137,822	358,851	465,869	397,925
Class Distribu-tion					

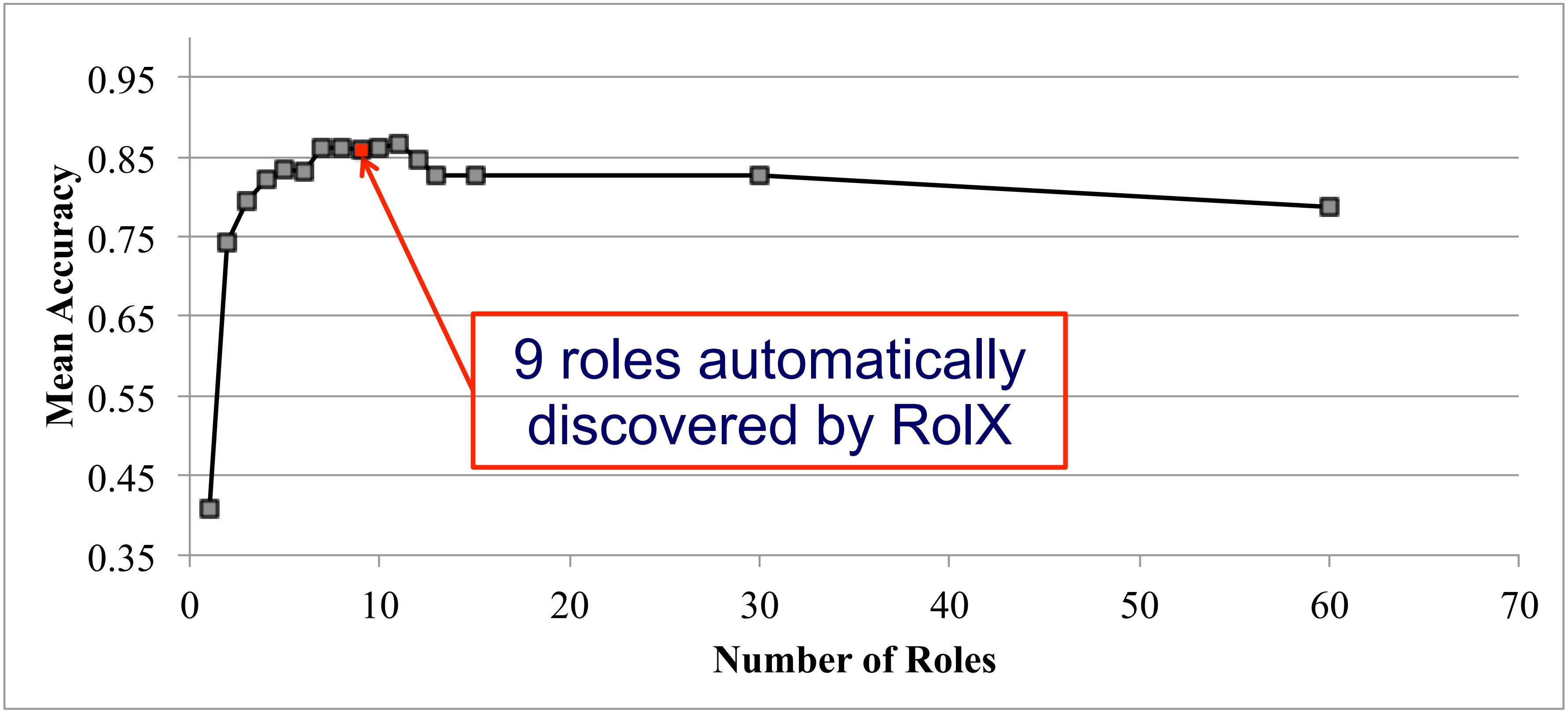
Web DNS P2P

Role Transfer Results



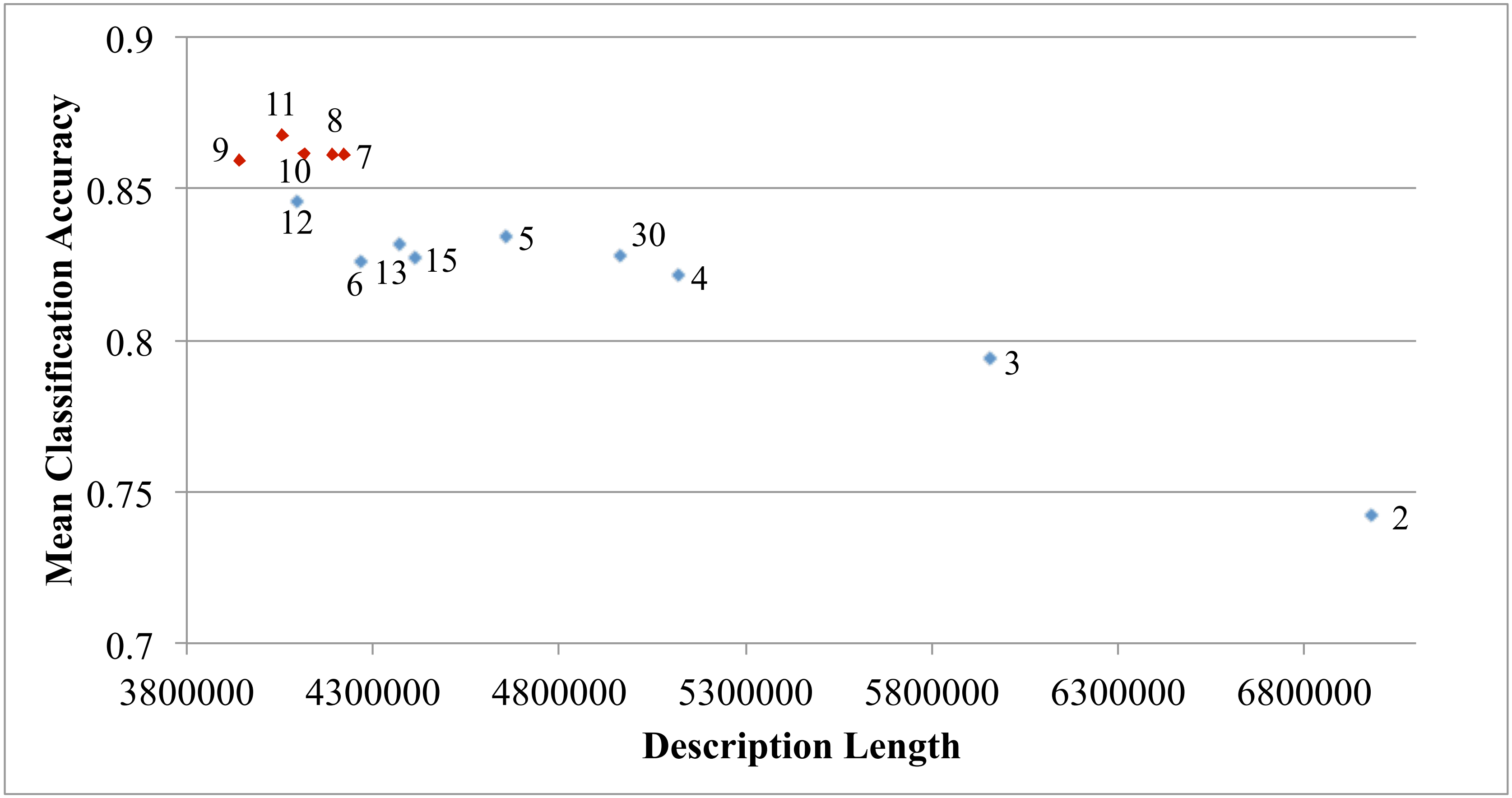
Roles generalize across disjoint networks & enable prediction without re-learning

Model Selection



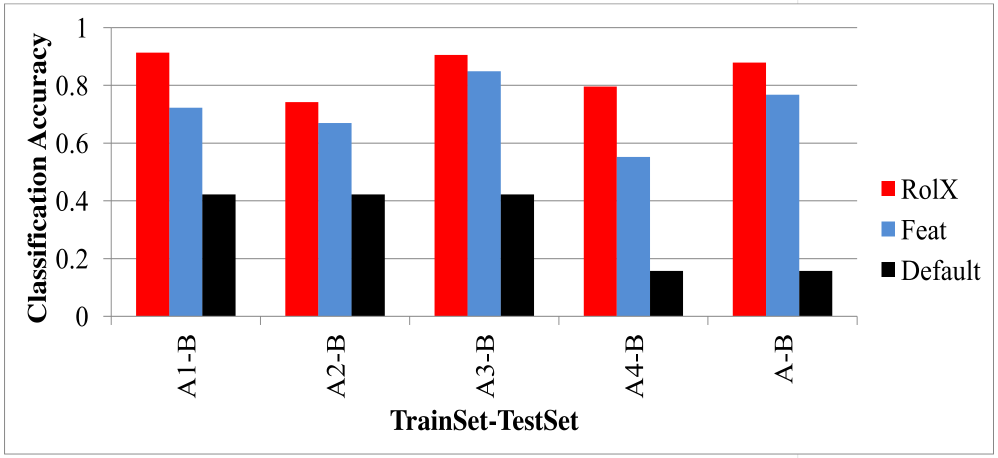
RolX selects high accuracy model sizes

Model Selection (continued)

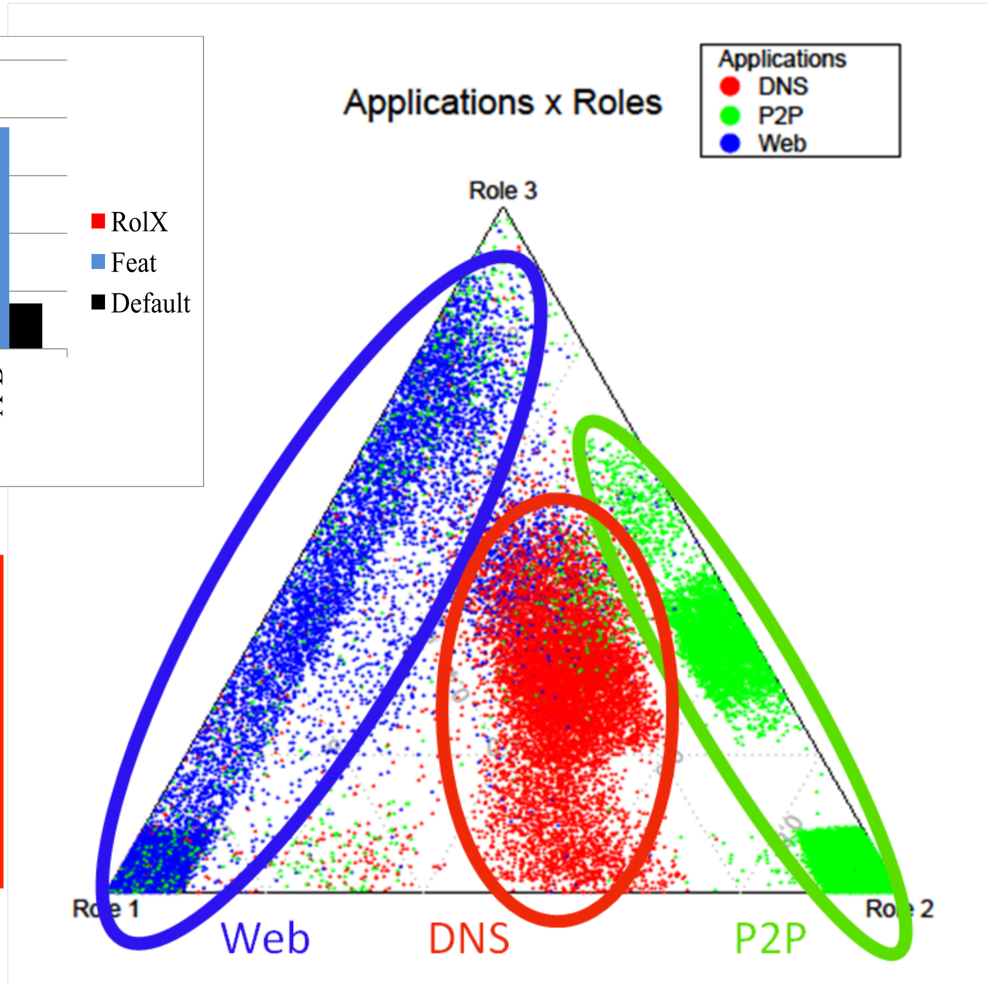


Classification accuracy is highest when RolX selection criterion is minimized

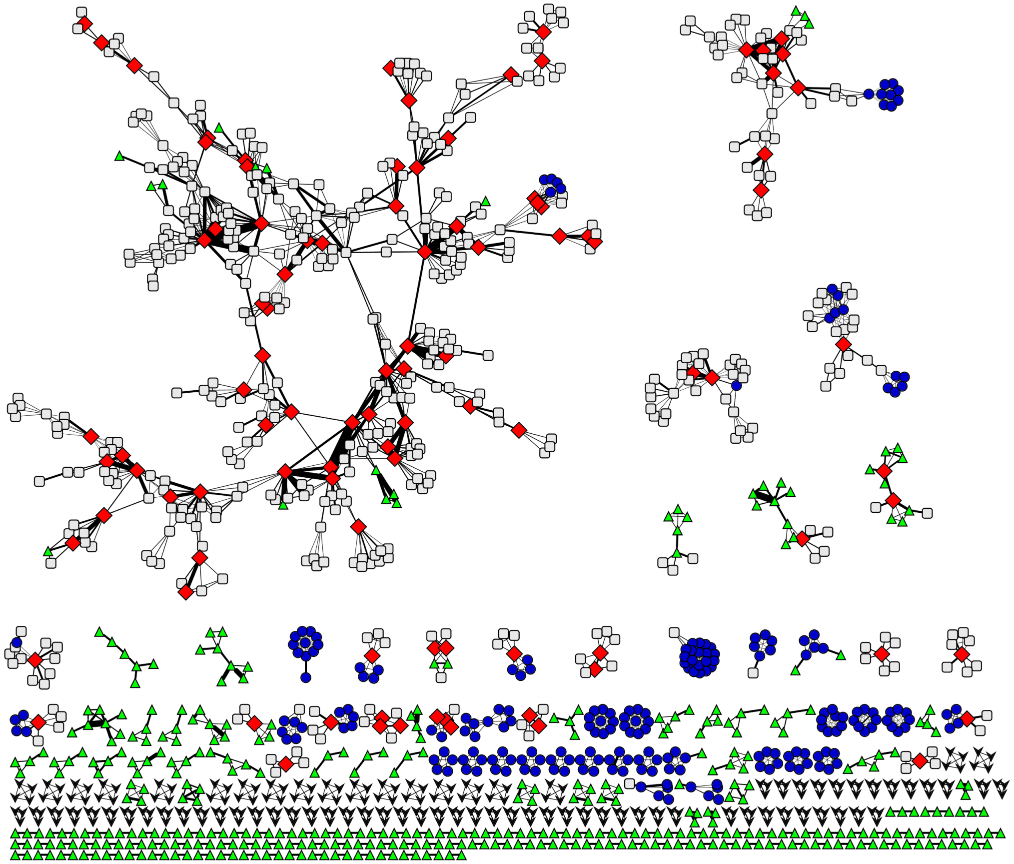
Role Space



IP trace classes are well-separated in the RolX **role space** with as few as 3 roles

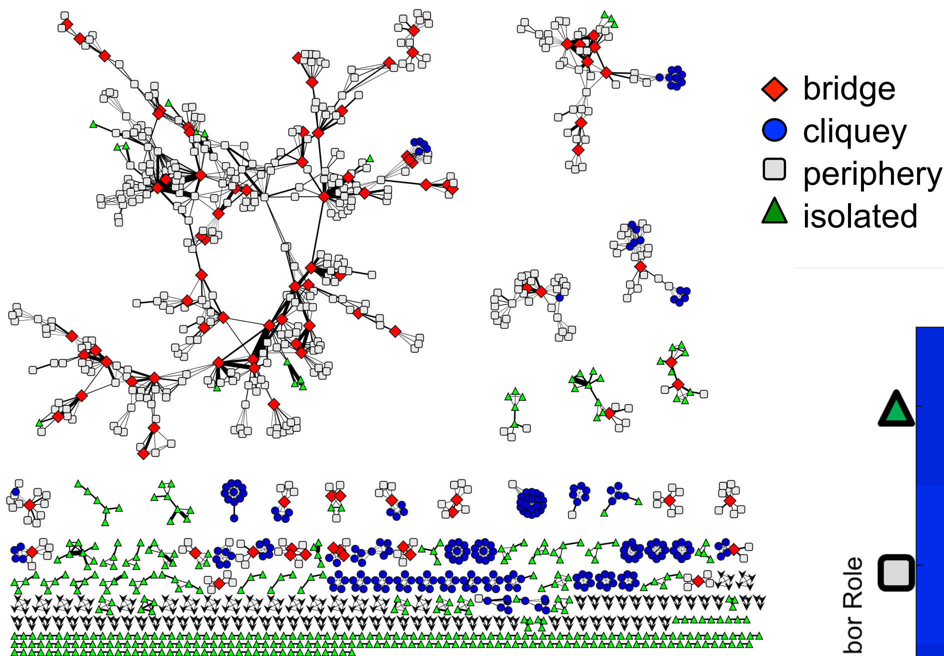


Automatically Discovered Roles



Network Science Co-authorship Graph
[Newman 2006]

Role Affinity Heat Map



Network Science Co-authorship Graph
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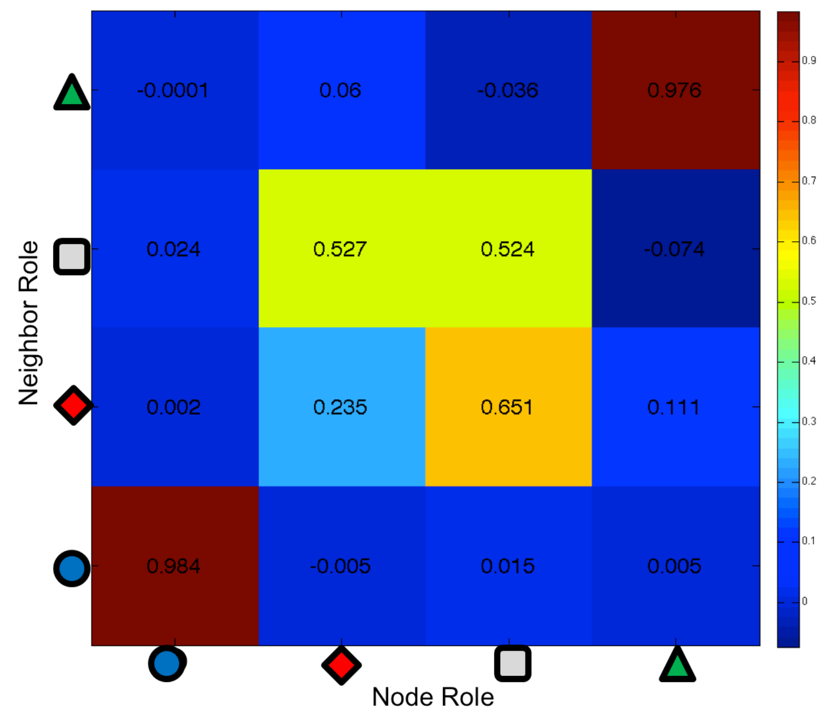
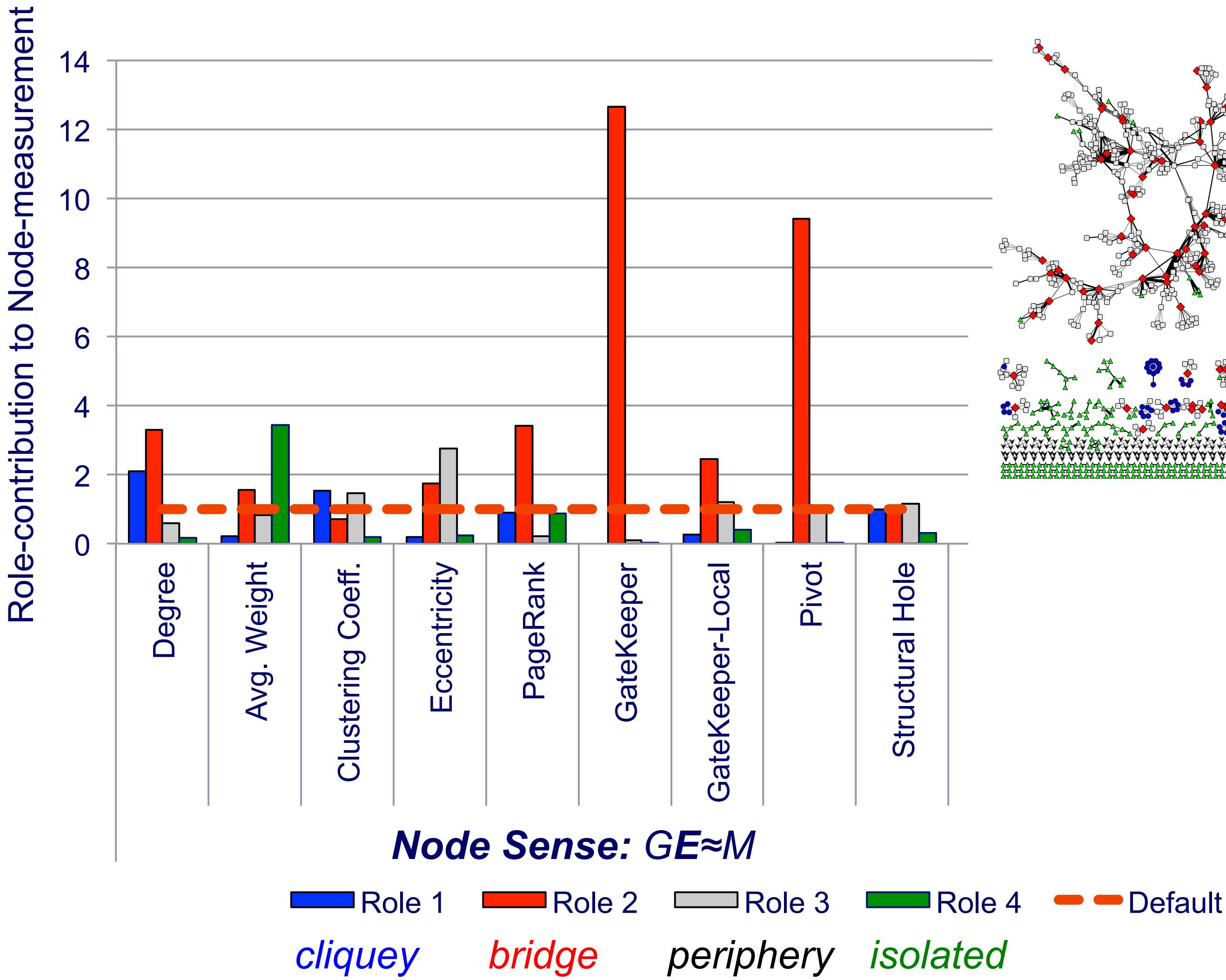
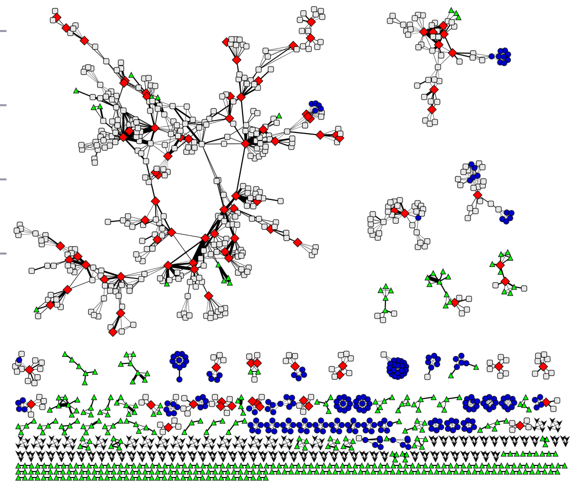


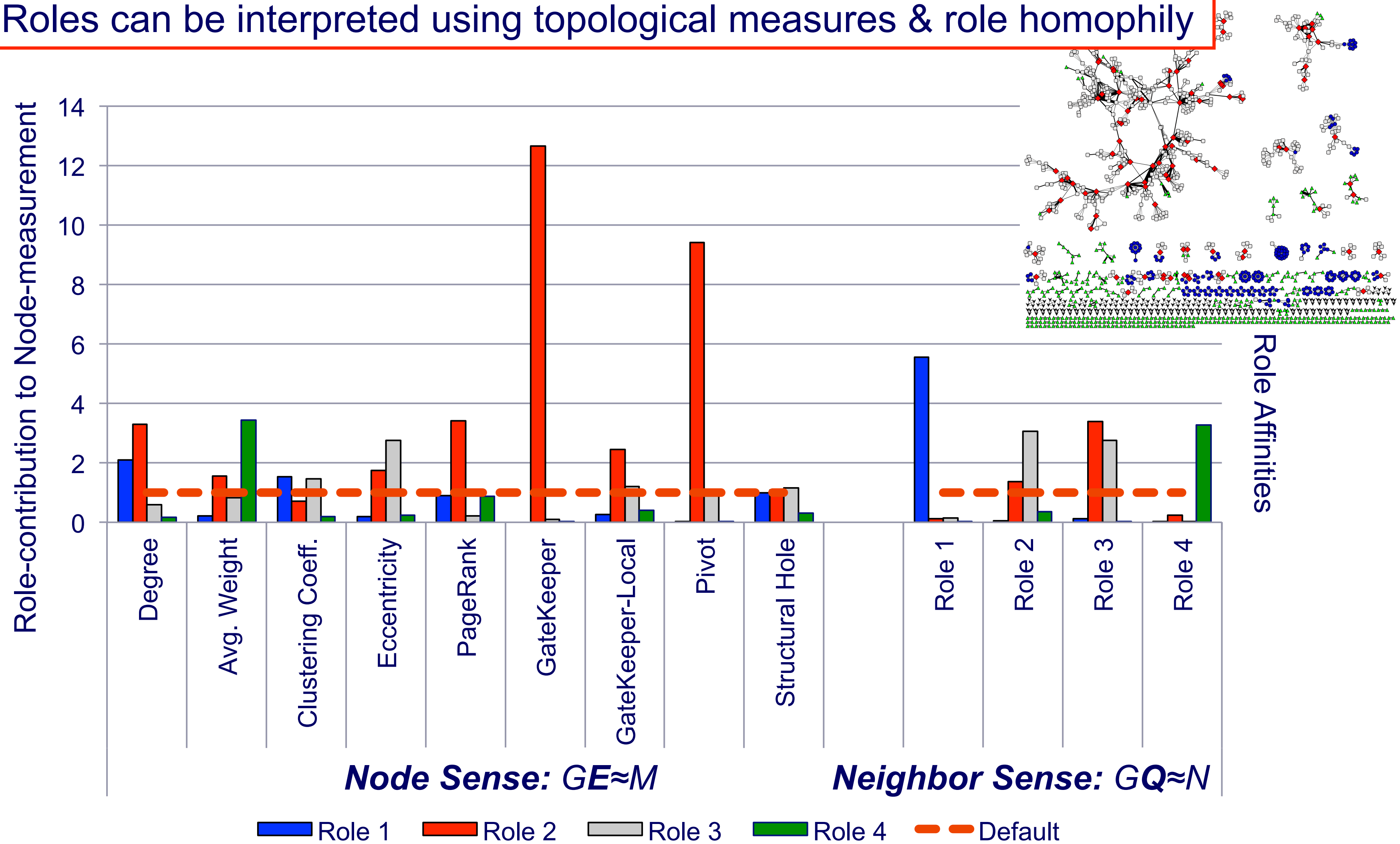
Making Sense of Roles





Making Sense of Roles

Roles can be interpreted using topological measures & role homophily

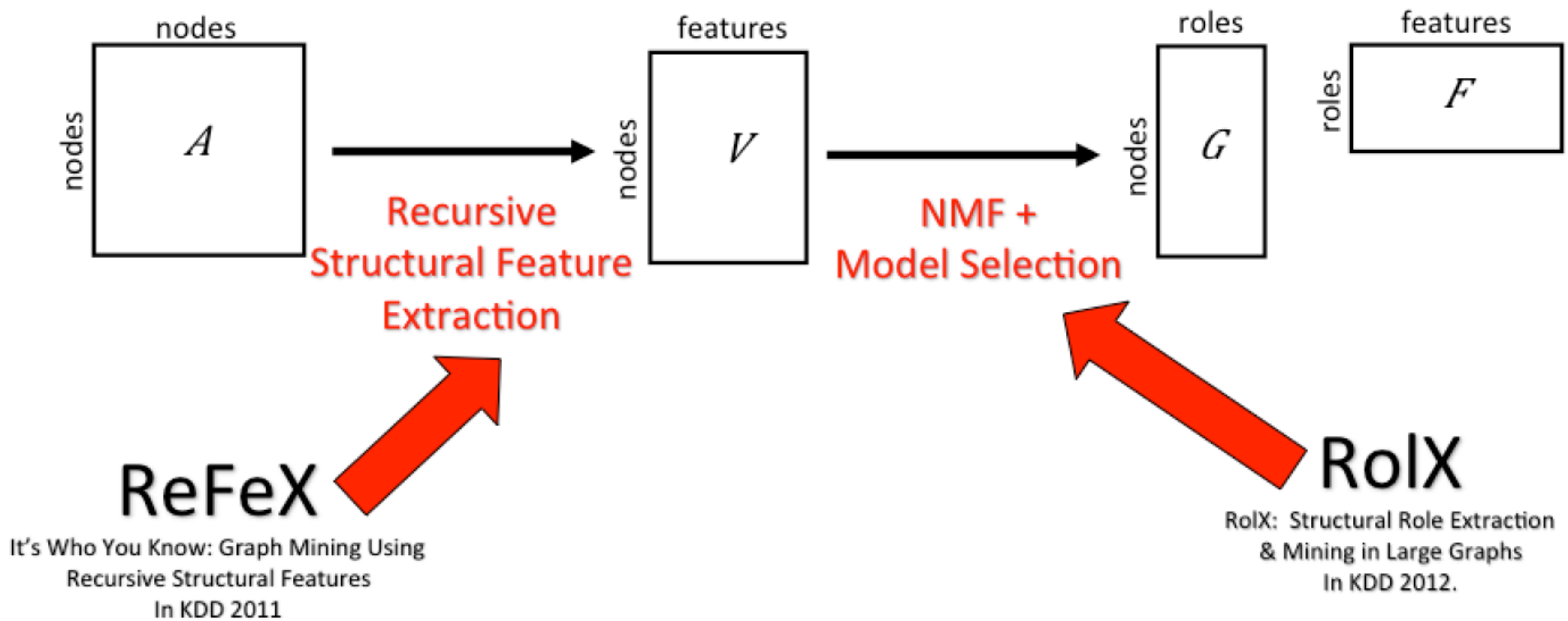


cliquey *bridge* *periphery* *isolated*

GLRD: Guided Learning for Role Discovery

- Introduced by Sean Gilpin et al.
- RolX is unsupervised
- What if we had guidance on roles?
  - Guidance as in weak supervision encoded as constraints
- Types of guidance
  - Sparse roles
  - Diverse roles
  - Alternative roles, given a set of existing roles

GLRD



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Structural Feature
Extraction
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NMF +
Model Selection
roles
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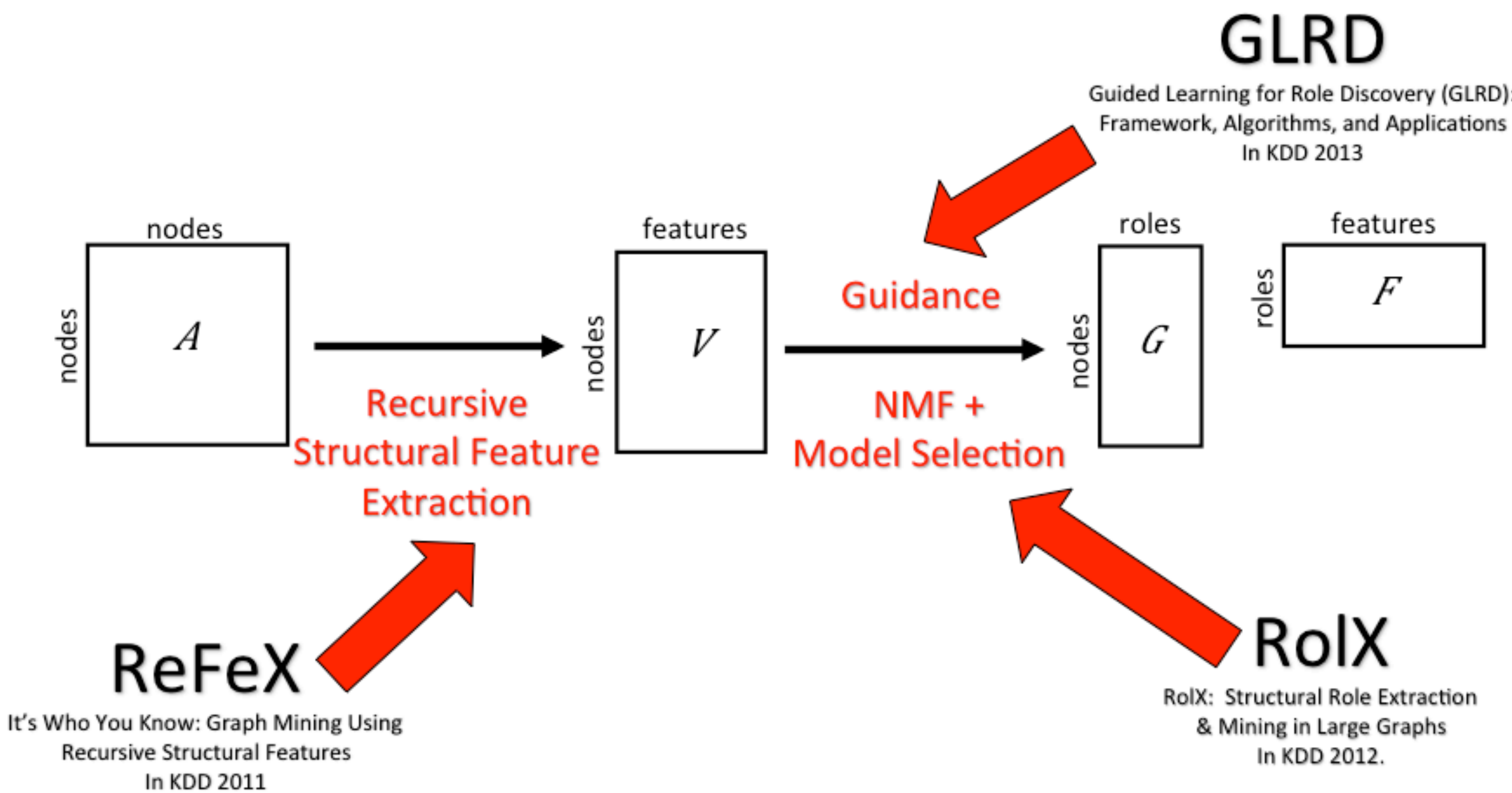
F
ReFeX
It's Who You Know: Graph Mining Using
Recursive Structural Features
In KDD 2011
RolX
RolX: Structural Role Extraction
& Mining in Large Graphs
In KDD 2012.

GLRD


GLRD
Guided Learning for Role Discovery (GLRD):
Framework, Algorithms, and Applications
In KDD 2013
nodes
nodes
A
Recursive
Structural Feature
Extraction
features
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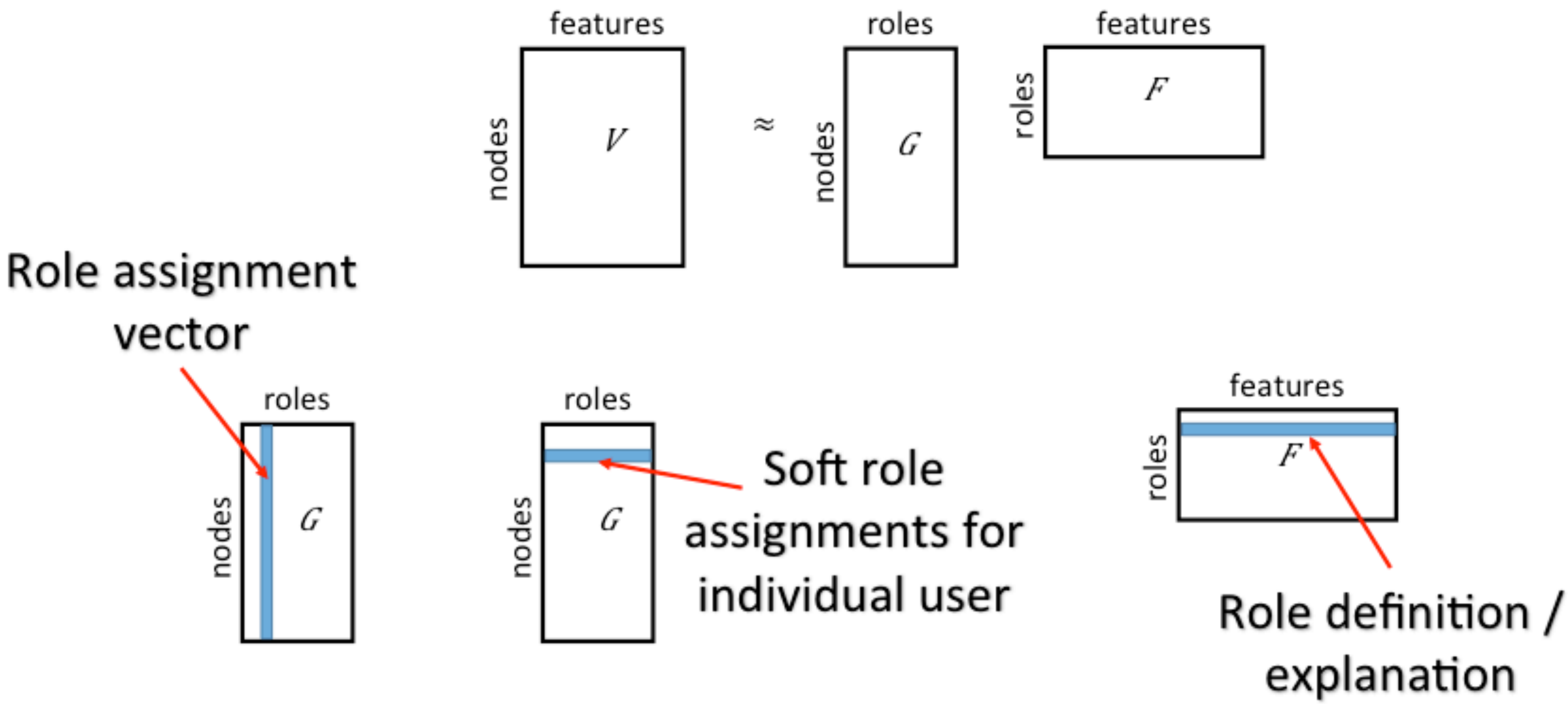
In KDD 2012.

Adding Constraints



GLRD Framework

- Constraints on columns of G (i.e., role assignments) or rows of F (i.e. role definitions) are convex functions

$$
\begin{aligned}
\underset{\mathbf{G},\mathbf{F}}{\text{minimize}} \quad & ||\mathbf{V} - \mathbf{GF}||_2 \\
\text{subject to} \quad & g_i(\mathbf{G}) \leq d_{Gi}, \; i = 1, \ldots, t_G \\
& f_i(\mathbf{F}) \leq d_{Fi}, \; i = 1, \ldots, t_F \\
\text{where} \;\; g_i \text{ and } f_i \;\; & \text{are convex functions.}
\end{aligned}
$$

- Use an alternative least squares (ALS) formulation
  - Do not alternate between solving for the entire G and F
  - Solve for one column of G or one row of F at a time
    - This is okay since we have convex constraints

Guidance Overview

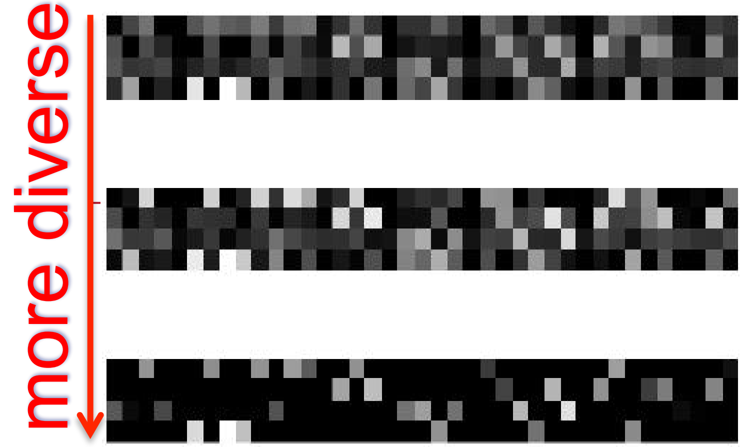
Guidance Type	Effect of **increasing** guidance	
	on role assignment (*G*)	on role definition (*F*)
Sparsity	Reduces the number of nodes with minority memberships in roles	Decreases likelihood that features with small explanatory benefit are included
Diversity	Limits the amount of allowable overlap in assignments	Roles must be explained with completely different sets of features
Alternative	Decreases the allowable similarity between the two sets of role assignments	Ensures that role definitions are very dissimilar between the two sets of role assignments

Sparsity

$$
\begin{aligned}
\underset{\mathbf{G},\mathbf{F}}{\text{argmin}} \quad & ||\mathbf{V} - \mathbf{G}\mathbf{F}||_2 \\
\text{subject to:} \quad & \mathbf{G} \geq 0, \mathbf{F} \geq 0 \\
& \forall i \quad ||\mathbf{G}_{\bullet\mathbf{i}}||_1 \leq \epsilon_G \\
& \forall i \quad ||\mathbf{F}_{\mathbf{i}\bullet}||_1 \leq \epsilon_F \\
\text{where} \quad & \epsilon_G \text{ and } \epsilon_F \text{ define upperbounds for the sparsity constraints (amount of allowable density).}
\end{aligned}
$$

Diversity

Goal: Find role assignments or definitions that are very different from each other



$$\underset{\mathbf{G},\mathbf{F}}{\text{argmin}} \quad ||\mathbf{V} - \mathbf{GF}||_2$$

$$\text{subject to:} \quad \mathbf{G} \geq 0, \mathbf{F} \geq 0$$

$$\forall i, j \quad \mathbf{G}_{\bullet i}^T \mathbf{G}_{\bullet j} \leq \epsilon_G \quad i \neq j$$

$$\forall i, j \quad \mathbf{F}_{i\bullet} \, \mathbf{F}_{j\bullet}^T \leq \epsilon_F \quad i \neq j$$

where ϵ_G and ϵ_F define upperbounds on how angularly similar role assignments and role definitions can be to each other.

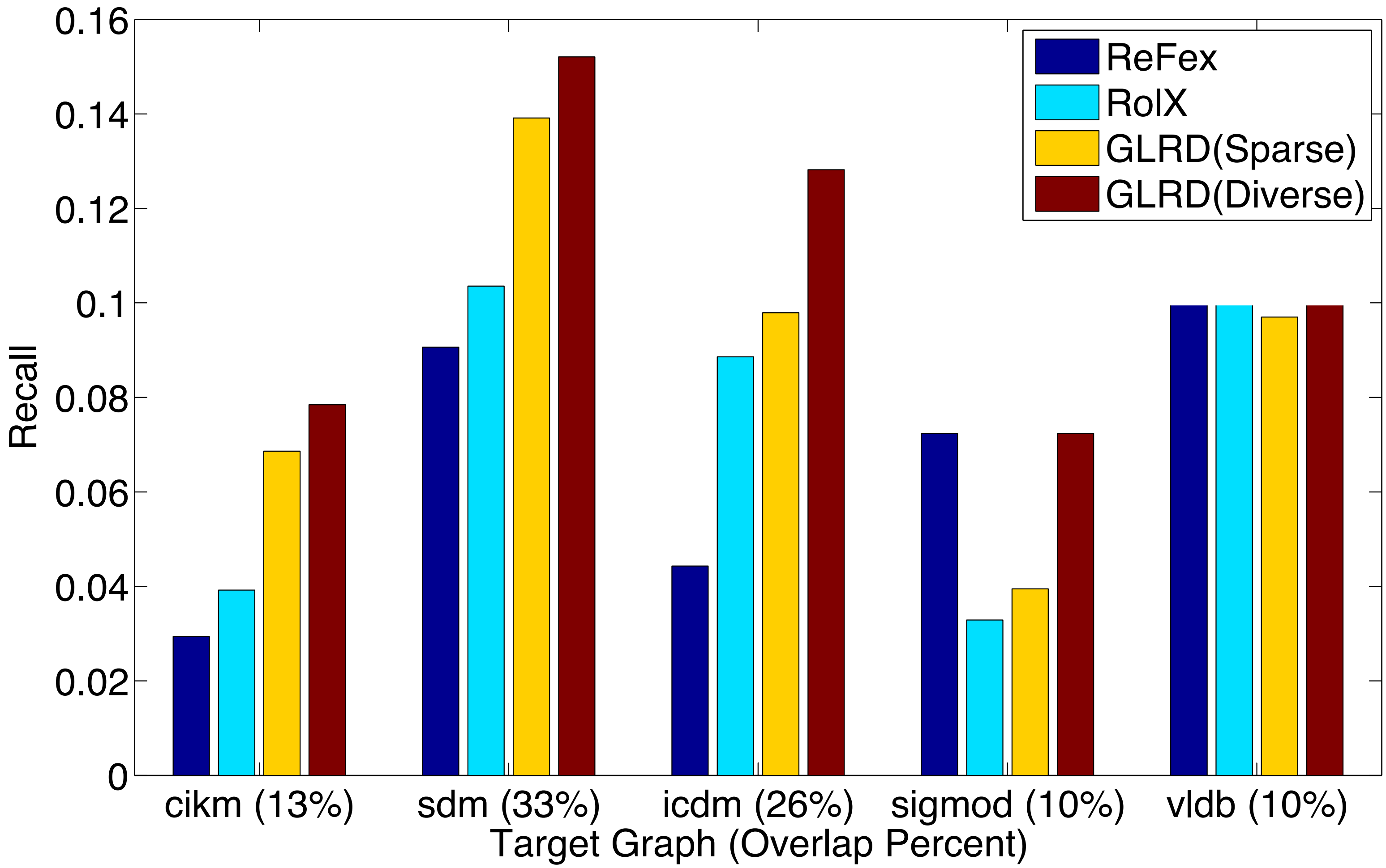
Diverse Roles and Sparse Roles

- Question: Can diversity and sparsity constraints create better role definitions?
- Conjecture: Better role definitions will better facilitate other problems such as identity resolution across graphs
- Experiment: Compare graph mining results using various methods for role discovery

Network	$\|V\|$	$\|E\|$	k	$\|LCC\|$	#CC
VLDB	1,306	3,224	4.94	769	112
SIGMOD	1,545	4,191	5.43	1,092	116
CIKM	2,367	4,388	3.71	890	361
SIGKDD	1,529	3,158	4.13	743	189
ICDM	1,651	2,883	3.49	458	281
SDM	915	1,501	3.28	243	165

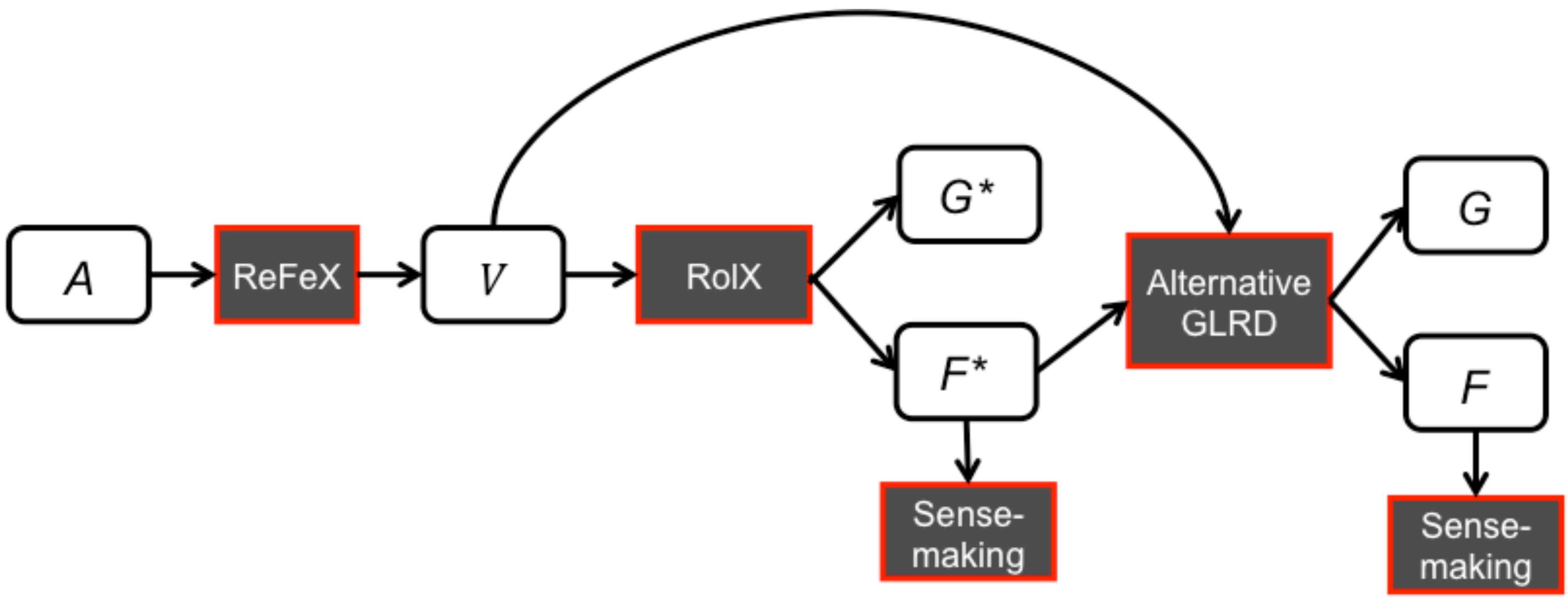
DBLP Co-authorship Networks from 2005-2009

Identity Resolution across Networks



Alternative Roles

- Question: Do alternative sets of roles exist in graphs and can they be discovered?

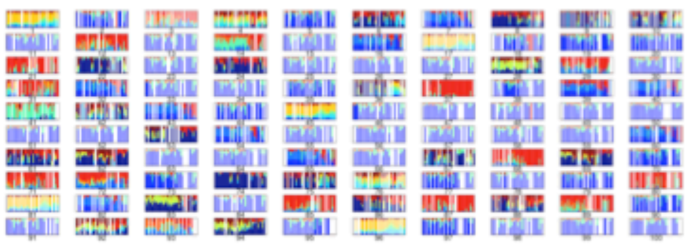


Slide from Rossi *et al.* WSDM 2013

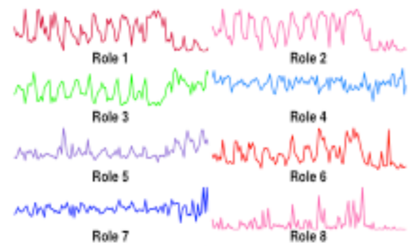
Modeling Dynamic Graphs with Roles

- Introduced by Rossi et al. WSDM 2013

1. **Identify** dynamic patterns in node behavior

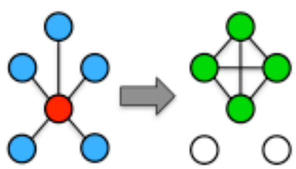


Evolving mixed-role memberships



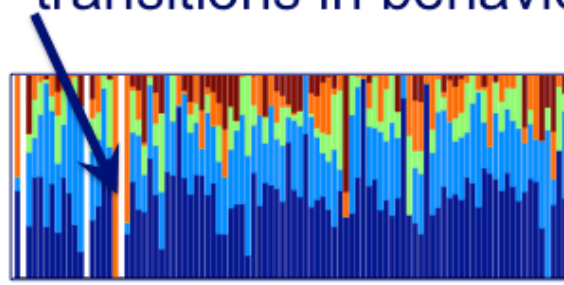
Role contributions

2. **Predict** future structural changes



Transition from star to clique

3. **Detect** unusual transitions in behavior



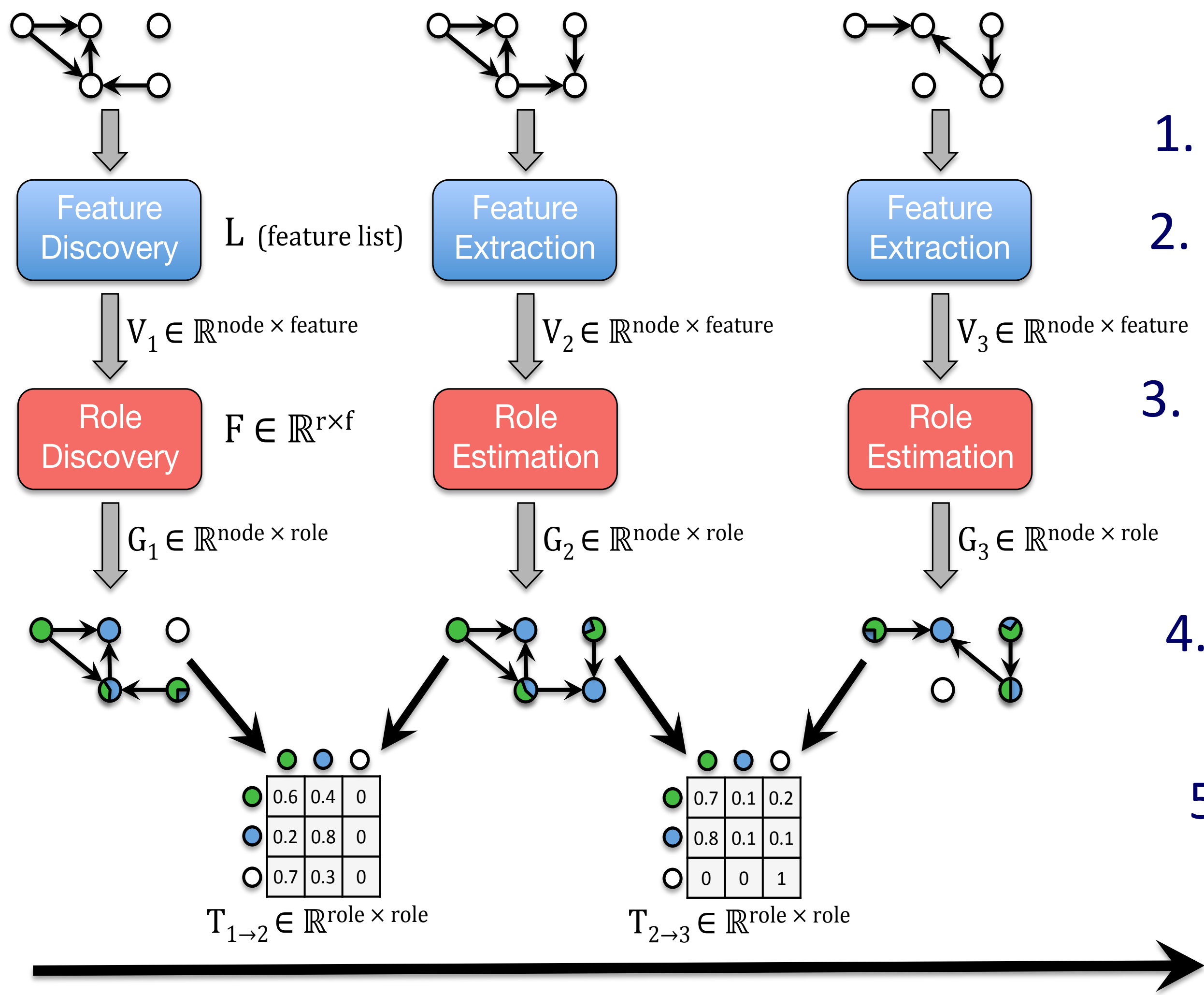
Slide from Rossi *et al.* WSDM 2013

Dynamic Behavioral Mixed-Membership (DBMM) Model

- Scalable for big graphs
- Easily parallelizable
- Non-parametric & data-driven
- Flexible and interpretable

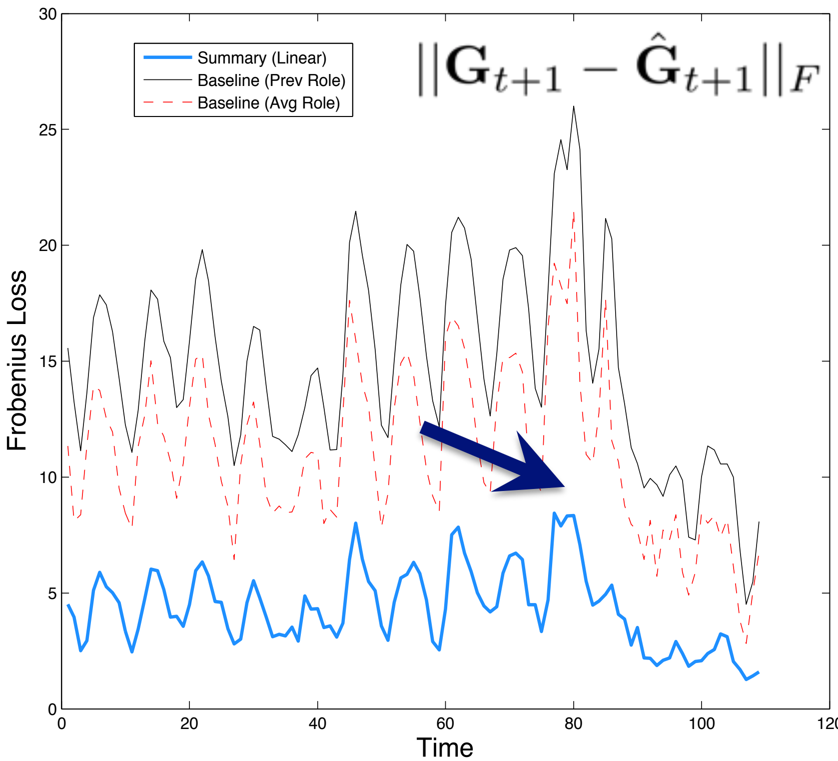
Slide from Rossi *et al.* WSDM 2013

Dynamic Behavioral Mixed-Membership (DBMM) Model



1. Compute set of features
2. Estimate the features on each snapshot graph
3. Learn roles from features using NMF, number of roles selected via MDL
4. Extract roles from each feature matrix over time
5. Use NMF to estimate transition model

Predicting Structural Behavior



Twitter

Given G_{t-1} and G_t find a transition model T that minimizes the functional:

$$f(\mathbf{G}_t, \mathbf{G}_{t-1}) = \frac{1}{2}||\mathbf{G}_t - \mathbf{G}_{t-1}\mathbf{T}||_F^2$$

All models predict G_{t+1} using G_t as

$$\mathbf{G}'_{\mathbf{t+1}} = \mathbf{G}_{\mathbf{t}}\mathbf{T}$$

Summary model: Weight training examples from *k* previous time-steps

Baseline models: Predict future role based on (1) previous role or (2) average role distribution

DBMM is more accurate at predicting future behavior than baselines.

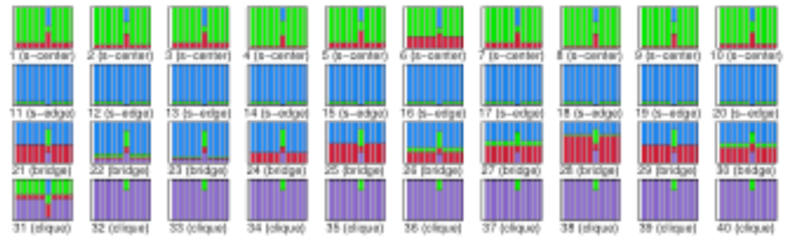
Slide from Rossi *et al.* WSDM 2013

Anomalous Structural Transitions

Problem: detect nodes with unusual structural transitions

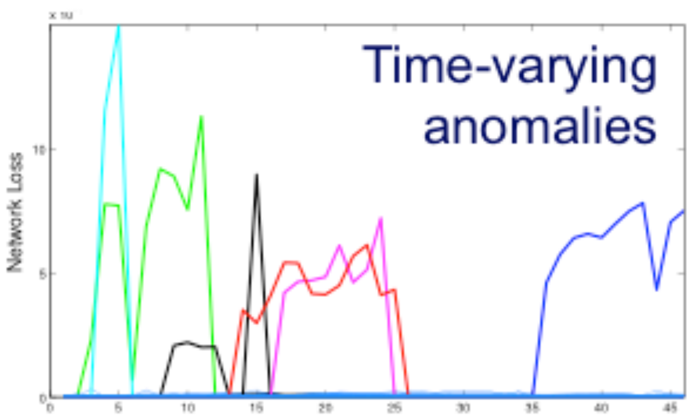
Anomaly score:

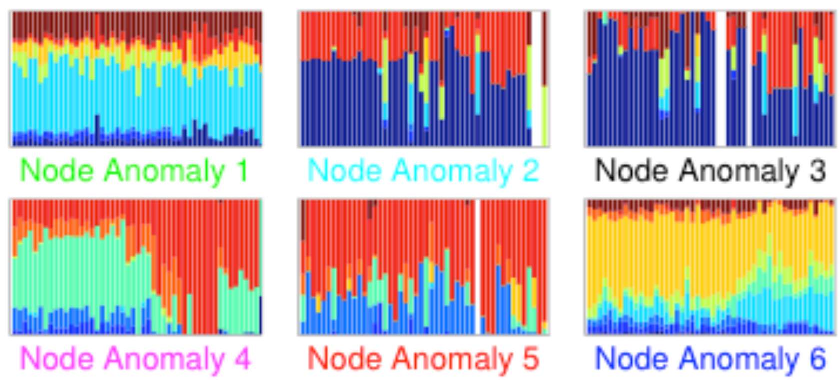
1. Estimate transition model T for *v*
2. Use it to predict *v*'s memberships
3. Take the difference from actual



Inject anomalies into synthetic data:
Detected 88.5% over 200 repeated trials

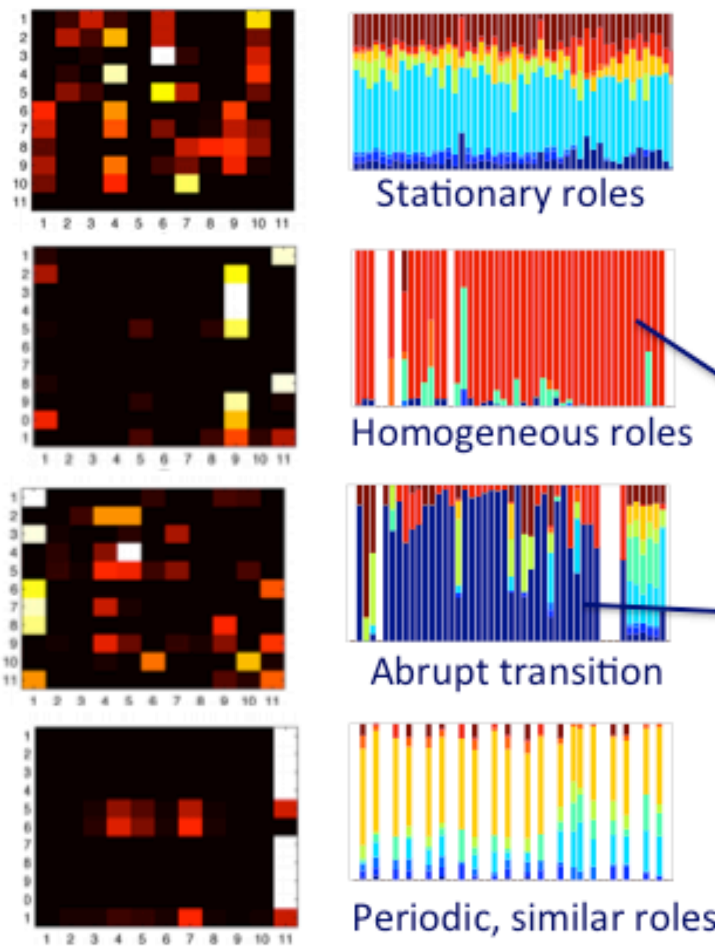
DBMM model finds nodes that are anomalous for only short time-periods





Slide from Rossi *et al.* WSDM 2013

Dynamic Network Analysis with Roles

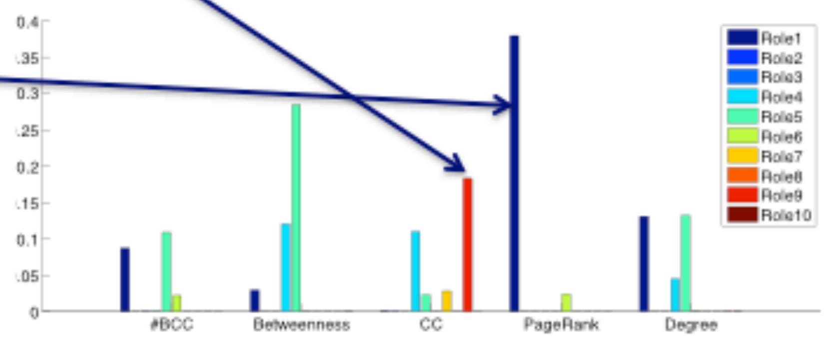


Roles exhibit many of the traditional time-series patterns

Roles are interpretable

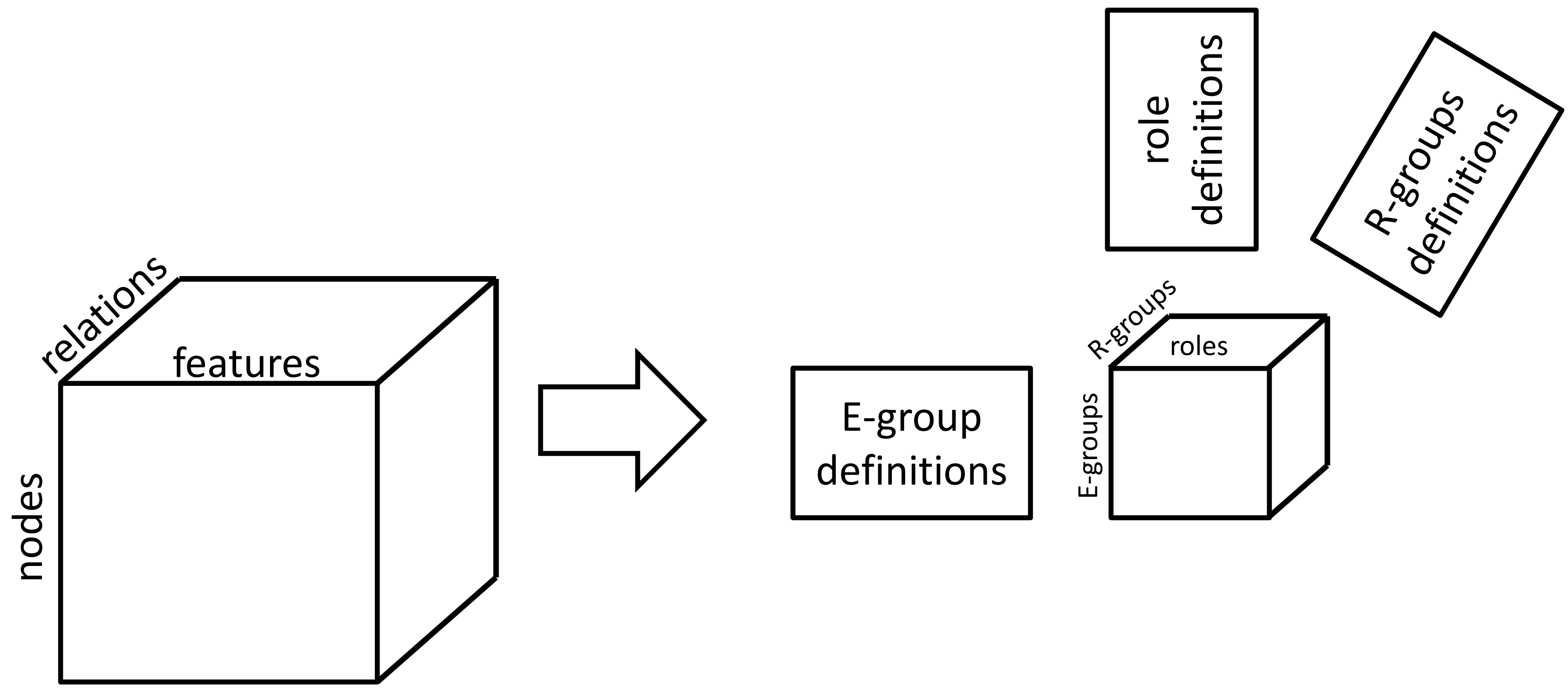
Fit role-model to matrix of network statistics:

$$\mathbf{G}_t\mathbf{E}_t \approx \mathbf{M}_t$$

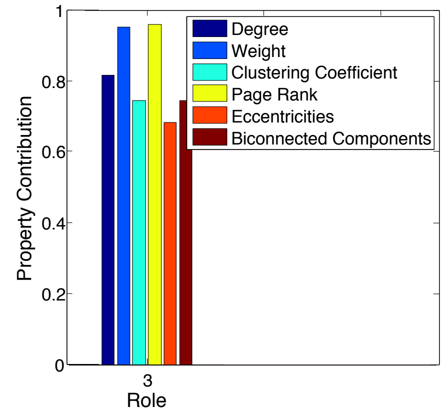


Roles Across Relations

- Role Discovery in Multi-Relational Graphs [Sean Gilpin, et al. under review]



A Pattern from the Core Tensor of the 110th Congress Co-sponsorship Graph

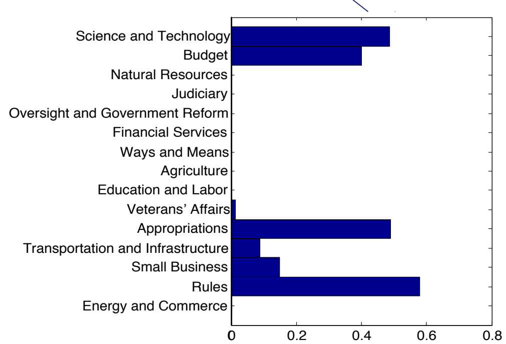


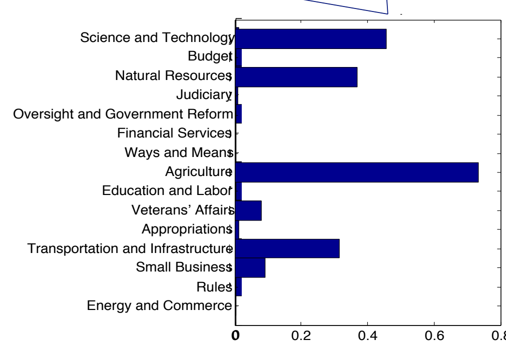
Roles

Name	Party	Exp
Hall, Ralph	R	16
Rodgers, Cathy	R	2
Myrick, Sue	R	12
Issa, Darrell	R	6
Drake, Thelma	R	2
Kuhl, Randy	R	2
Poe, Ted	R	2
Boozman, John	R	6
Conaway, Michael	R	2
Wamp, Zach	R	12

Name	Party	Exp
Jackson-Lee, Sheila	D	12
Cohen, Steve	D	0
Hare, Phil	D	0
Grijalva, Raul	D	4
English, Phil	R	12
Honda, Michael	D	6
McCotter, Thaddeus	R	4
Filner, Bob	D	14
Hinchey, Maurice	D	14
Gonzalez, Charles	D	8

E-groups





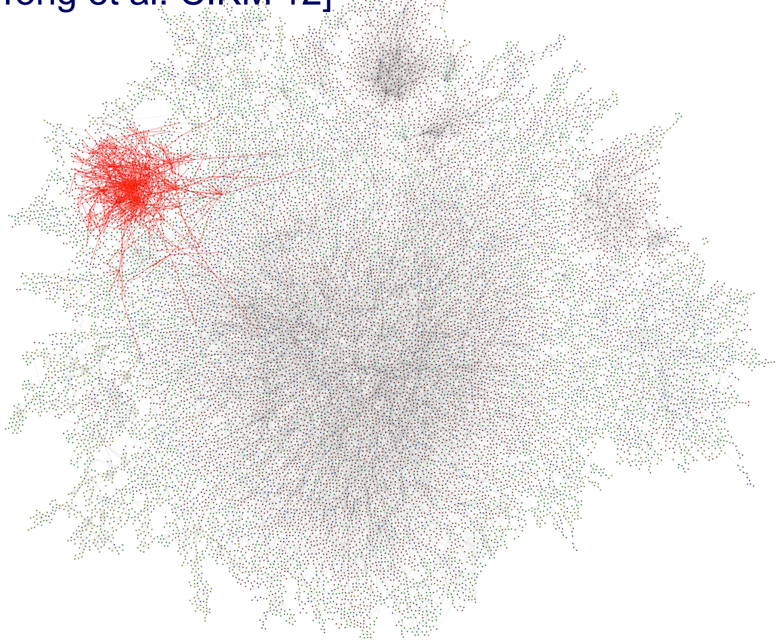
R-groups

Using Roles to Minimize Dissemination on Graphs

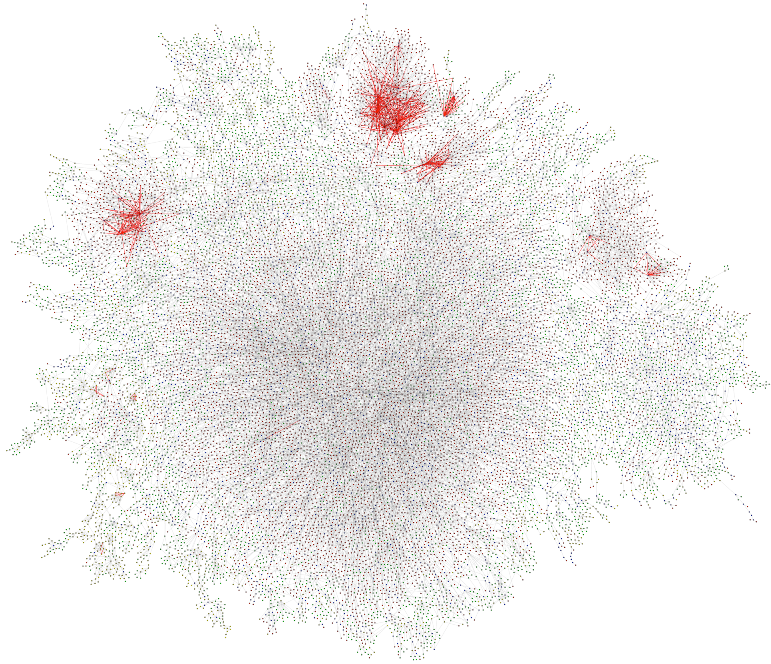
- Learn to predict which *k* edges to cut to minimize dissemination on an unseen graph
  - [Long T. Le, TER, Hanghang Tong. under review]

NetMelt on Yahoo! IM

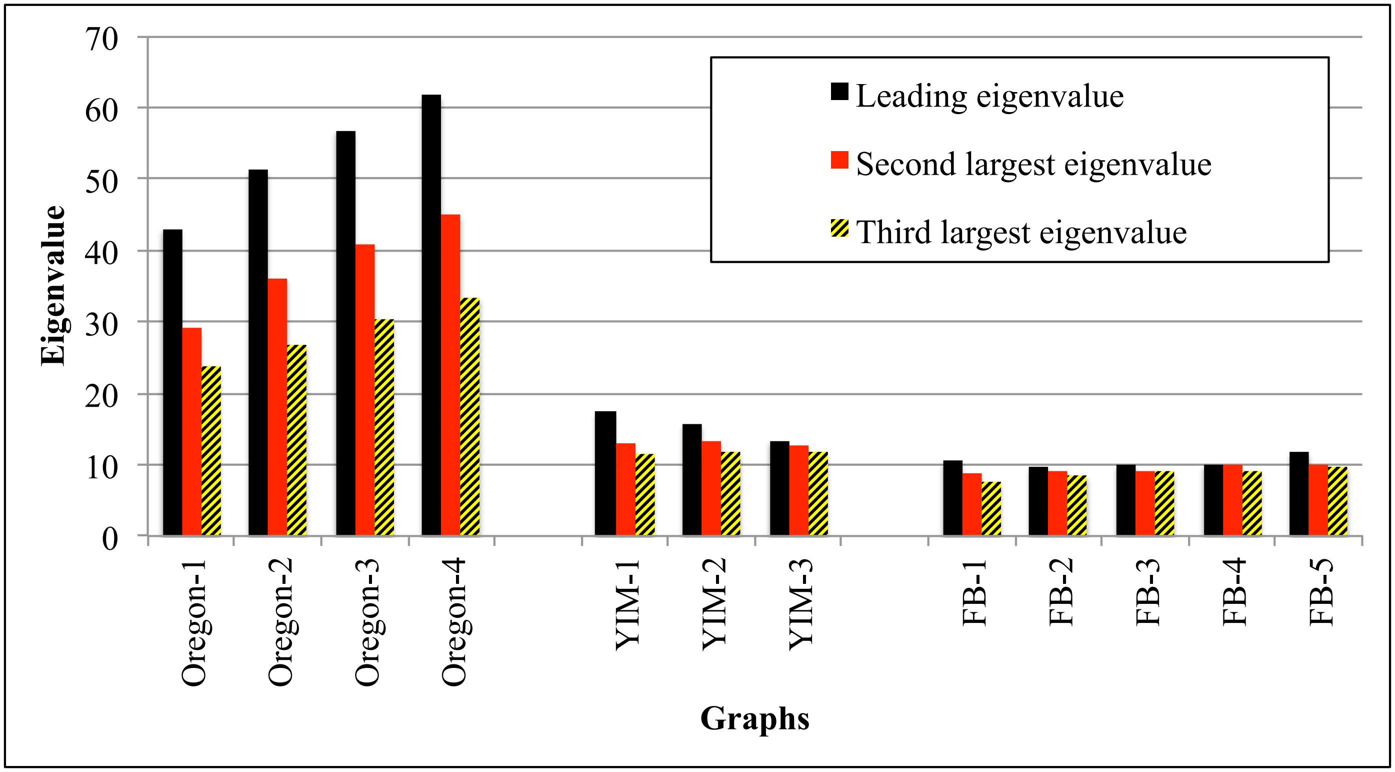
[Tong et al. CIKM'12]



RoleLearnλ on Yahoo! IM

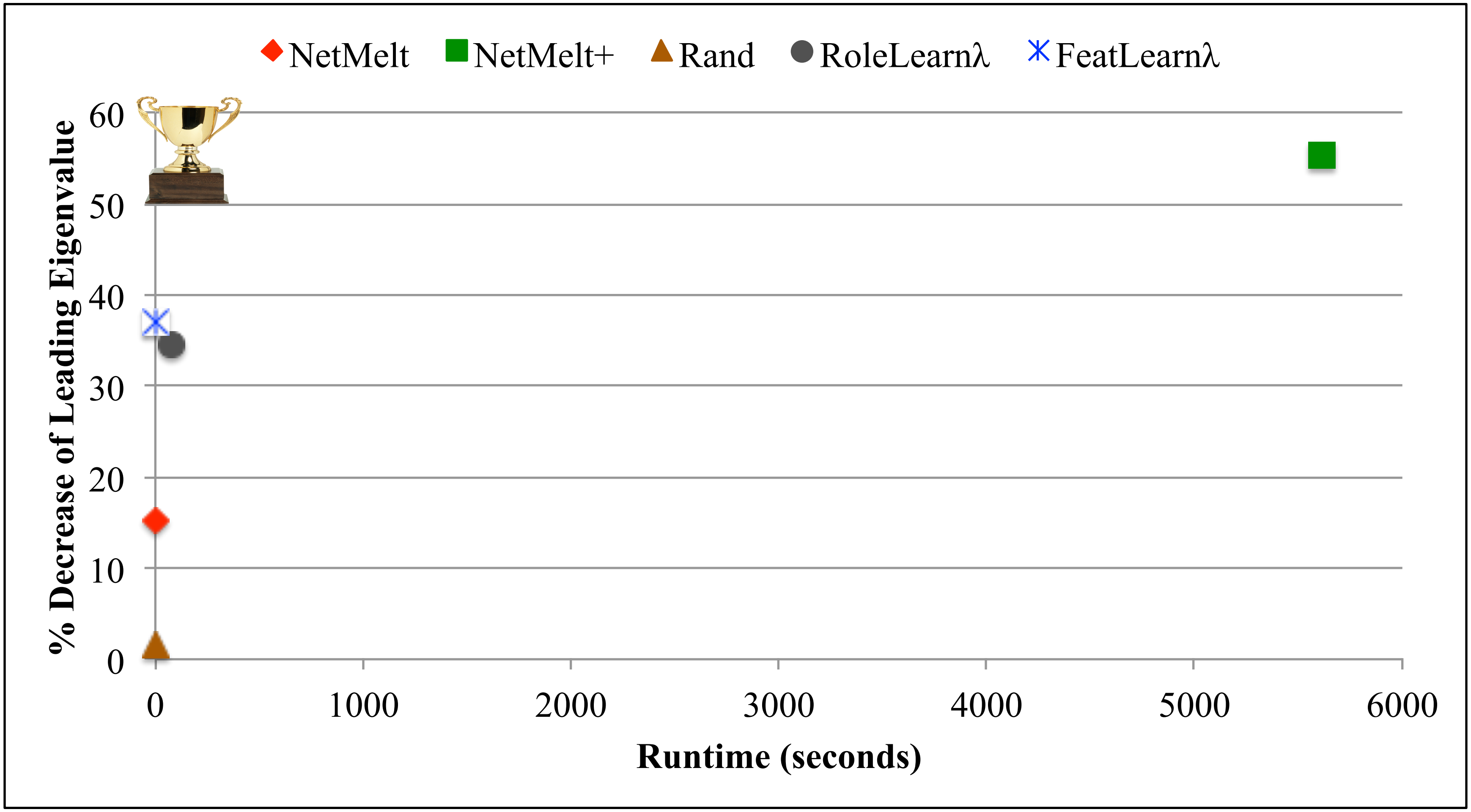


$\lambda_1 - \lambda_2$ is Small (Especially in Social Graphs)

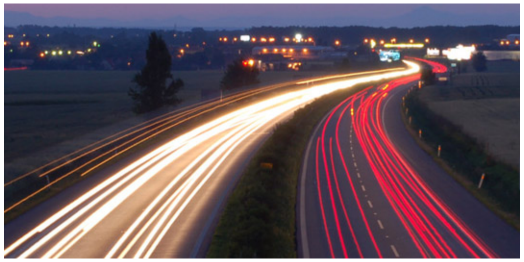


Our new problem formulation:
Learn to predict which edges to cut.

Yahoo! IM (% Drop in λ vs. Runtime)



Roadmap



- Node Roles
  - What are roles
  - Roles and communities
  - Roles and equivalences (from sociology)
  - Roles (from data mining)
  - Summary
- Node Proximity
- Summary

Summary

- Roles
  - Structural behavior ("function") of nodes
  - Complementary to communities
  - Previous work mostly in sociology under equivalences
  - Recent graph mining work produces mixed-membership roles, is fully automatic and scalable
  - Can be used for many tasks: transfer learning, re-identification, anomaly detection, etc
  - Extensions: including guidance, modeling dynamic networks, etc

Roles: Regular Equivalence vs. Role Discovery

	Role Discovery	Regular Equivalence
Mixed-membership over roles	✓	
Automatically selects the best model	✓	
Can incorporate arbitrary features	✓	
Uses structural features	✓	
Uses structure	✓	✓
Generalizes across disjoint networks (longitudinal & cross-sectional)	✓	?
Scalable (linear on # of edges)	✓	
Guidance	✓	

Acknowledgement

- LLNL: Brian Gallagher, Keith Henderson
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- CMU: Danai Koutra
- UC Berkeley: Lei Li
- UC Davis: Ian Davidson, Sean Gilpin
- Rutgers: Long Le

Thanks to: LLNL, NSF, IARPA, DARPA, DTRA.

Papers at http://eliassi.org/pubs.html

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- Sean Gilpin, Tom Kuo, Tina Eliassi-Rad, Ian Davidson: Roles across relations: Role discovery in multi-relational graphs. **under review**, 2014.
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- Ryan A. Rossi, Brian Gallagher, Jennifer Neville, Keith Henderson: Role-dynamics: fast mining of large dynamic networks. **WWW** (Companion Volume) 2012: 997-1006.
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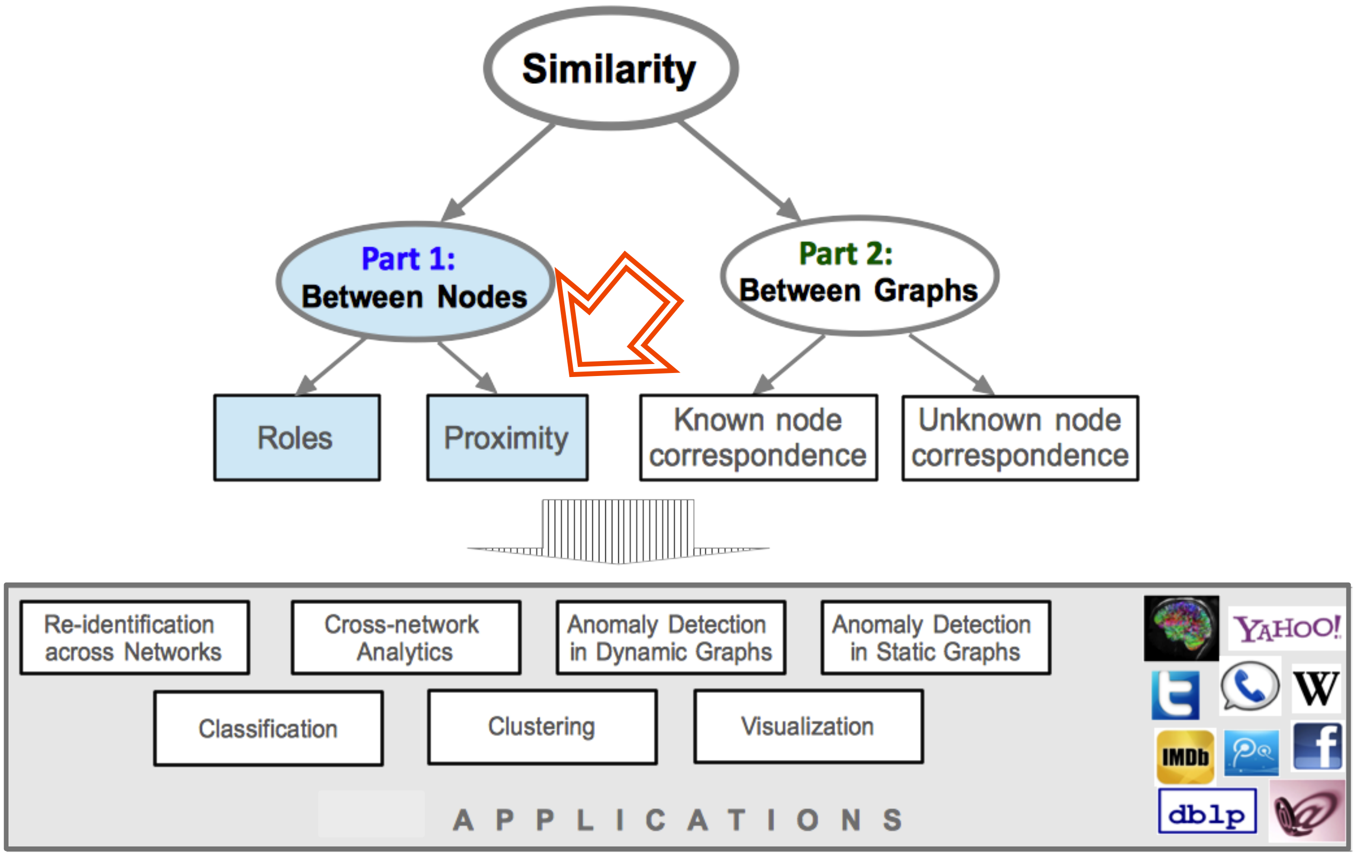
Next


Similarity
Part 1:
Between Nodes
Part 2:
Between Graphs
Roles
Proximity
Known node correspondence
Unknown node correspondence
Re-identification across Networks
Cross-network Analytics
Anomaly Detection in Dynamic Graphs
Anomaly Detection in Static Graphs
Classification
Clustering
Visualization
A P P L I C A T I O N S
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