# Discovering Roles and Anomalies in Graphs: Theory and Applications

## Part 1: Roles

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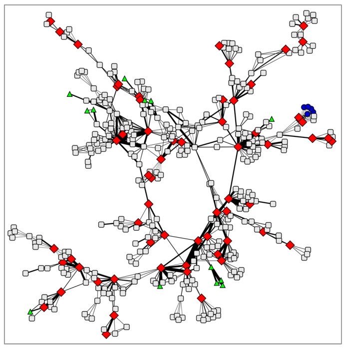
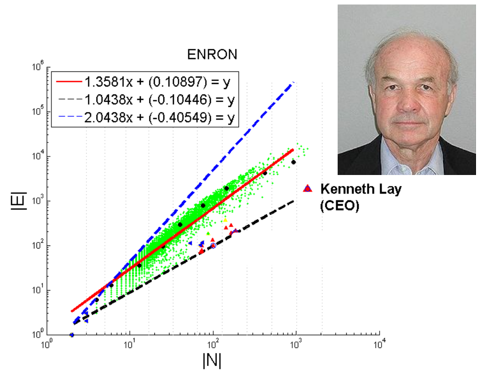
ECML PKDD 2013 Tutorial

# Overview





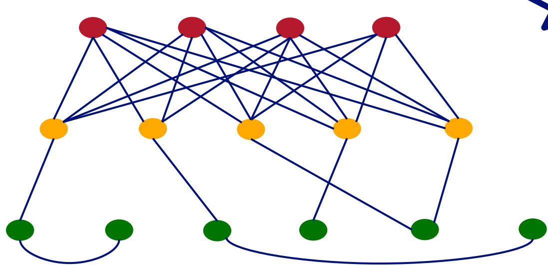

Features

Roles

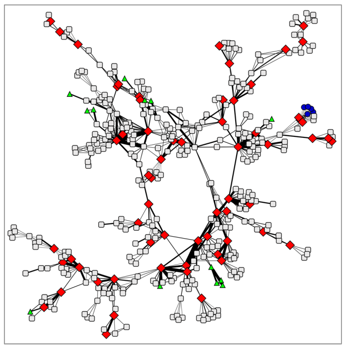
Anomalies

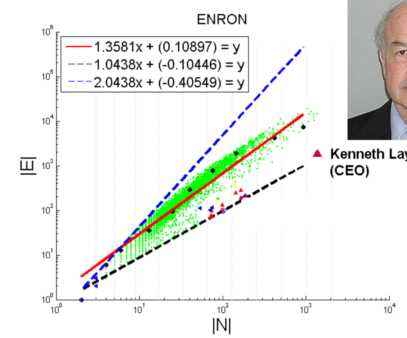
= rare roles

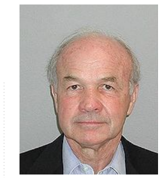
Patterns



# Overview





Features

Roles

Anomalies

= rare roles

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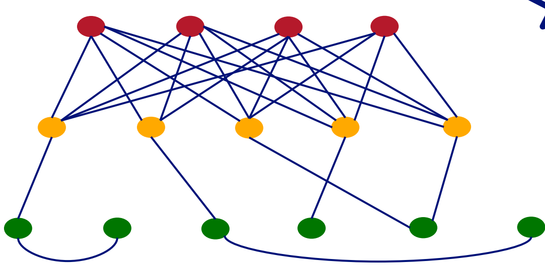
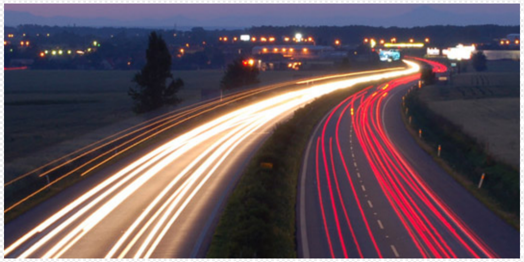


# Roadmap

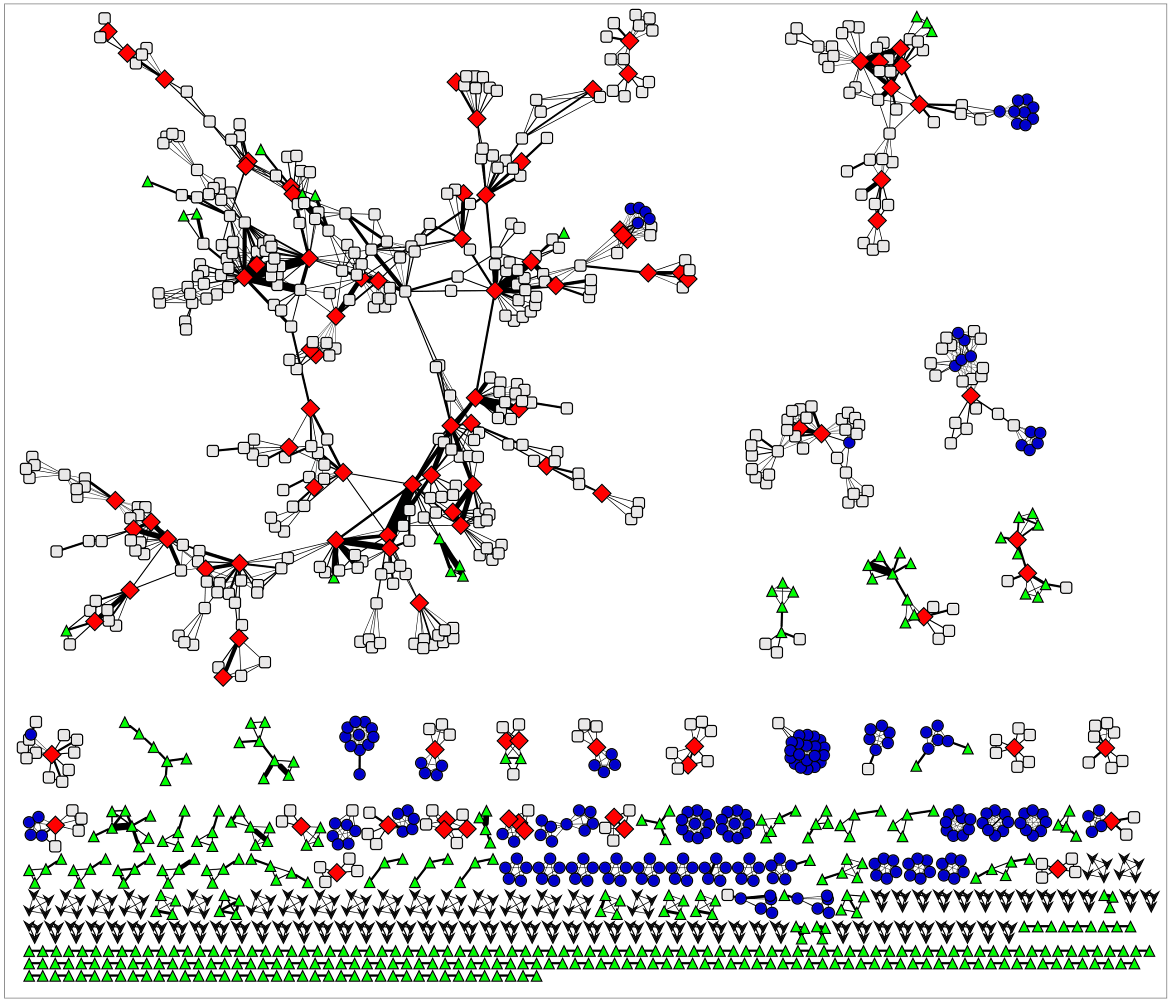
- What are roles
- Roles and communities
- Roles and equivalences (from sociology)
- Roles (from data mining)
- Summary



# 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
  - …

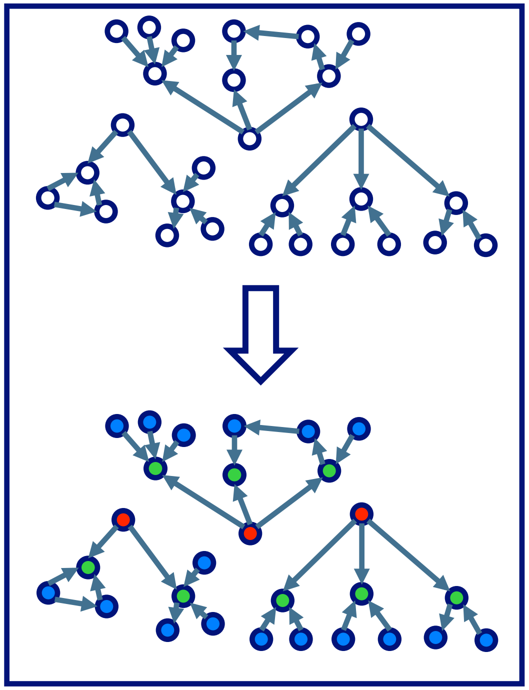
# Example of Roles



◆ centers of stars
● members of cliques
□ peripheral nodes

# Why are roles important?

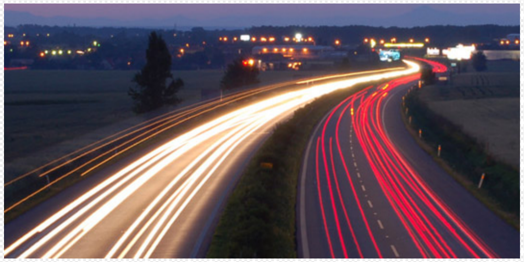
## Role Discovery



- 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



- What are roles
- $\boxed{\text{Roles and communities}}$
- Roles and equivalences (from sociology)
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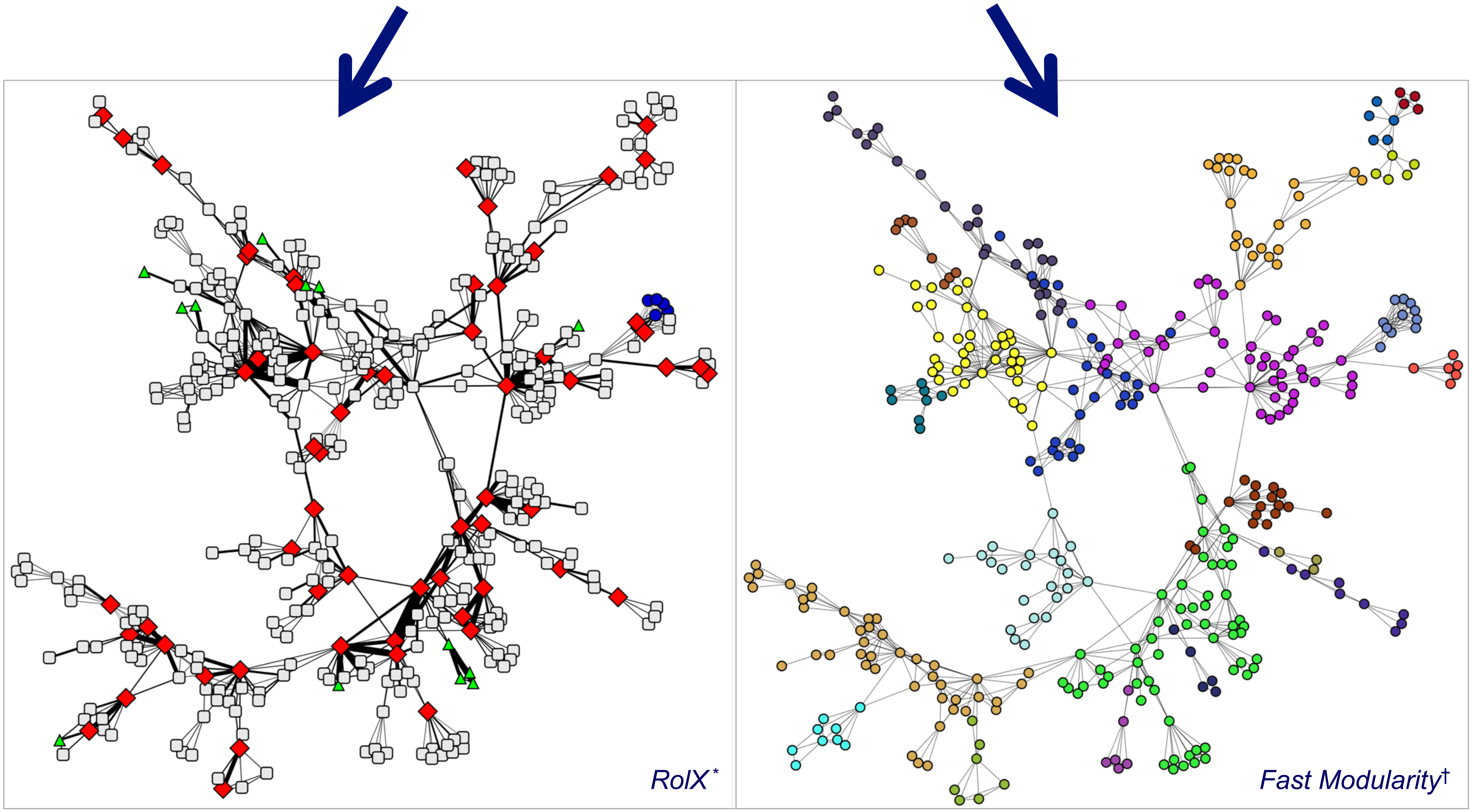
- Summary

# Roles and Communities

- Roles group nodes with similar structural properties
- Communities group nodes that are well-connected to each other
- Roles and communities are complementary

# Roles and Communities



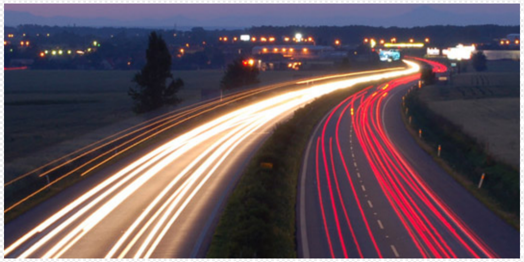

* Henderson, et al. 2012; † Clauset, et al. 2004

# Roles and Communities

Consider the social network of a CS dept

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

# Roadmap



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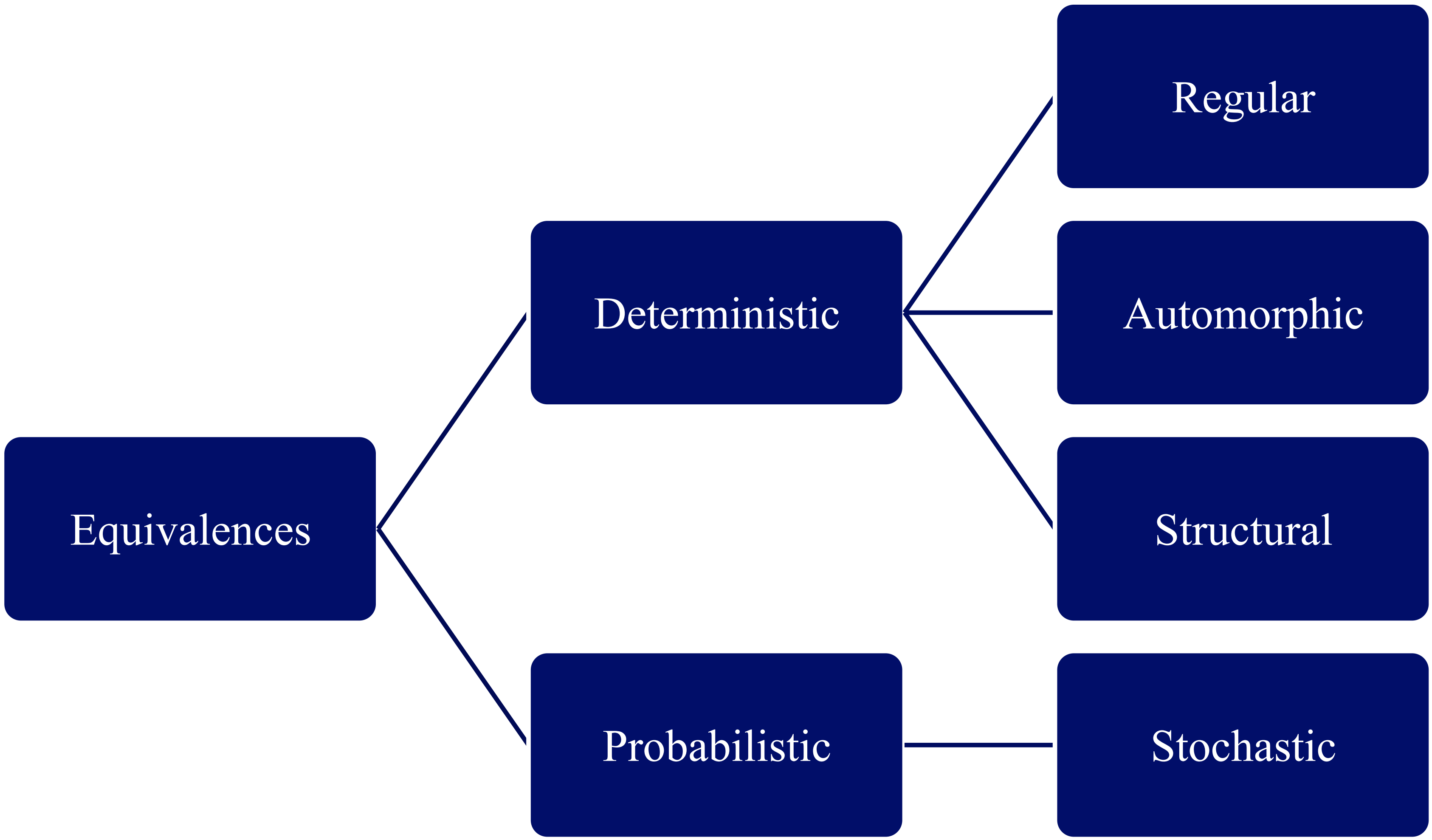
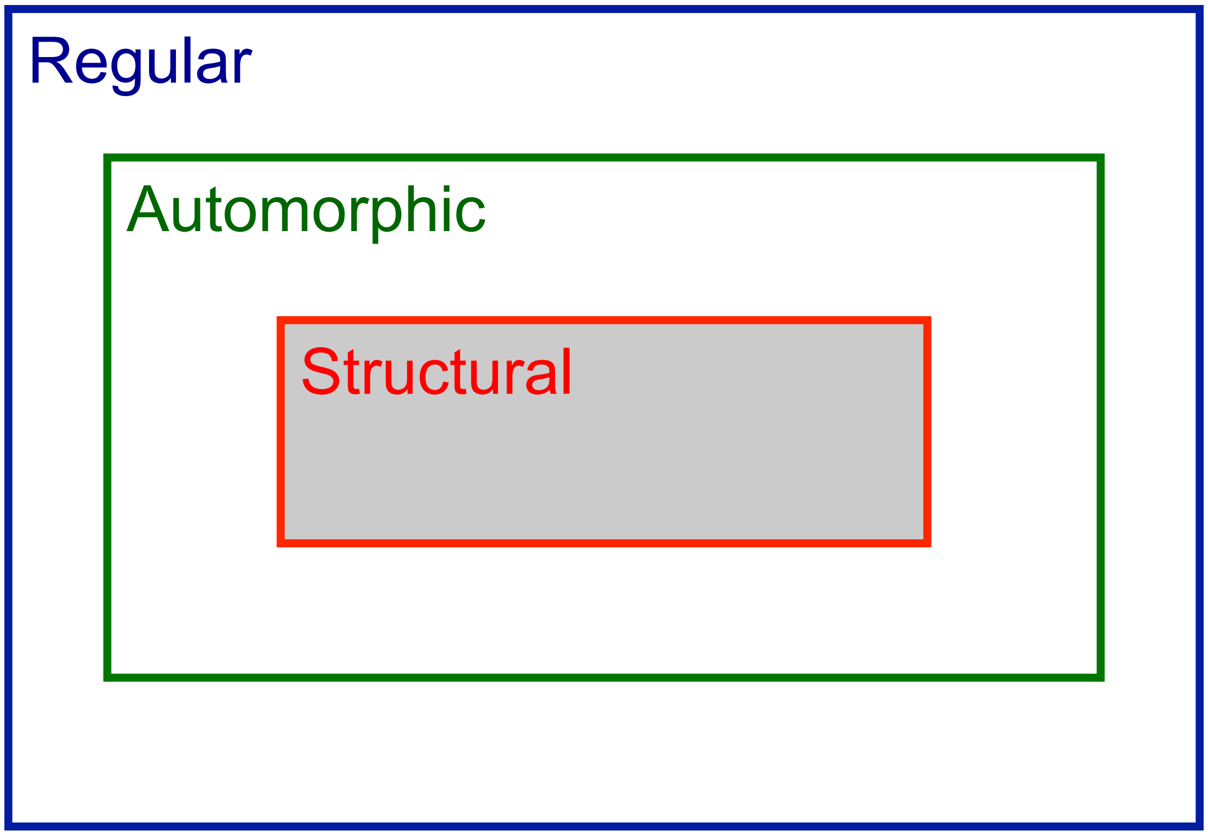
# Equivalences

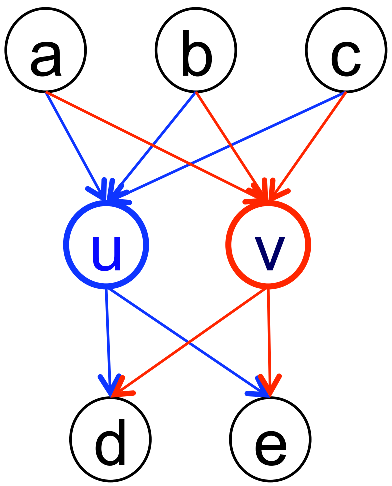


# Deterministic Equivalences



# 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]
- A hierarchical divisive approach
    1. Starting with the adjacency matrix, repeatedly calculate Pearson correlations between rows 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
- Successive split can be applied to submatrices in order to produce a hierarchy (where every node has a unique position)

# Structural Equivalence: Algorithms

- STRUCUTRE [Burt 1976]
- A hierarchical agglomerative approach
  1. For each node $i$, create its ID vector by concatenating its row and column vectors from the adjacency matrix
  2. For every pair of nodes $\langle i, j \rangle$, measure the square root of sum of squared differences between the corresponding entries in their ID vectors
  3. Merge entries in hierarchical fashion as long as their difference is less than some threshold $\alpha$

# Structural Equivalences: Algorithms

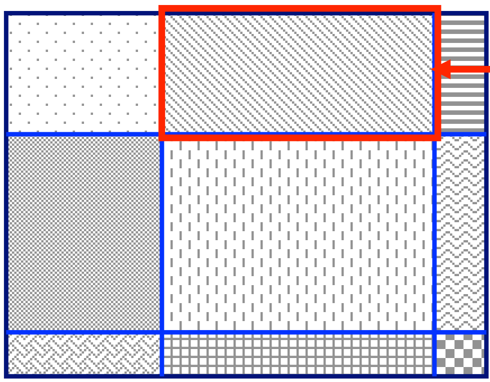
- Combinatorial optimization approaches
  - Numerical optimization with tabu search [UCINET]
  - Local optimization [Pajek]
- Partition the sociomatrices into blocks based on a cost function that minimizes the sum of within block variances
  - Basically, minimize the sum of code cost within each block

# Cross-Associations (XA)

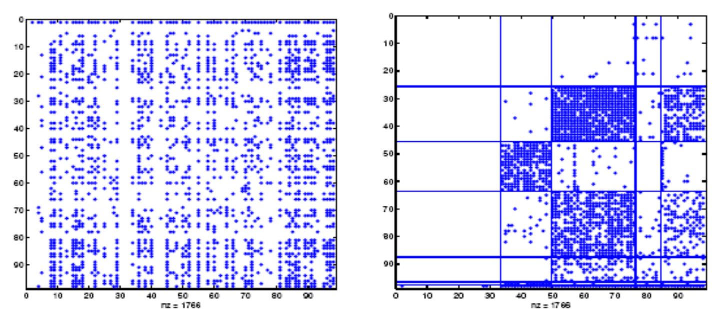
- [Chakrabarti+, KDD 2004]
- Minimize total encoding cost of the adjacency matrix

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

Binary Matrix

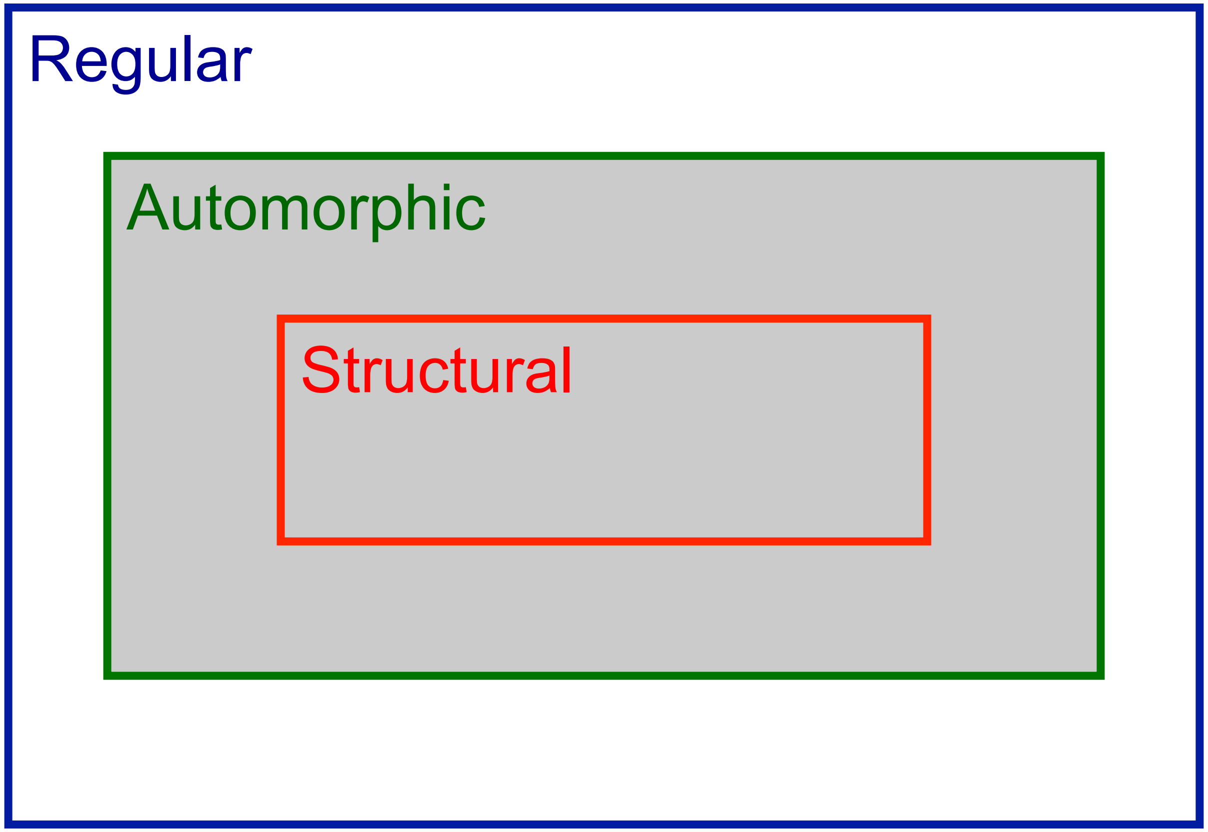


$p_i^1 = n_i^1 / (n_i^1 + n_i^0)$



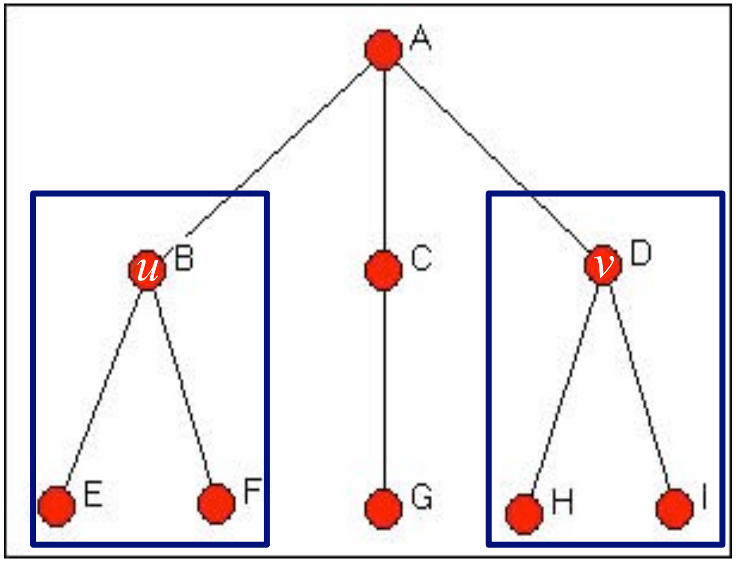
(a) before (b) after

# Deterministic Equivalences



# Automorphic Equivalence

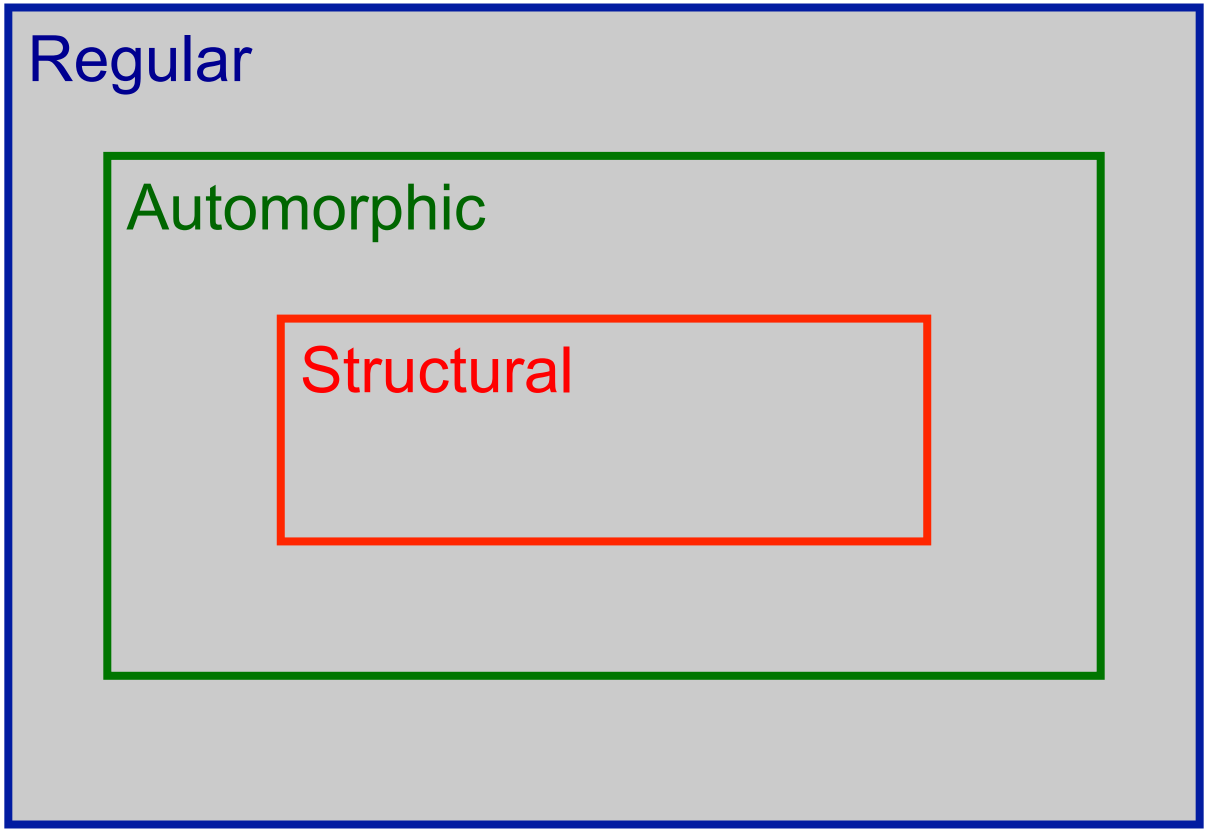
- [Borgatti, et al. 1992; Sparrow 1993]
- Two nodes *u* and *v* are automorphically equivalent if all the nodes can be relabeled to form an isomorphic graph with the labels of *u* and *v* interchanged
  - Swapping *u* and *v* (possibly along with their neighbors) does not change graph distances
- Two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



# Automorphic Equivalence: Algorithms

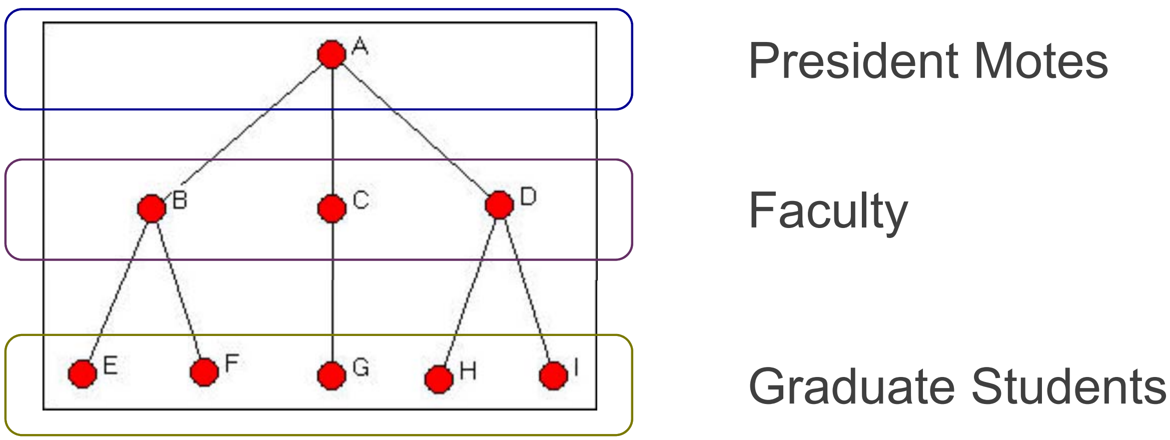
- Sparrow (1993) proposed an algorithm that scales linearly to the number of edges
- Use numerical signatures on degree sequences of neighborhoods
- Numerical signatures use a unique transcendental number like π, which is independent of any permutation of nodes
- Suppose node *i* has the following degree 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

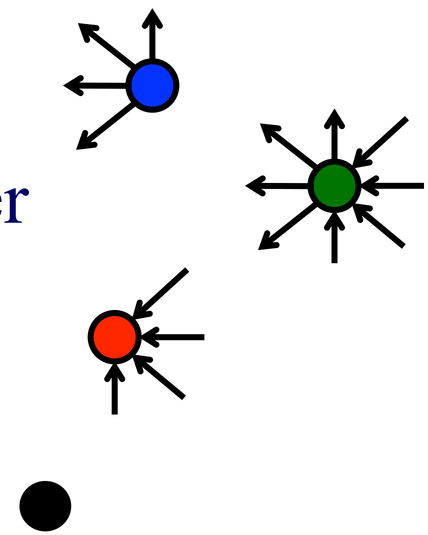
- [Everett & Borgatti, 1992]
- Two nodes *u* and *v* are regularly equivalent *if* they are equally related to equivalent others




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
## (continued)

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



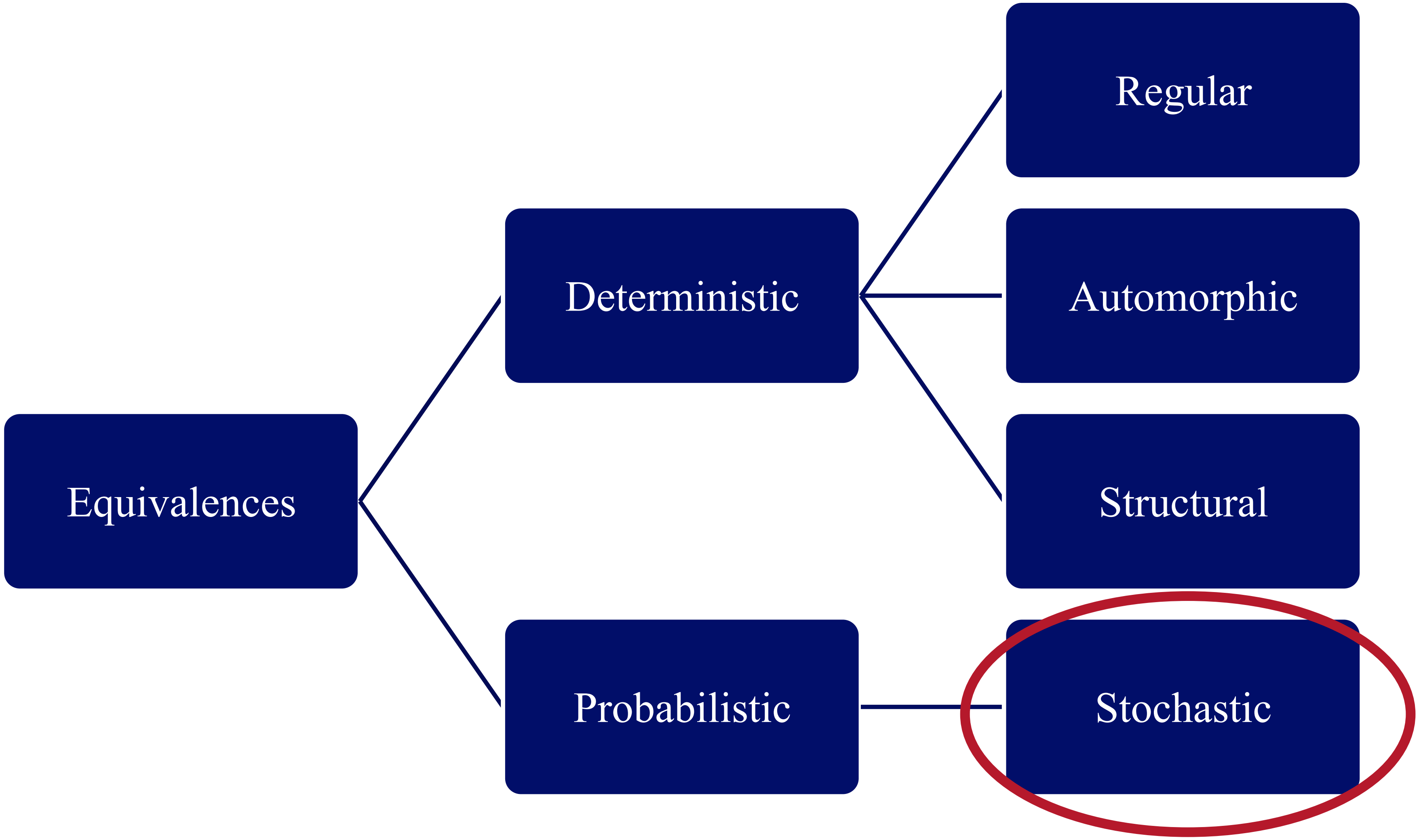
# Regular Equivalence
## (continued)

- 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

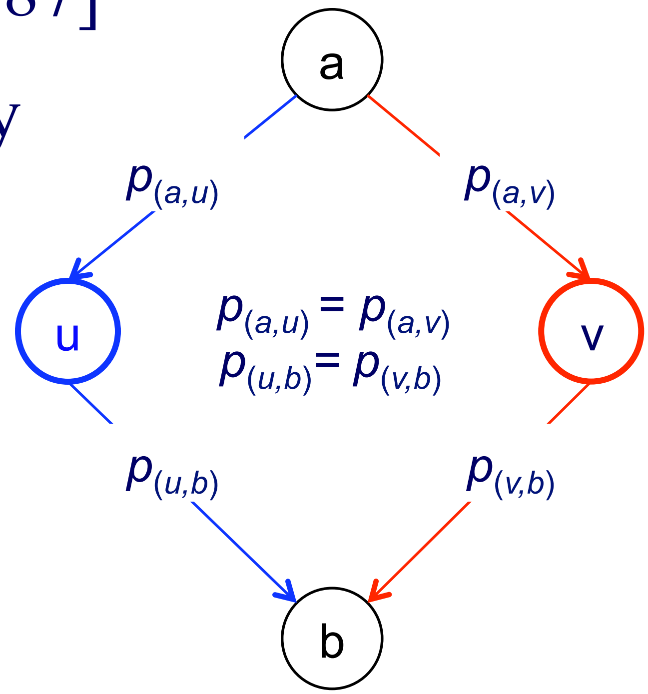
- Many algorithms exist here
- Basic notion
  – Profile each node's neighborhood by the presence of nodes of other "types"
  – Nodes are regularly equivalent to the extent that they have similar "types" of other nodes at similar distances in their neighborhoods

# Equivalences



# Stochastic Equivalence

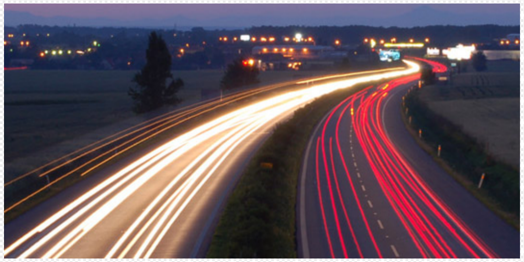
- [Holland, et al. 1983; Wasserman & Anderson, 1987]
- Two nodes are stochastically equivalent if they are "exchangeable" w.r.t. a probability distribution
- Similar to structural equivalence but probabilistic



# 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

# Roadmap



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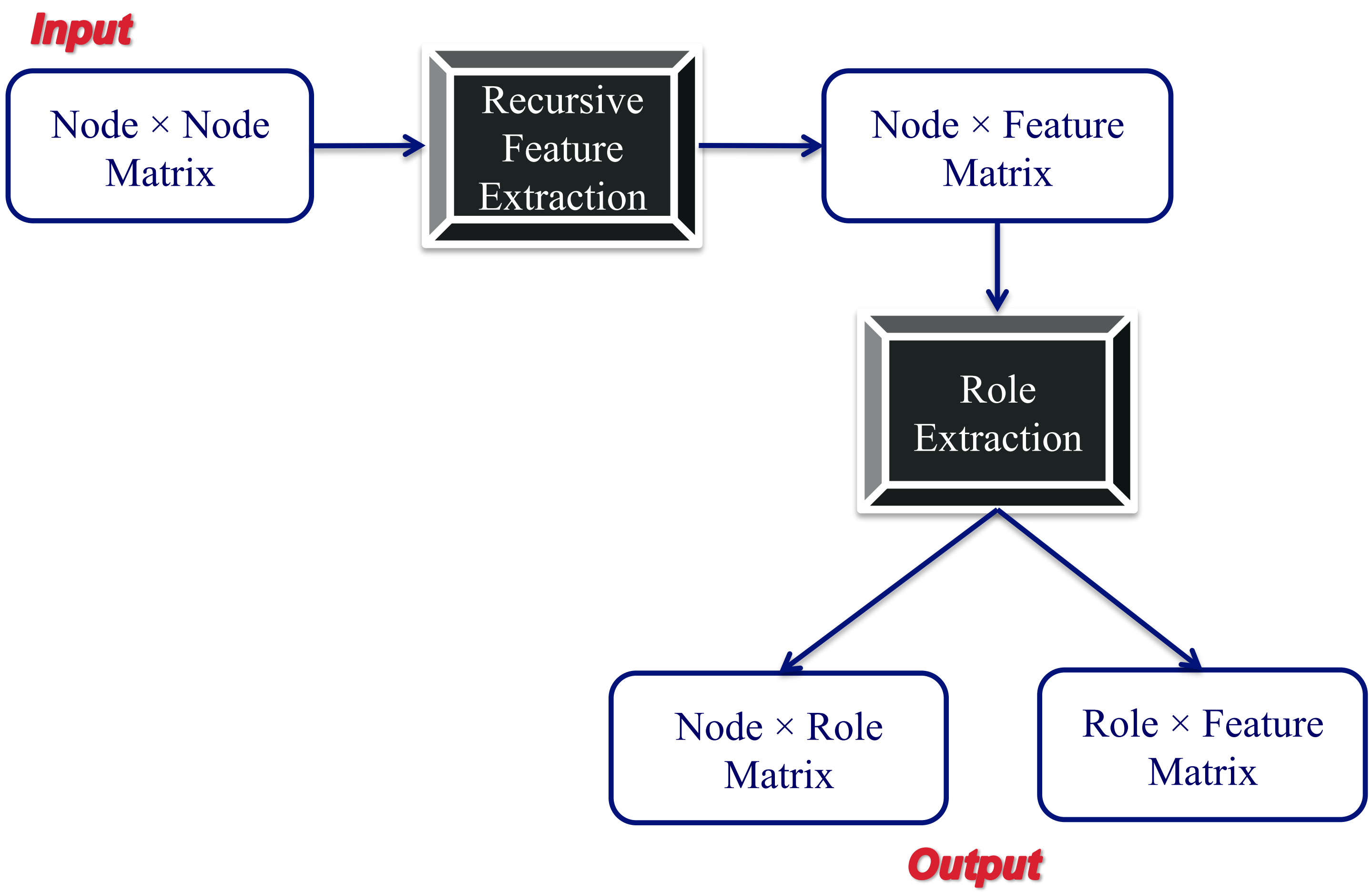
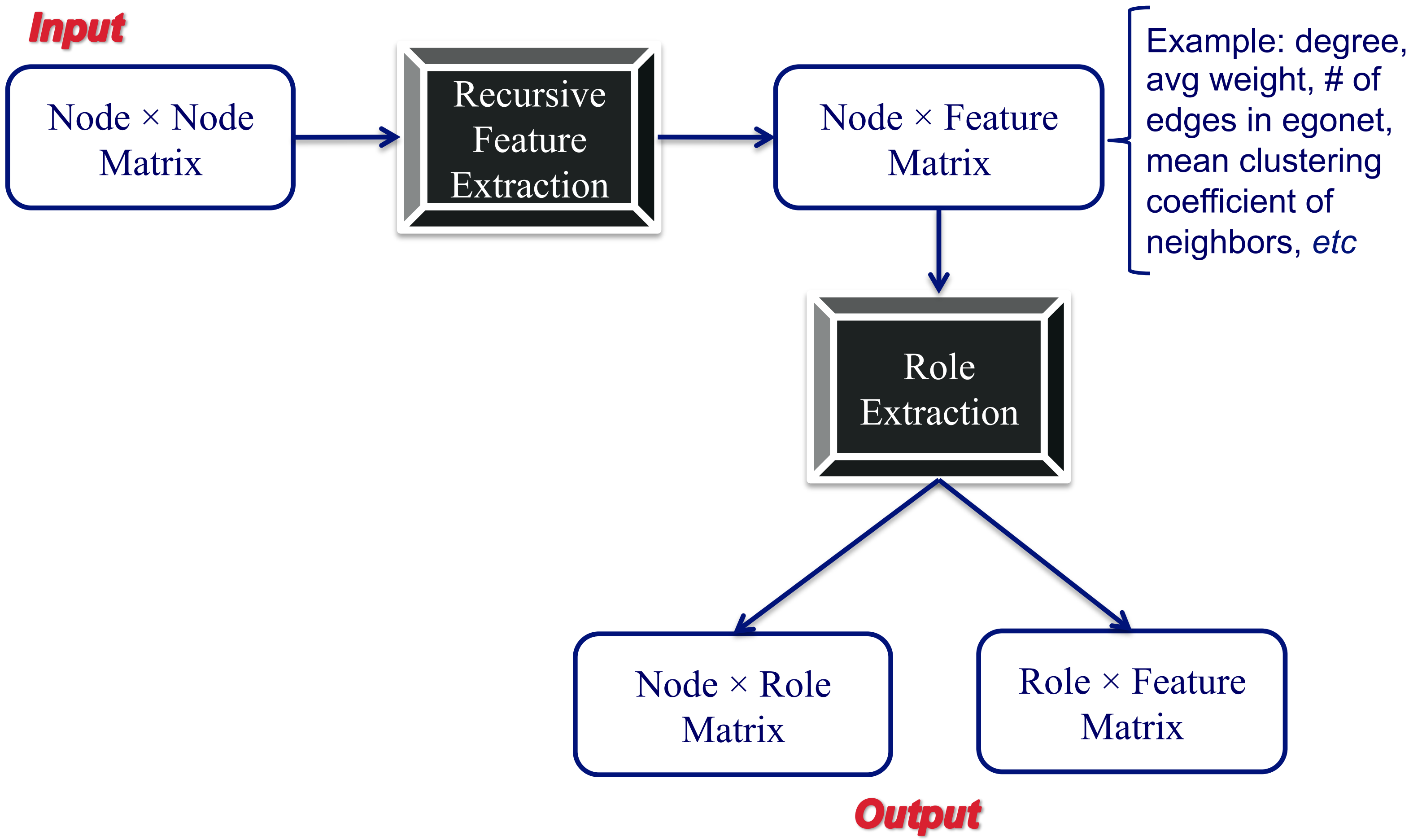
# RolX: Role eXtraction

- 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

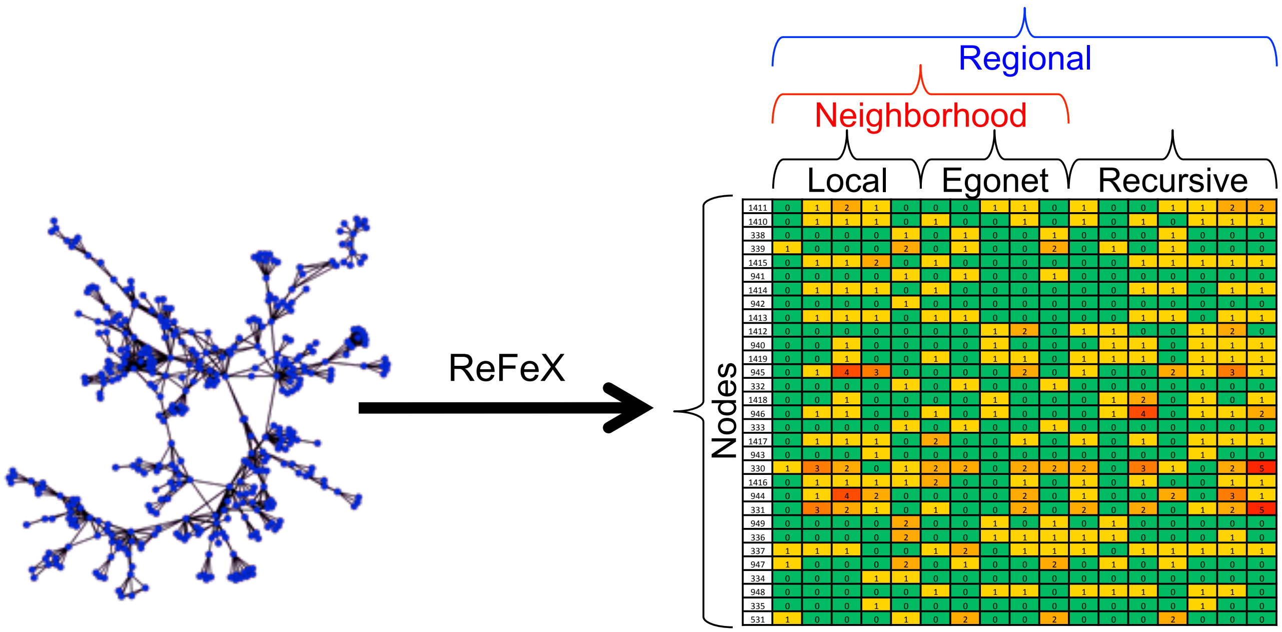


# RolX: Flowchart



# Recursive Feature Extraction

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



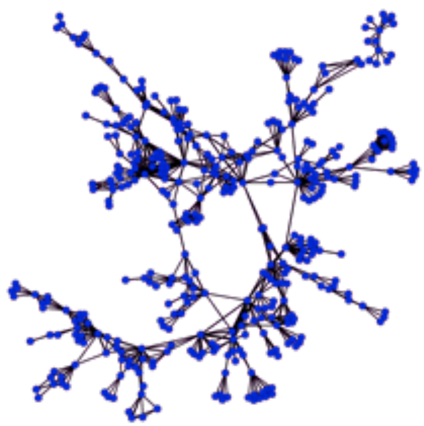

- Neighborhood features: What is your connectivity pattern?
- Recursive Features: To what *kinds* of nodes are you connected?

# Propositionalisation (PROP)

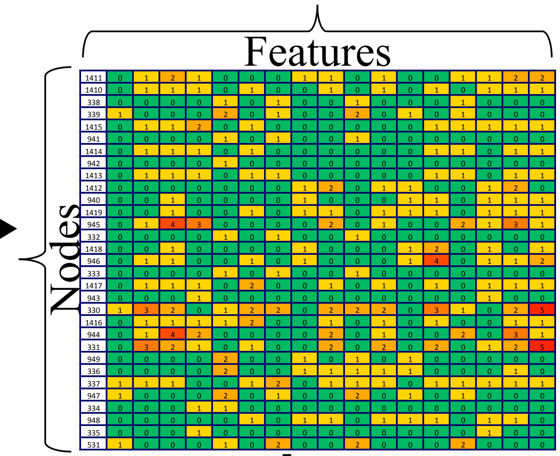
- [Knobbe, et al. 2001; Neville, et al. 2003; Krogel, et al. 2003]
- From multi-relational data mining with roots in Inductive Logic Programming (ILP)
- Summarizes a multi-relational dataset (stored in multiple tables) into a propositional dataset (stored in a single “target” table)
- Derived attribute-value features describe properties of individuals
- Related more to recursive structural features than structural roles

# Role Extraction

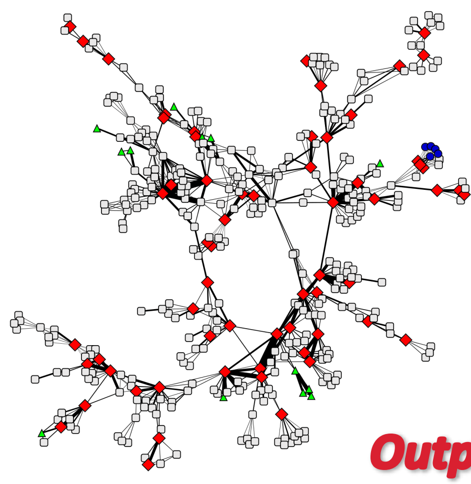
***Input***



Recursively extract features

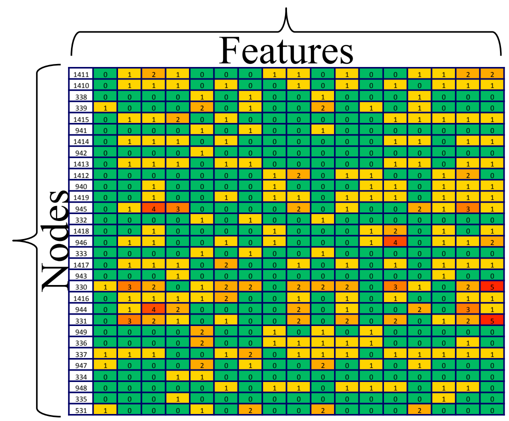



Automatically factorize roles

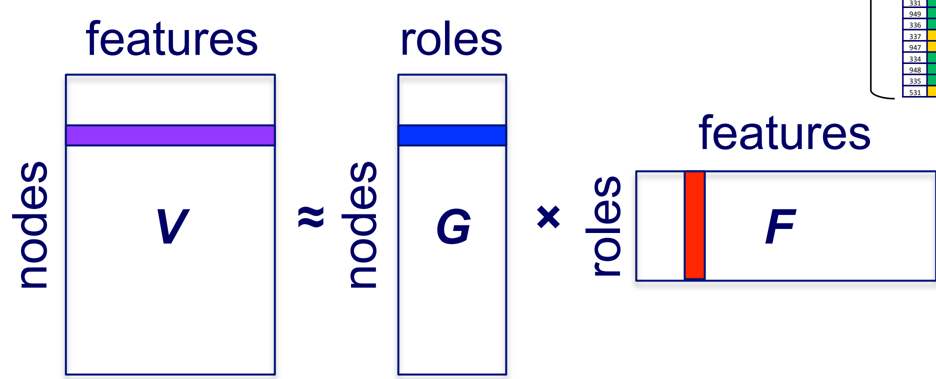


***Output***

# 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 $V \approx GF$




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

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

# Role Extraction: Model Selection

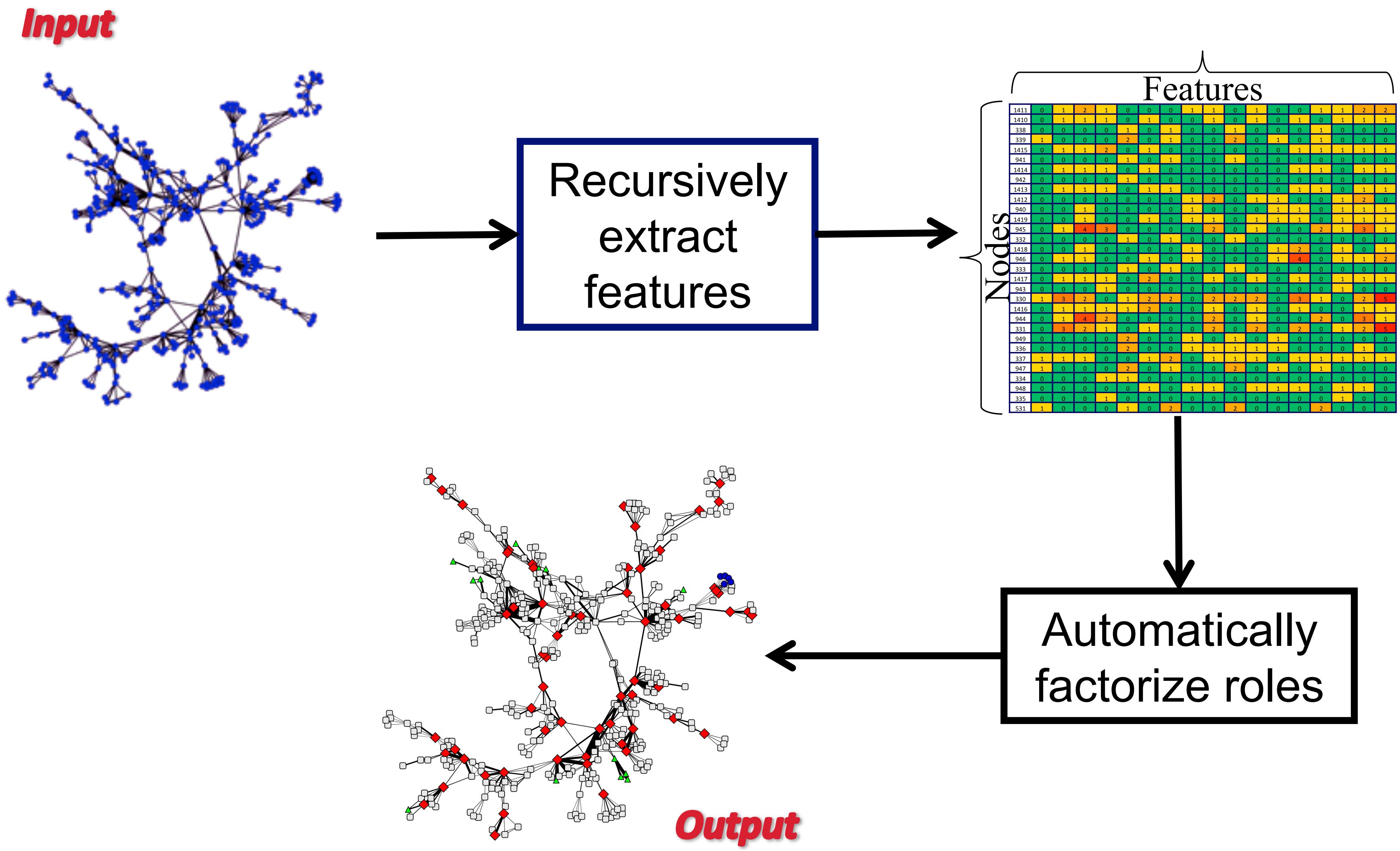
- Roles summarize behavior
  - Or, they compress the feature matrix, *V*
- Use MDL to select the model size *r* that results in the best compression
  - *L*: description length
  - *M*: # of bits required to describe the model
  - *E*: cost of describing the reconstruction errors in *V – GF*
  - Minimize $L = M + E$
    - 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



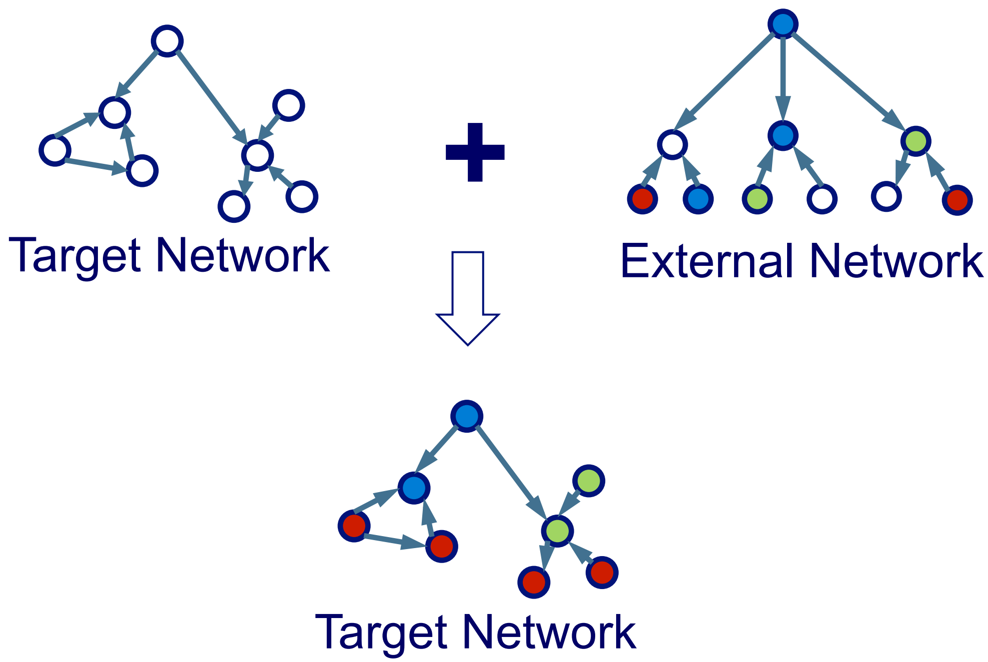
# Experiments on Role Discovery

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

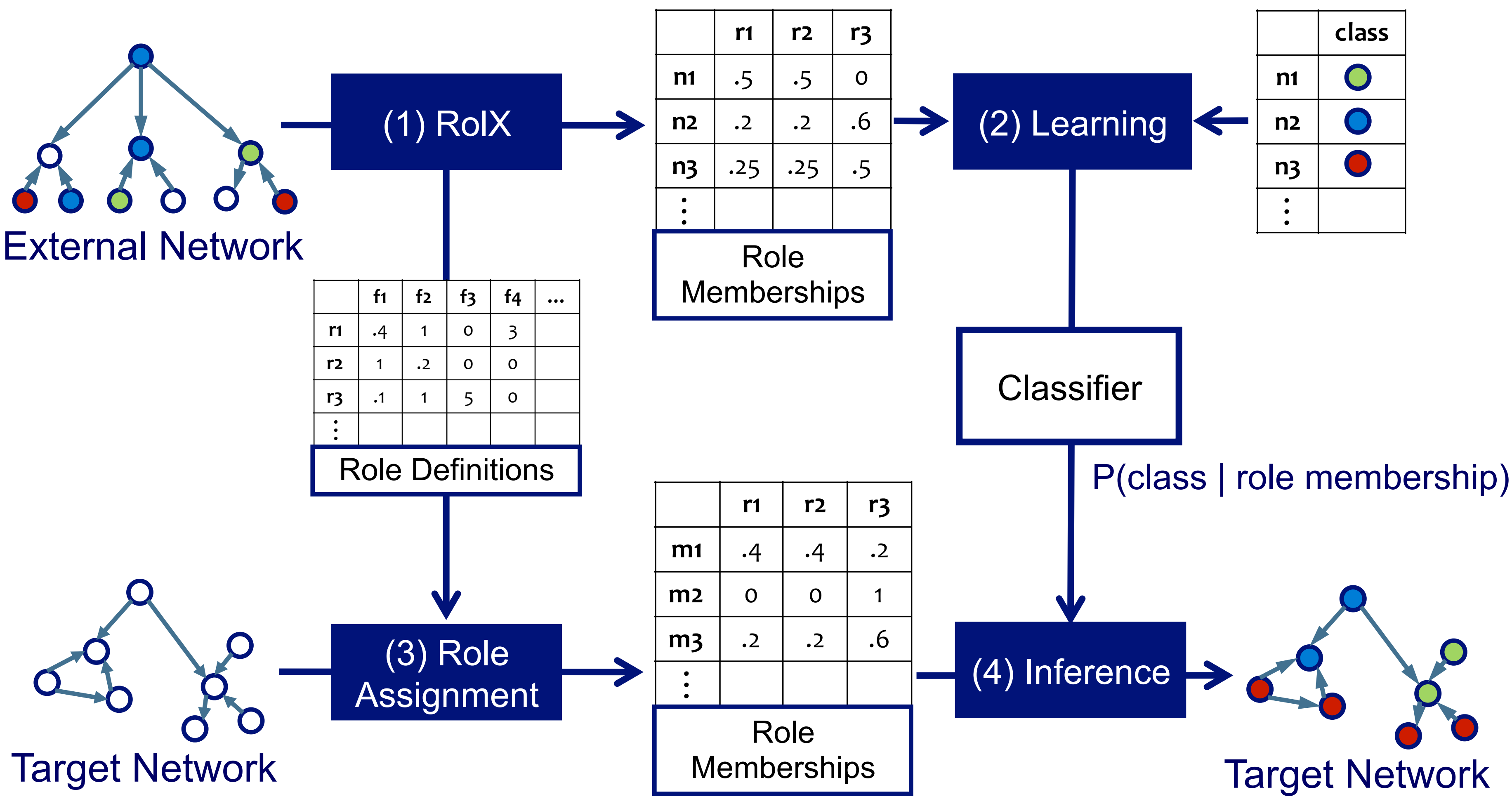
Details in Henderson *et al.* KDD 2012

# Role Transfer

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



# Role Transfer = RolX + SL



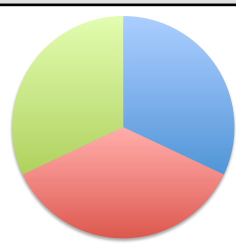
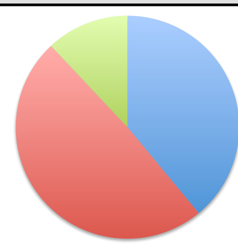
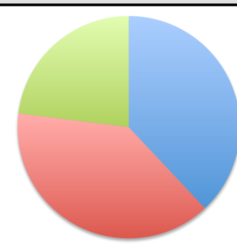
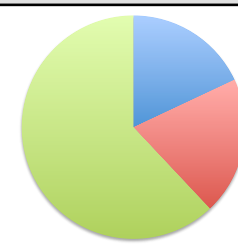
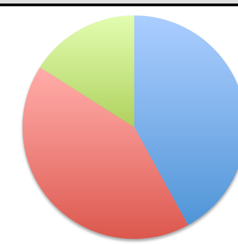

| | r1 | r2 | r3 |
|---|---|---|---|
| n1 | .5 | .5 | 0 |
| n2 | .2 | .2 | .6 |
| n3 | .25 | .25 | .5 |
| ⋮ | | | |

| | class |
|---|---|
| n1 | |
| n2 | |
| n3 | |
| ⋮ | |

| | f1 | f2 | f3 | f4 | … |
|---|---|---|---|---|---|
| r1 | .4 | 1 | 0 | 3 | |
| r2 | 1 | .2 | 0 | 0 | |
| r3 | .1 | 1 | 5 | 0 | |
| ⋮ | | | | | |

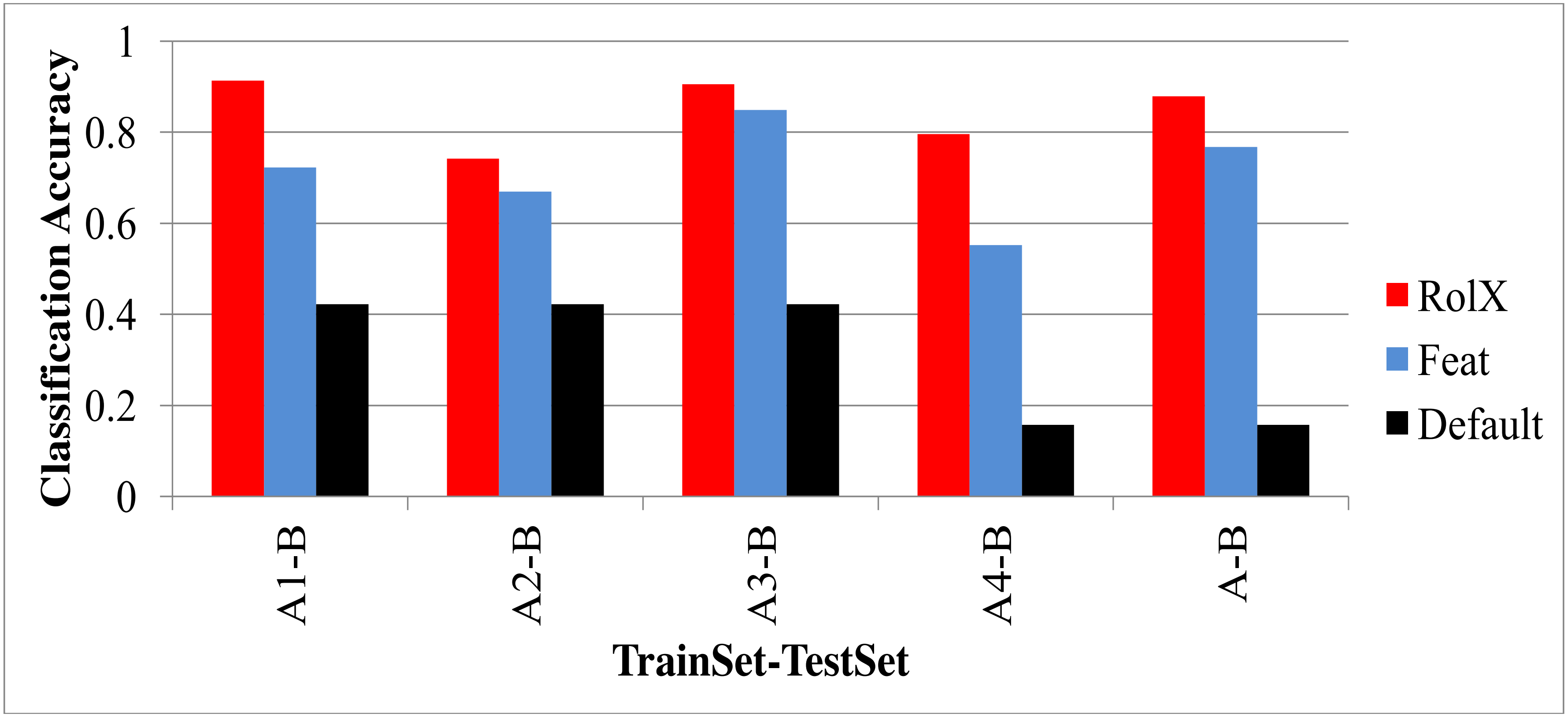
| | r1 | r2 | r3 |
|---|---|---|---|
| m1 | .4 | .4 | .2 |
| m2 | 0 | 0 | 1 |
| m3 | .2 | .2 | .6 |
| ⋮ | | | |

# 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 |  |  |  |  |  |

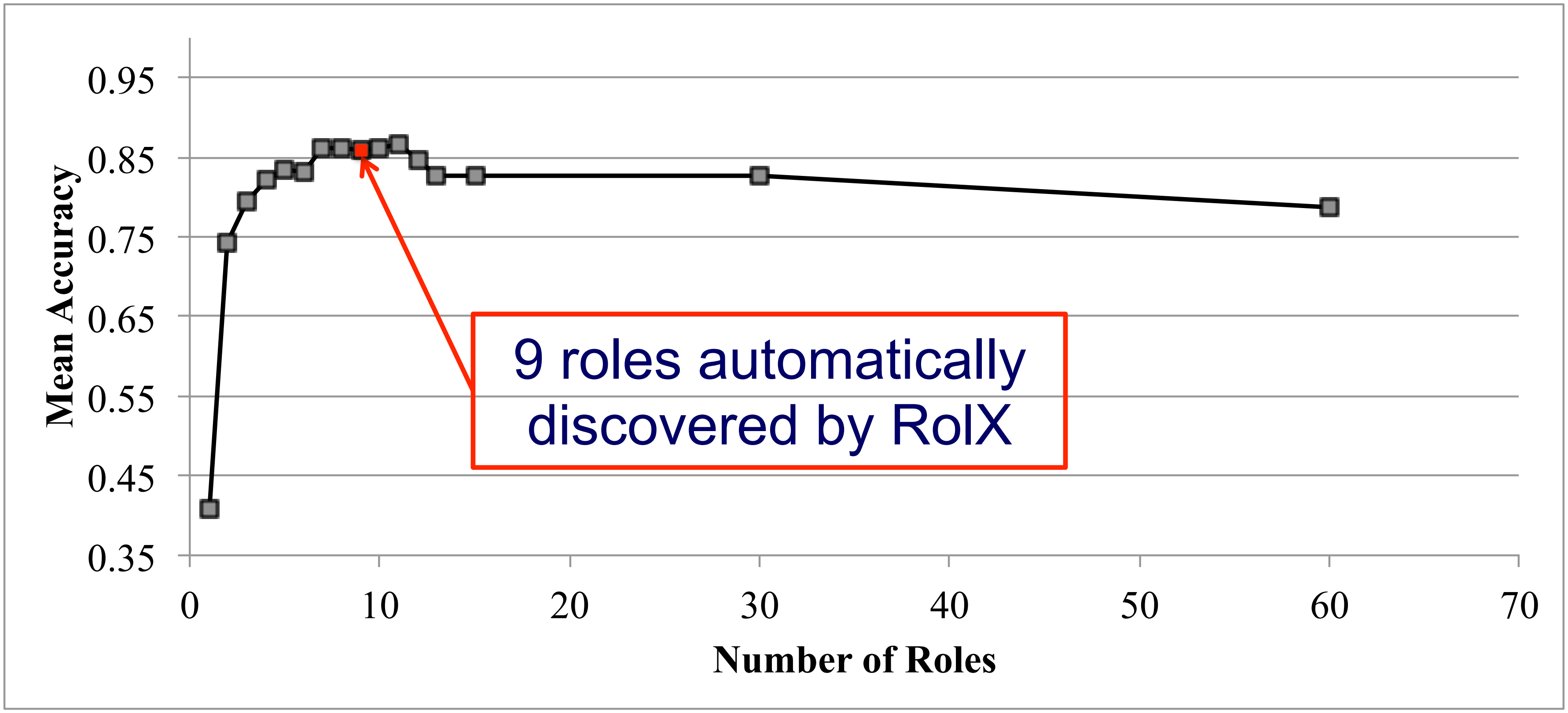
Web DNS P2P

# Role Transfer Results



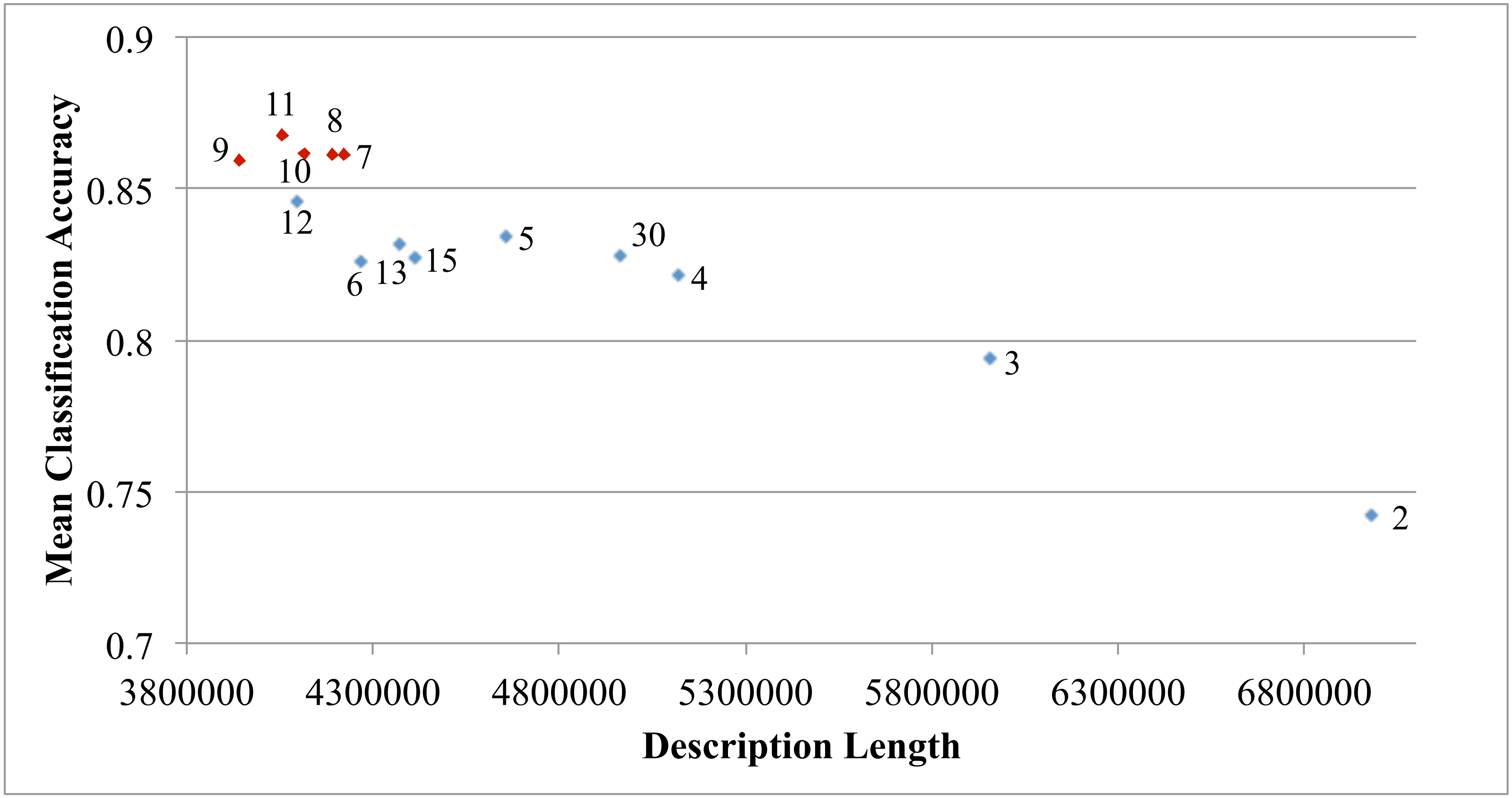

Roles generalize across disjoint networks & enable prediction without re-learning

# Model Selection



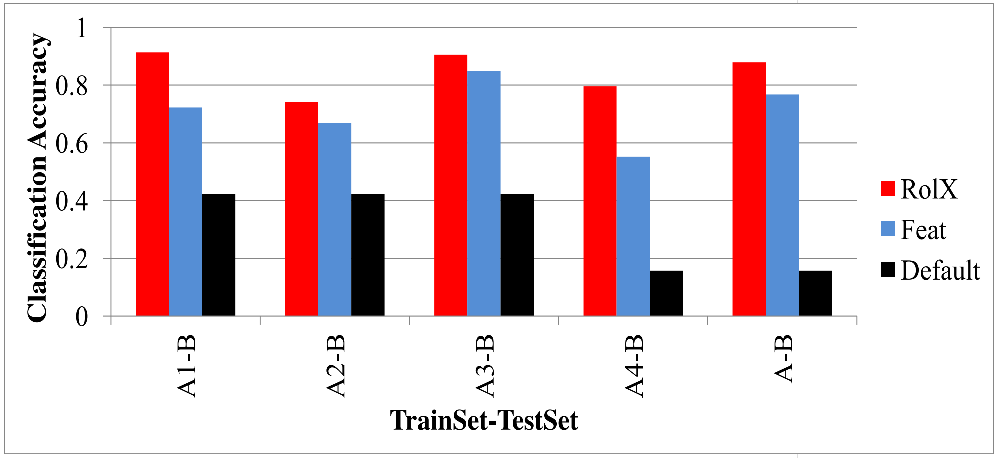

RolX selects high accuracy model sizes

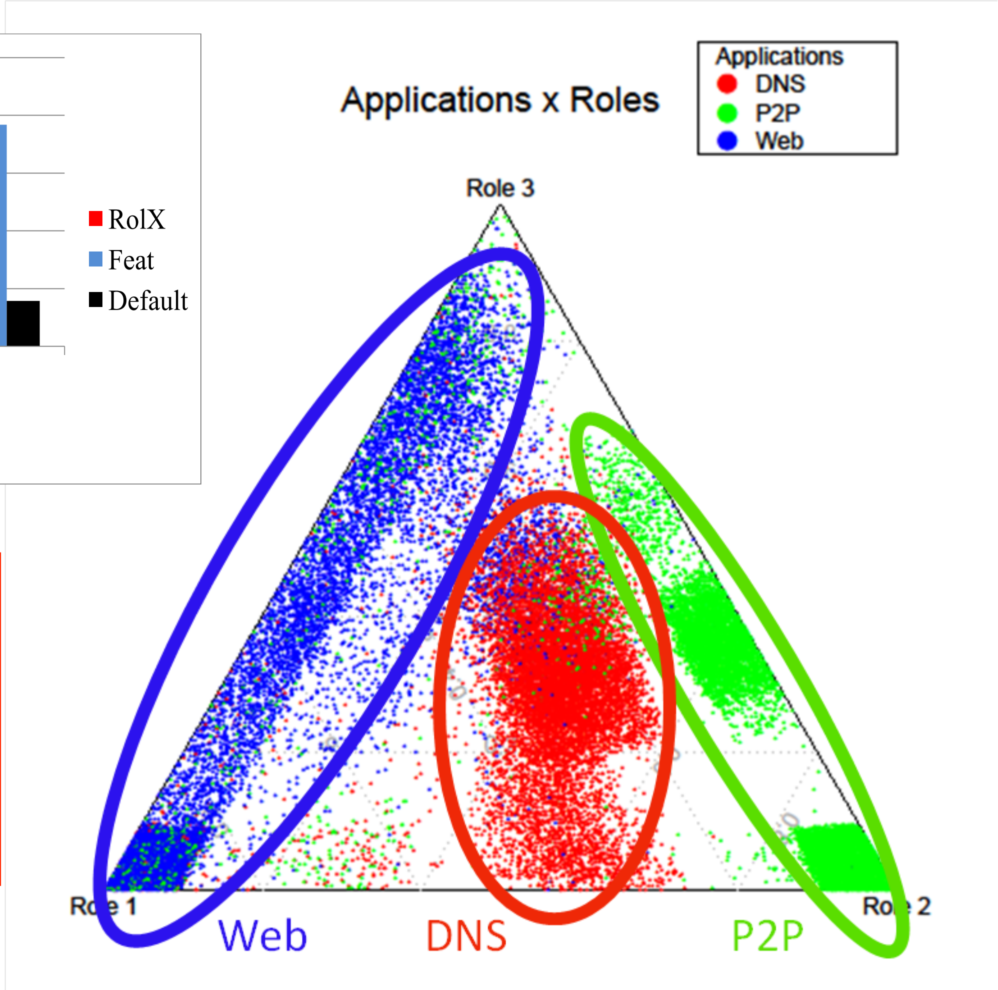
# Model Selection (continued)




Classification accuracy is highest when RolX selection criterion is minimized

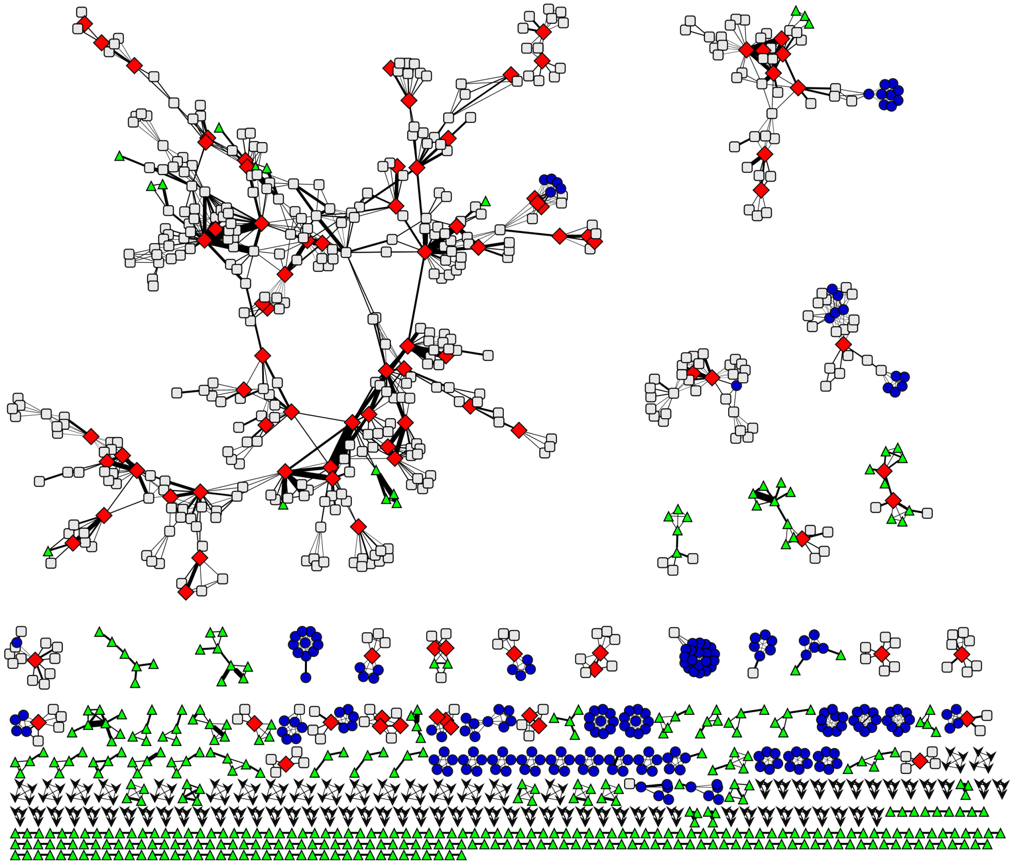
# Role Space



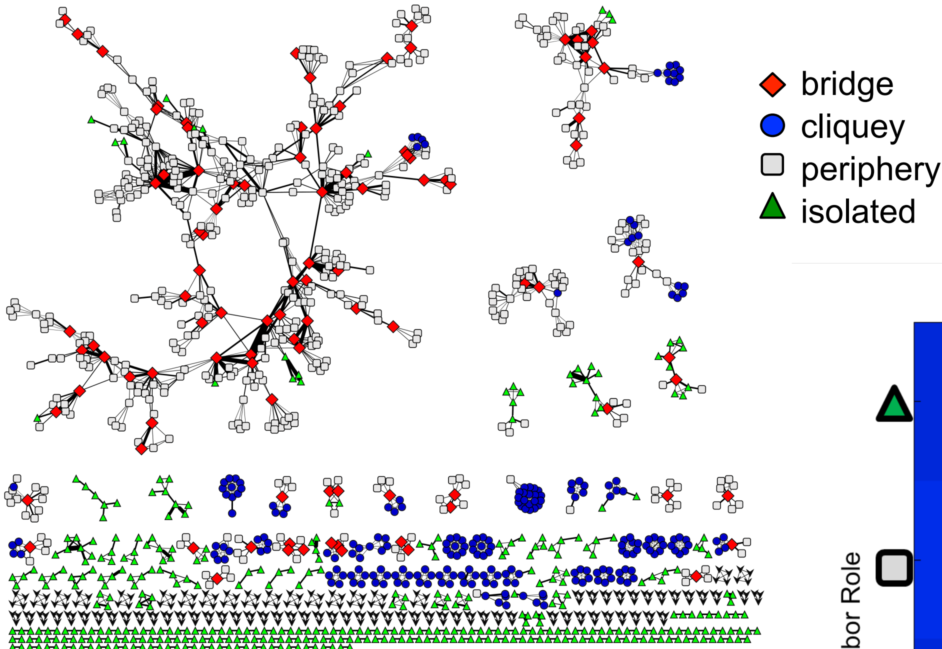

IP trace classes are well-separated in the RolX **role space** with as few as 3 roles

# Automatically Discovered Roles

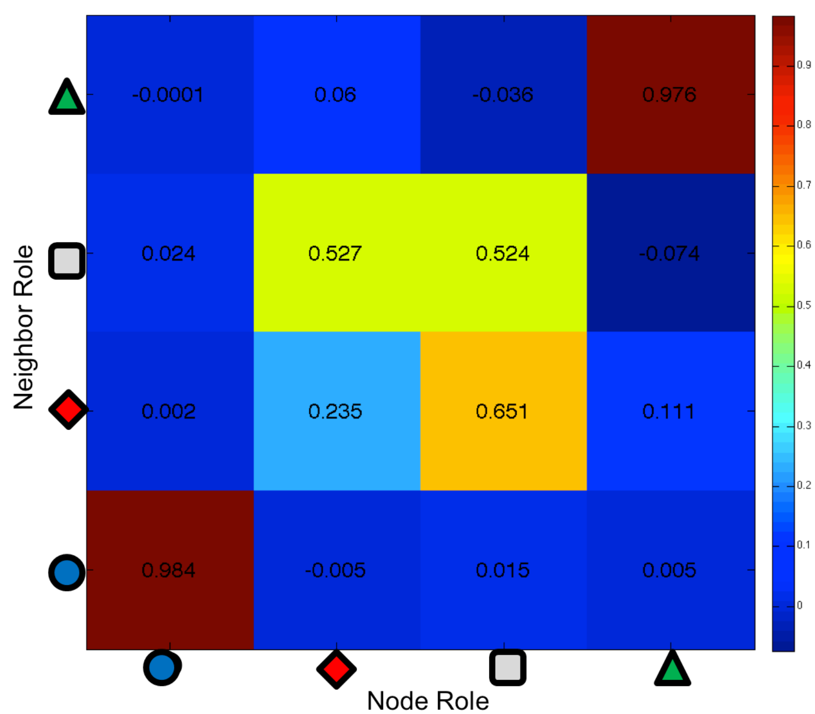


*Network Science Co-authorship Graph*
[Newman 2006]

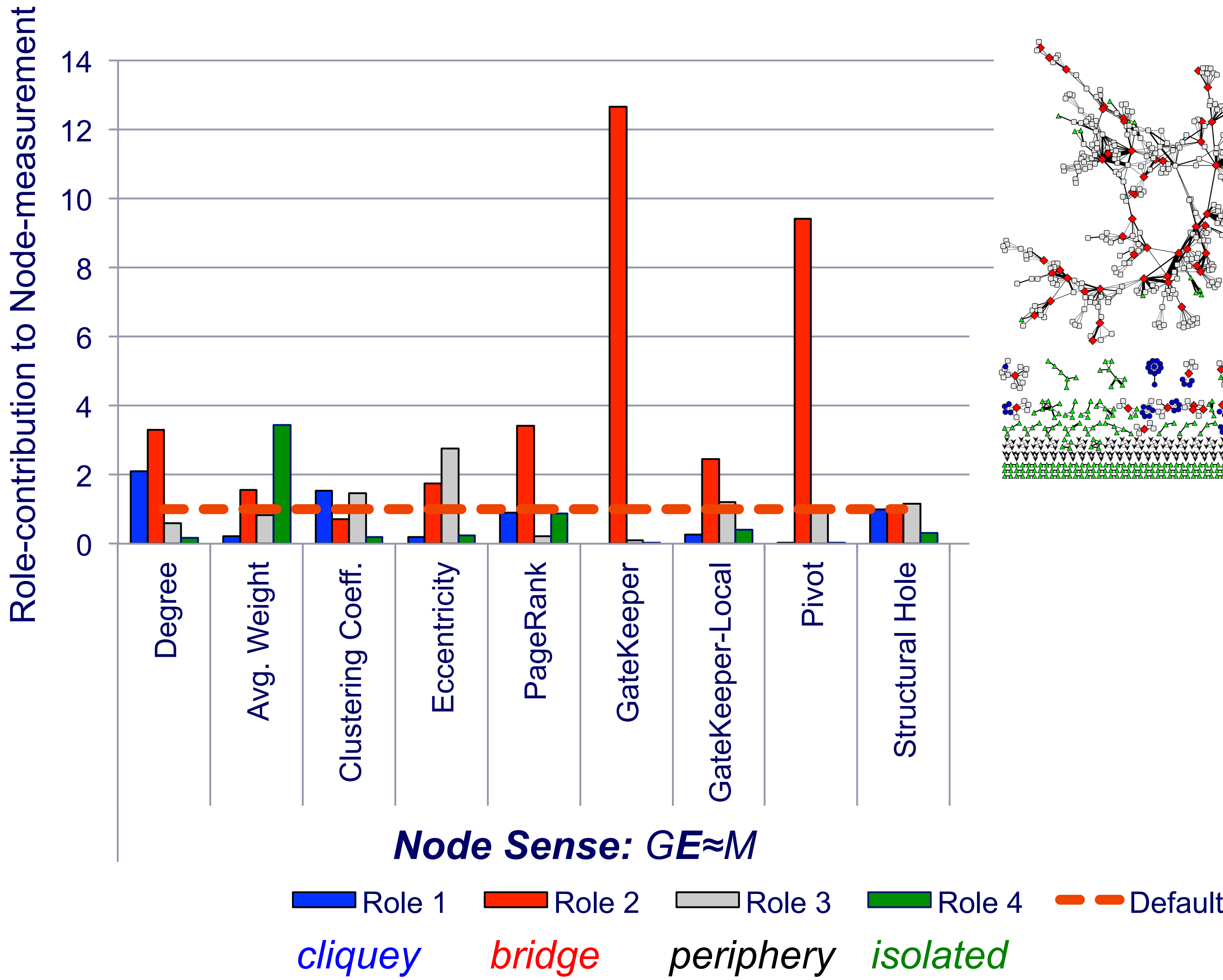
# Role Affinity Heat Map

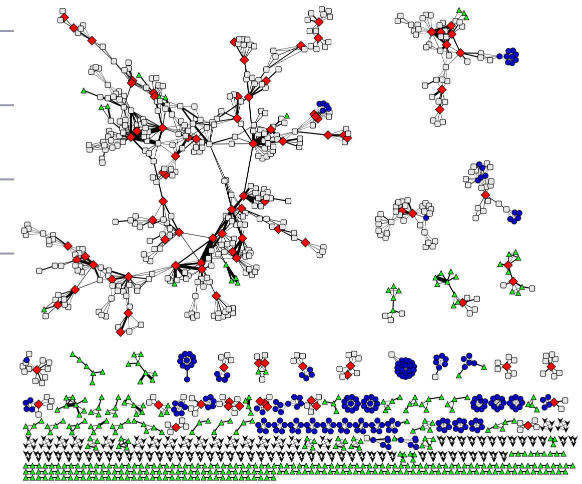



*Network Science Co-authorship Graph*
[Newman 2006]



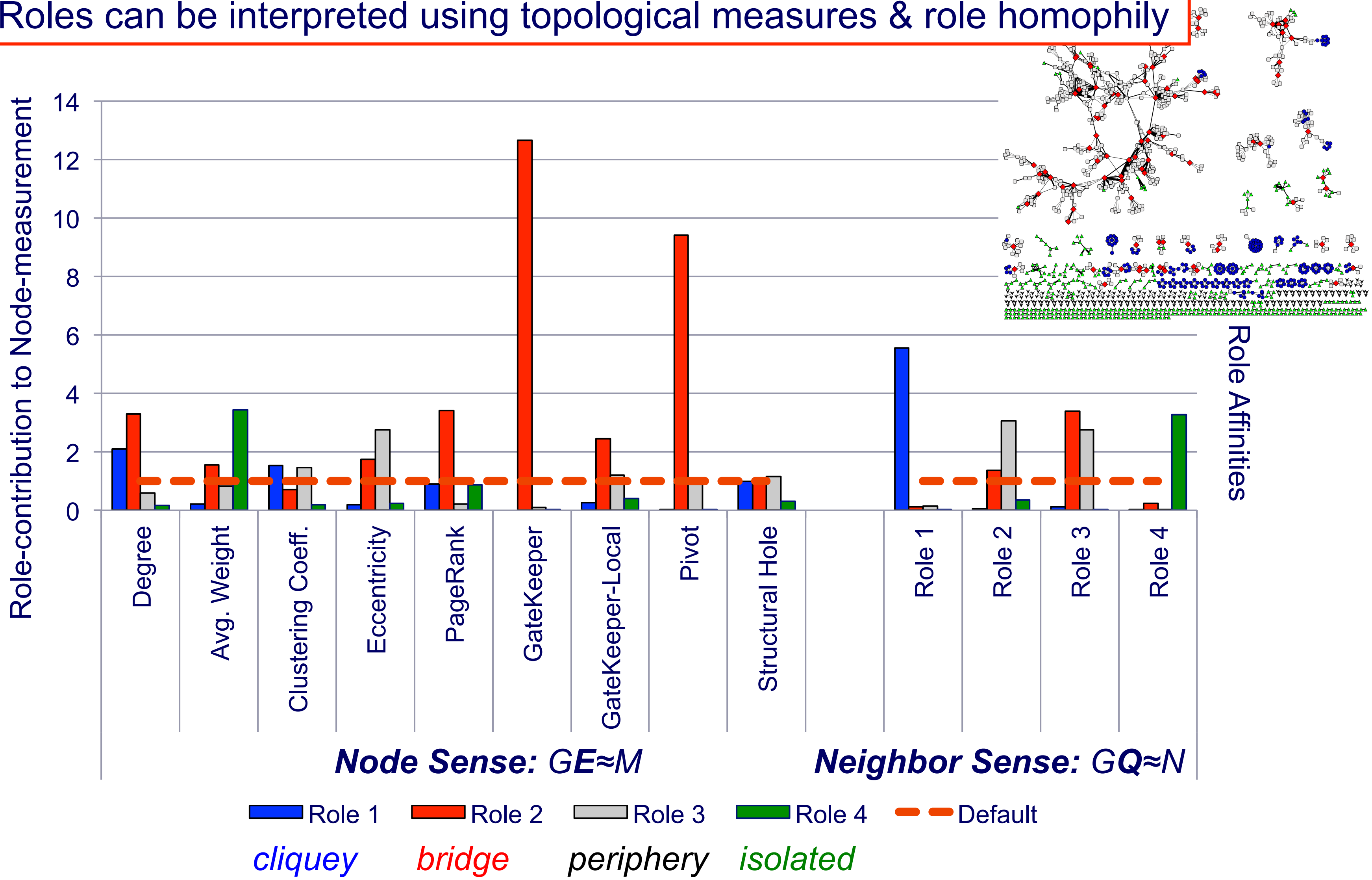
# Making Sense of Roles



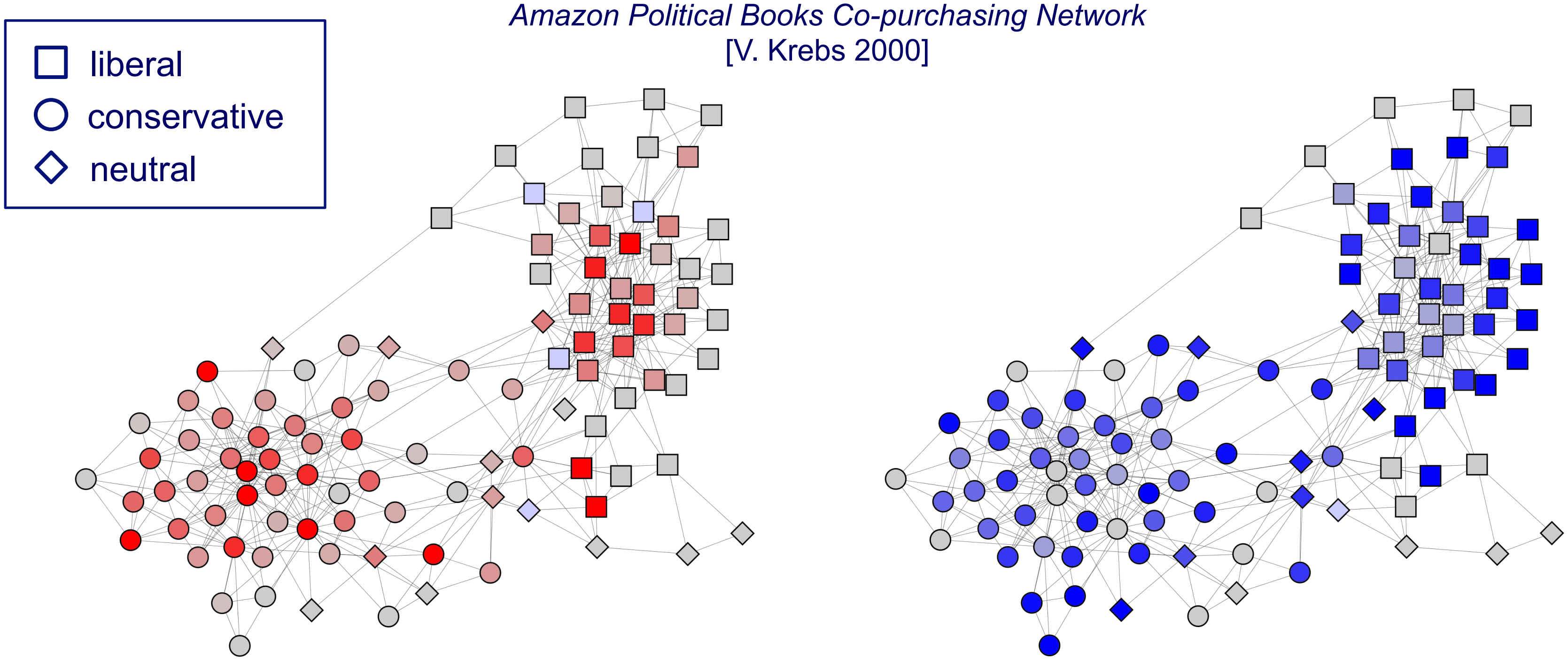
# Making Sense of Roles

Roles can be interpreted using topological measures & role homophily



# Mixed Membership over Roles

*Amazon Political Books Co-purchasing Network*
[V. Krebs 2000]

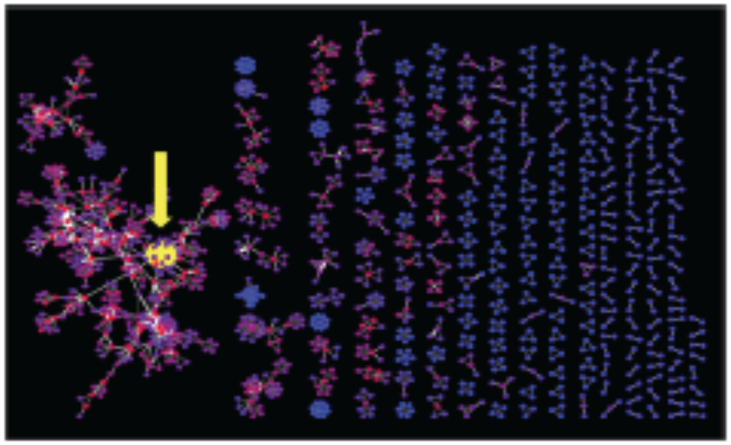



Bright red nodes are locally central nodes

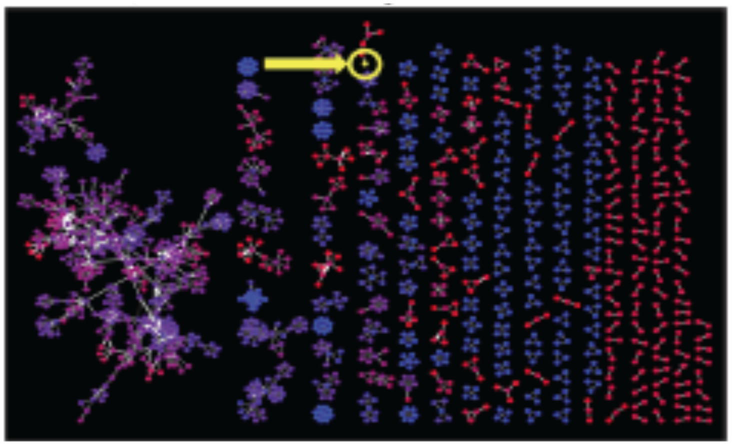
Bright blue nodes are peripheral nodes

Purchasing behavior of customers is captured by separating the "locally central" books from the "locally peripheral" books

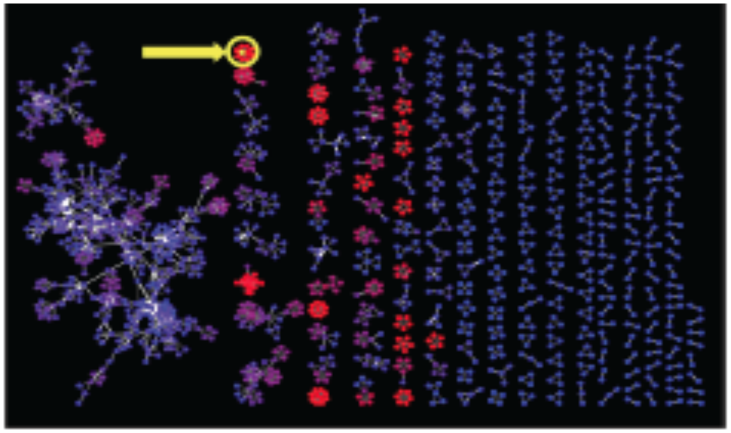
# Role Query



Node Similarity for M.E.J. Newman (***bridge***)



Node Similarity for J. Rinzel (***isolated***)



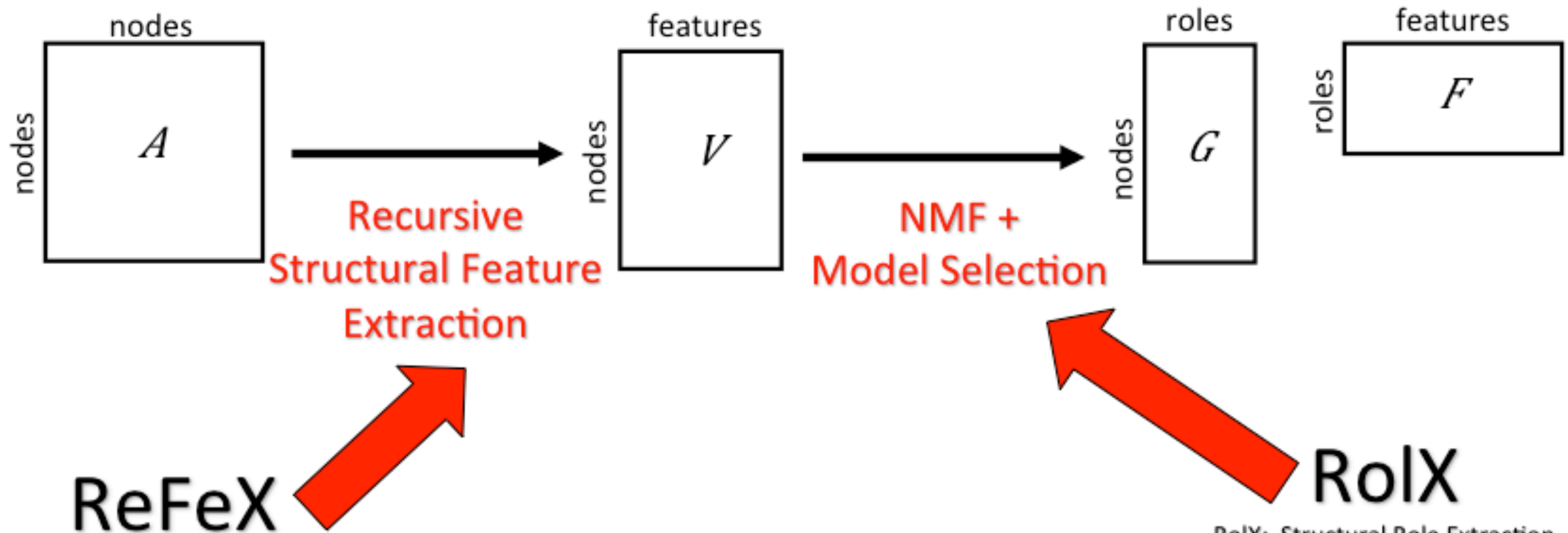
Node Similarity for F. Robert (***cliquey***)

Mixed-membership roles enable us to measure similarity of nodes based on their role memberships

# 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

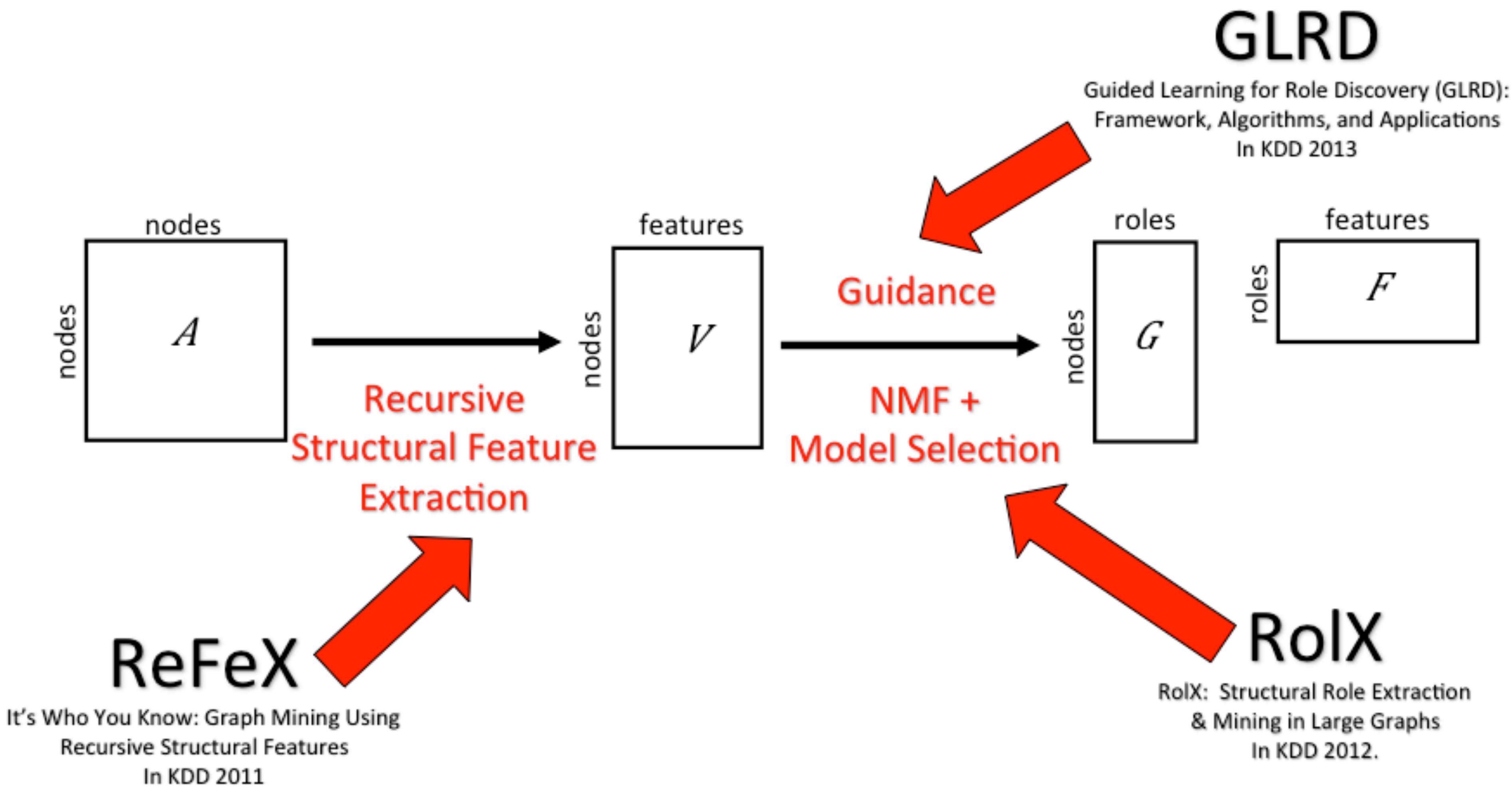
# GLRD



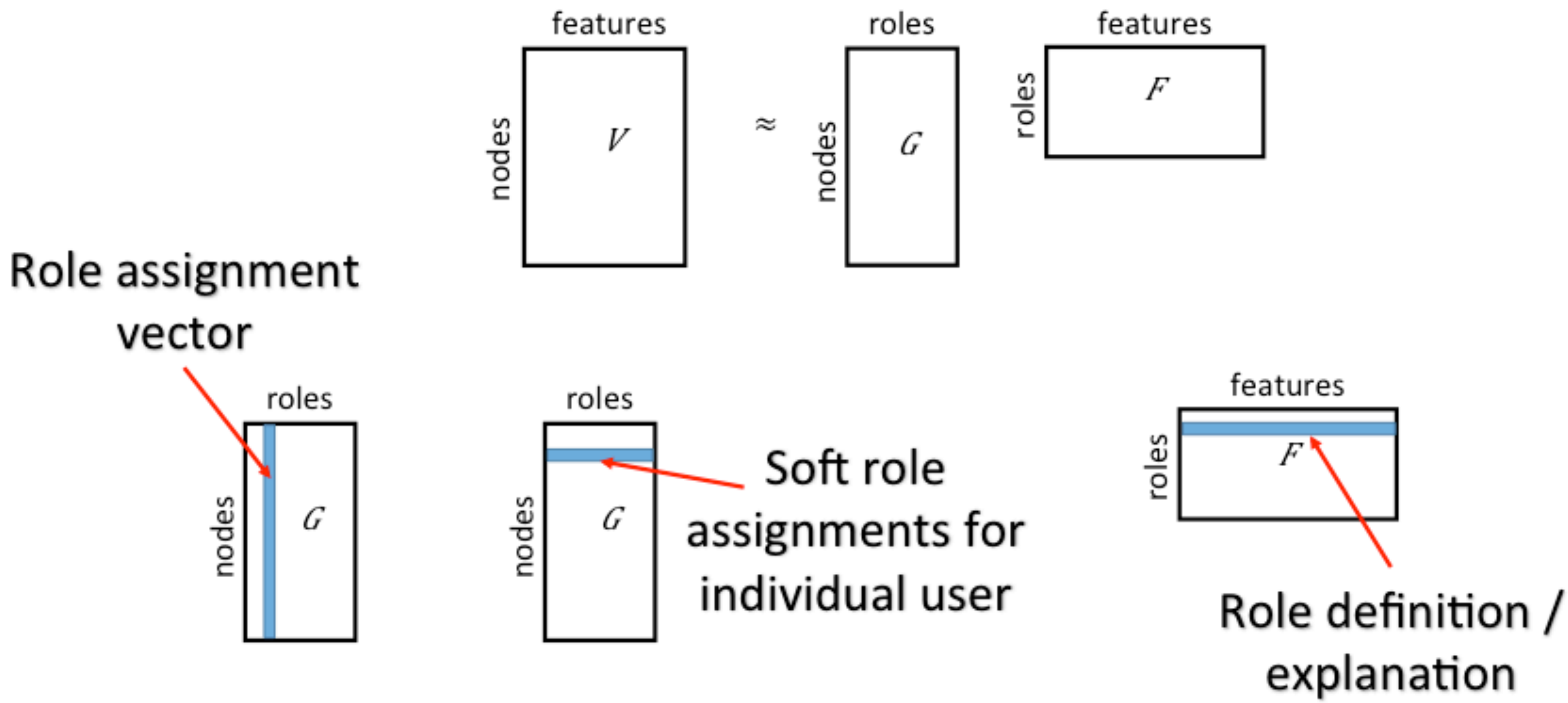

It's Who You Know: Graph Mining Using Recursive Structural Features In KDD 2011

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
nodes
V
Guidance
NMF + Model Selection
roles
nodes
G
features
roles
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.

# Adding Constraints



# GLRD Framework

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

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

where $g_i$ and $f_i$ are convex functions.

- 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

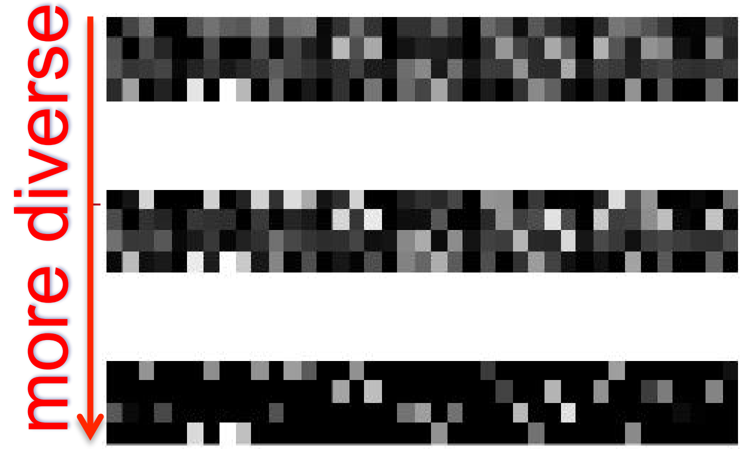
| Guidance Type | Effect of increasing guidance | |
|---|---|---|
| | on role assignment ($G$) | on role definition ($F$) |
| Sparsity | Reduces the number of nodes with minority memberships in roles | Decreases likelihood that features with small explanatory benefit are included |
| Diversity | Limits 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

$$
\begin{aligned}
\underset{\mathbf{G},\mathbf{F}}{\operatorname{argmin}} \quad & ||\mathbf{V} - \mathbf{G}\mathbf{F}||_2 \\
\text{subject to:} \quad & \mathbf{G} \geq 0, \mathbf{F} \geq 0 \\
& \forall i \quad ||\mathbf{G}_{\bullet \mathbf{i}}||_1 \leq \epsilon_G \\
& \forall i \quad ||\mathbf{F}_{\mathbf{i} \bullet}||_1 \leq \epsilon_F
\end{aligned}
$$

where $\epsilon_G$ and $\epsilon_F$ define upperbounds for the sparsity constraints (amount of allowable density).

# Diversity




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

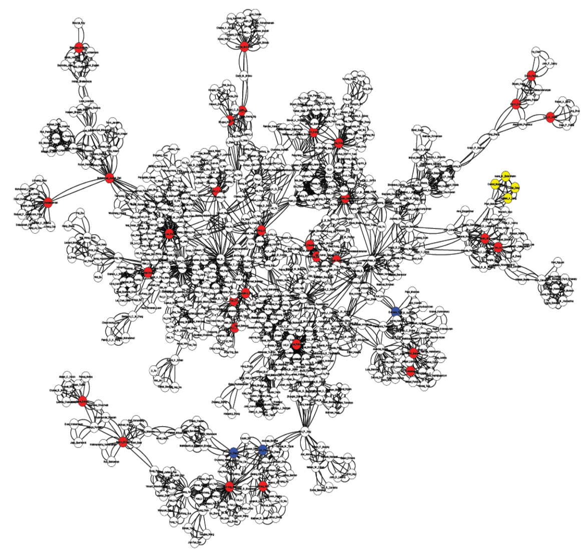
subject to: $\quad \mathbf{G} \geq 0, \mathbf{F} \geq 0$

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

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

where $\quad \epsilon_G$ and $\epsilon_F$ define upperbounds on how angularly similar role assignments and role definitions can be to each other.

# Alternativeness



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

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

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

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

where $\epsilon_G$ and $\epsilon_F$ define upperbounds on how similar the results can be to $\mathbf{G}^*$ and $\mathbf{F}^*$.

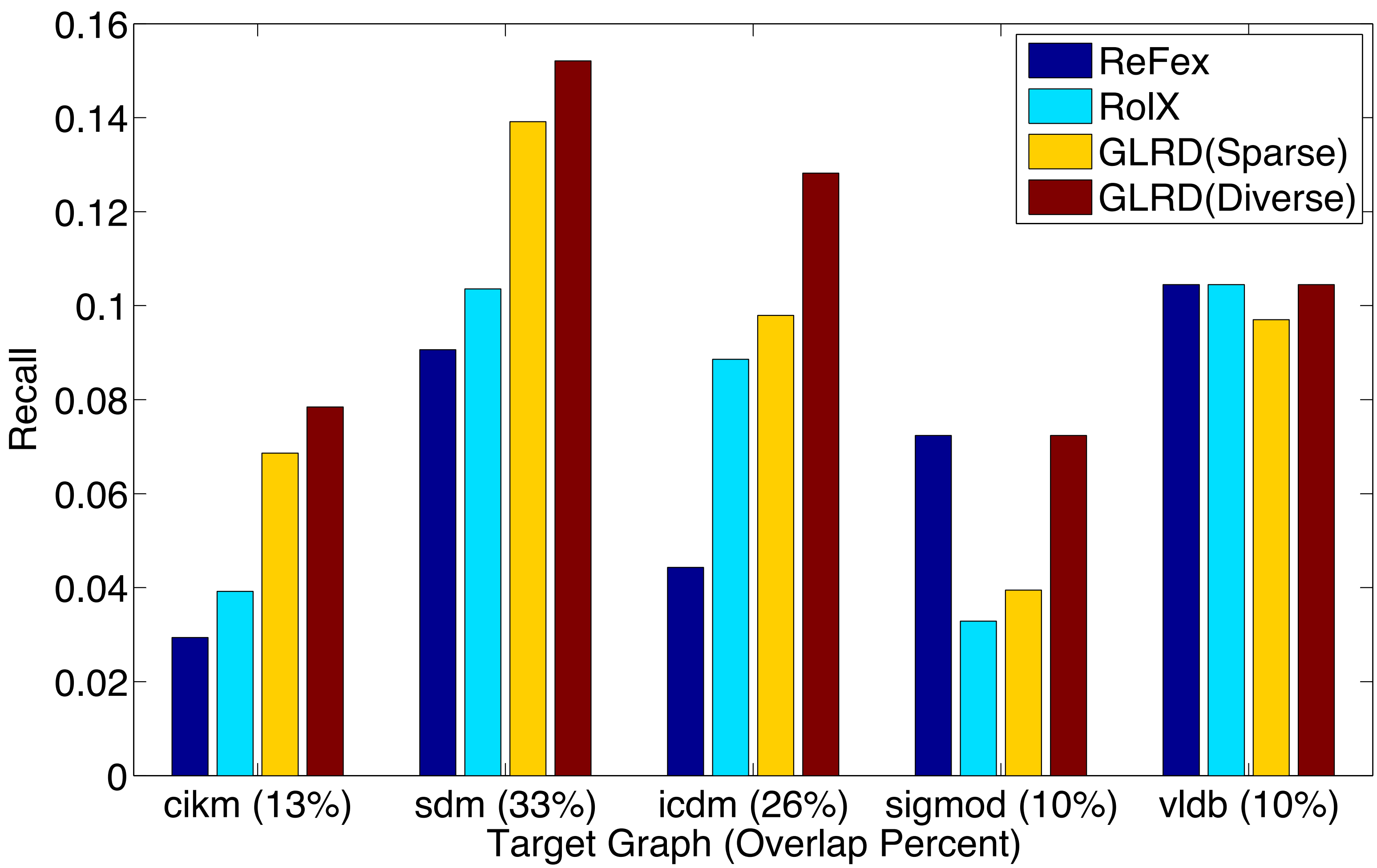
# Diverse Roles and Sparse Roles

- 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 |

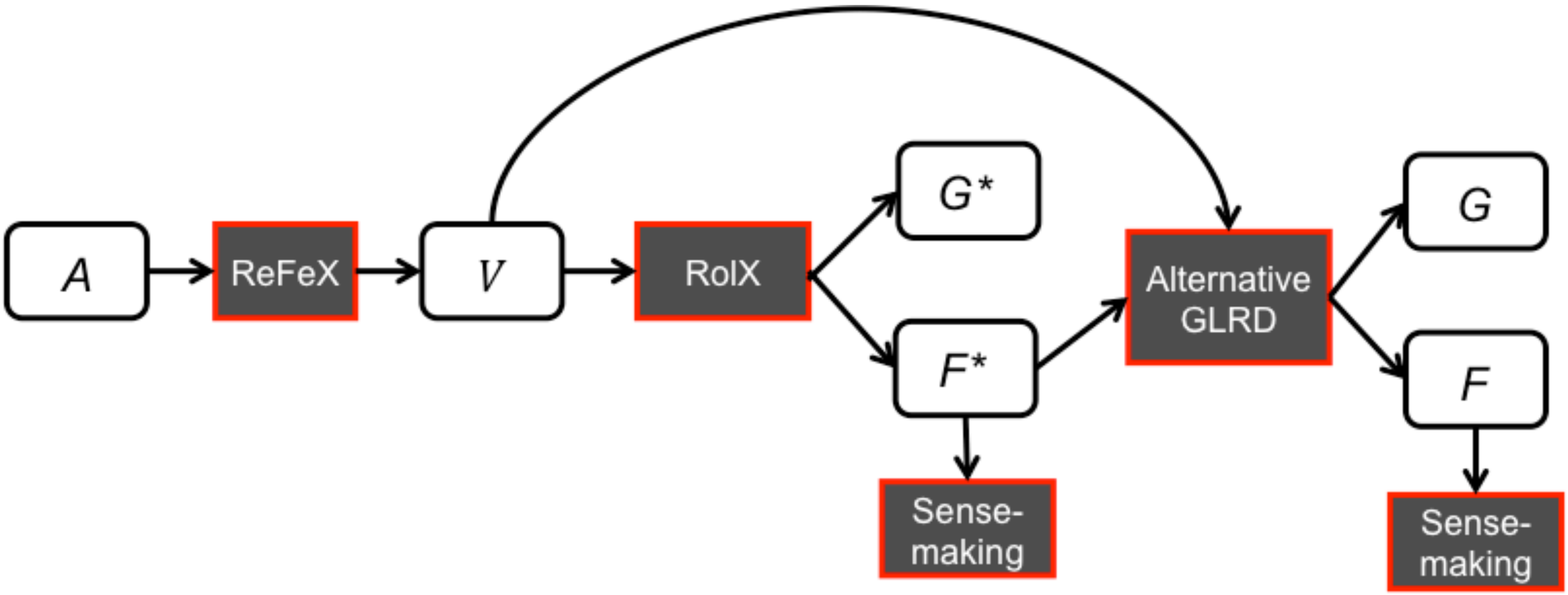
DBLP Co-authorship Networks from 2005-2009

# Identity Resolution across Networks

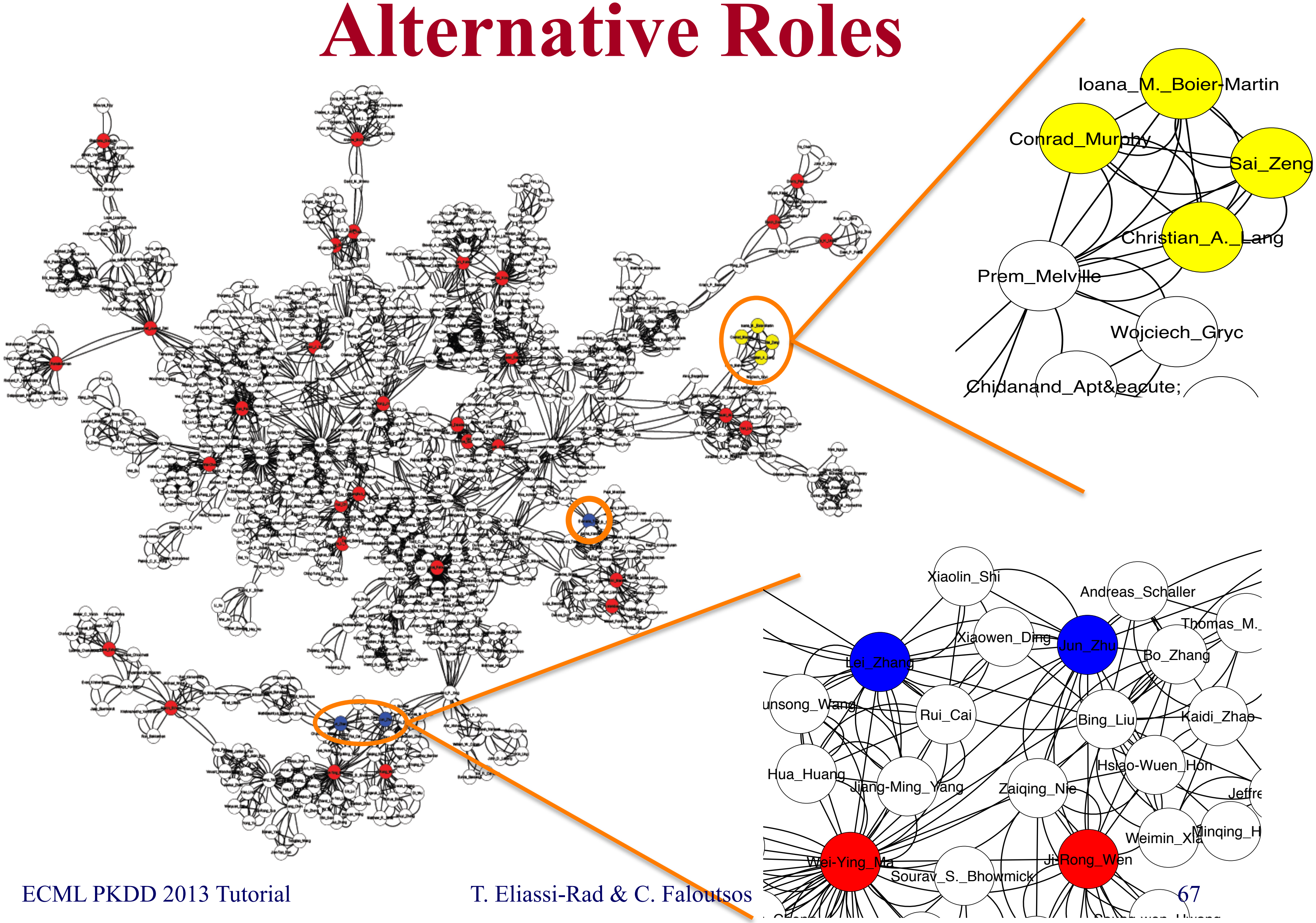


# Alternative Roles

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



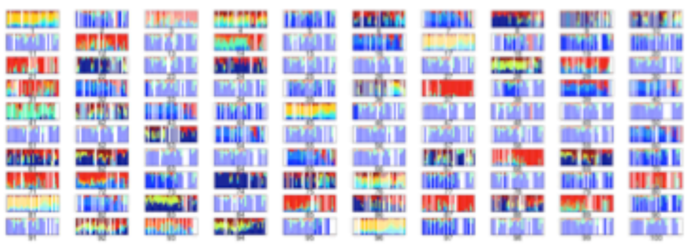
# Alternative Roles



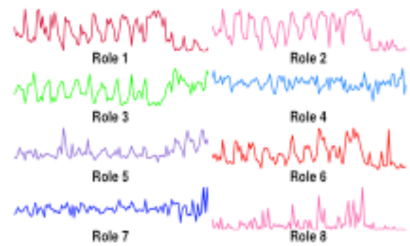
# Modeling Dynamic Graphs with Roles

- Introduced by Rossi *et al.* WSDM 2013

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

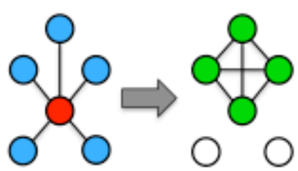


*Evolving mixed-role memberships*



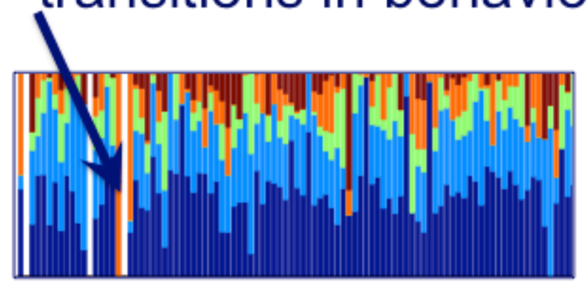

*Role contributions*

2. **Predict** future structural changes



*Transition from star to clique*

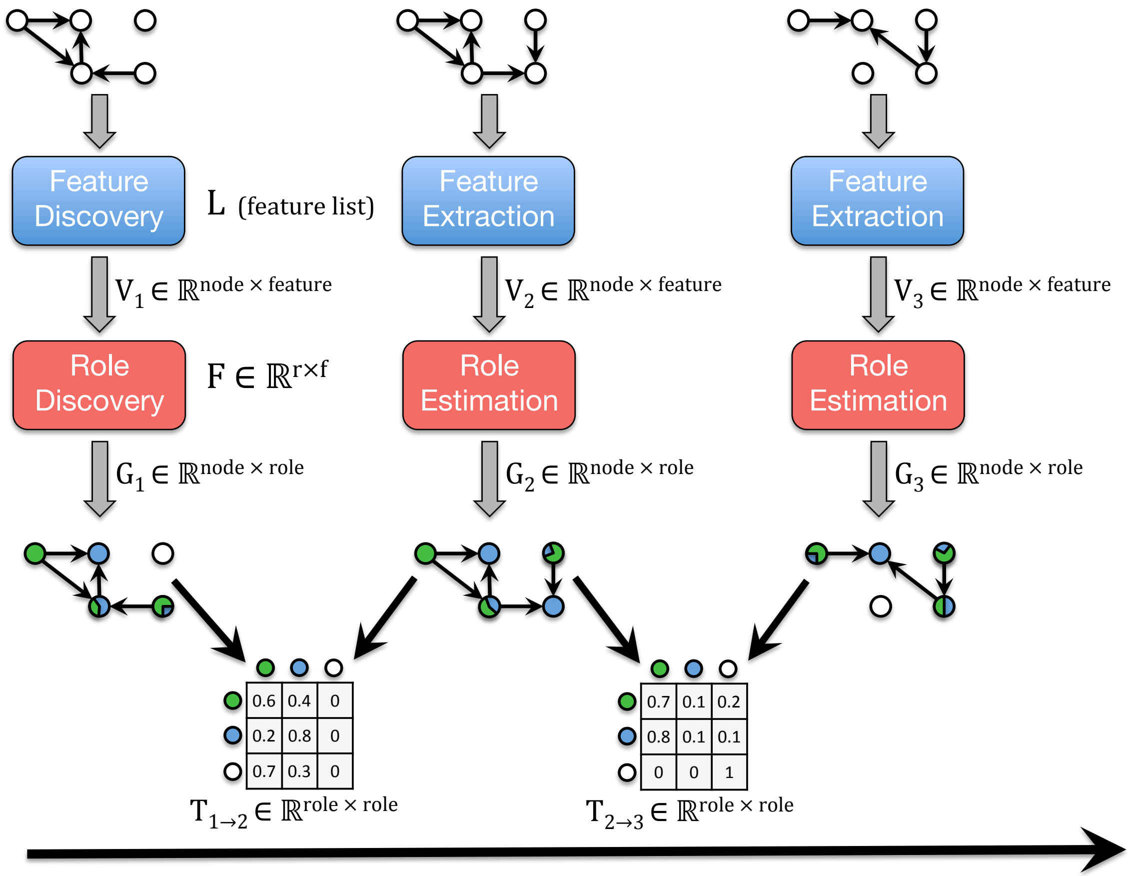
3. **Detect** unusual transitions in behavior



# Dynamic Behavioral Mixed-Membership (DBMM) Model

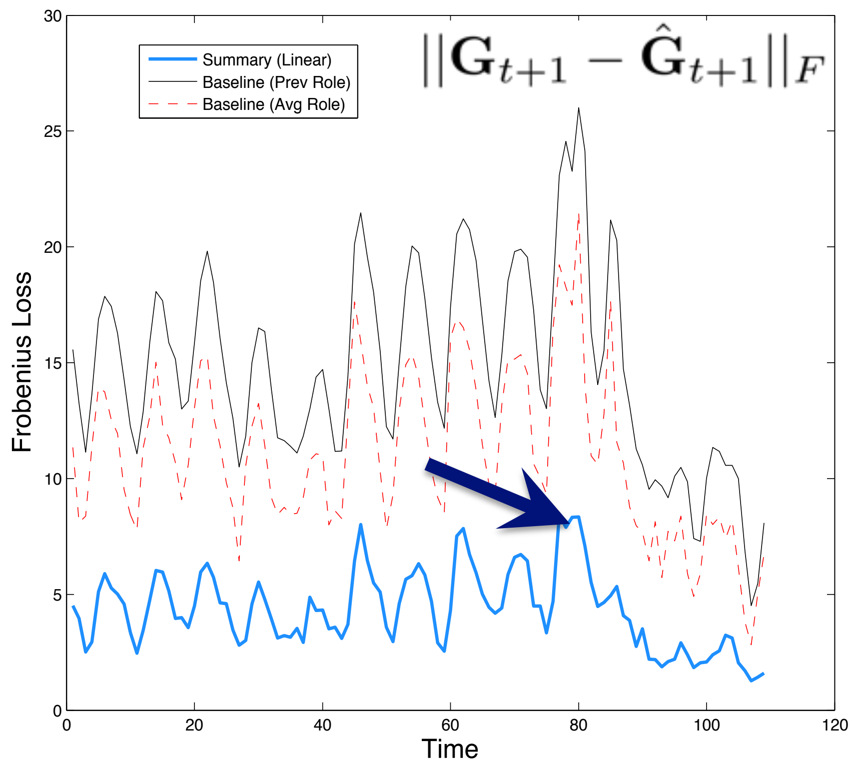
- Scalable for **BIG** graphs
- Easily parallelizable
- Non-parametric & data-driven
- Flexible and interpretable

# 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

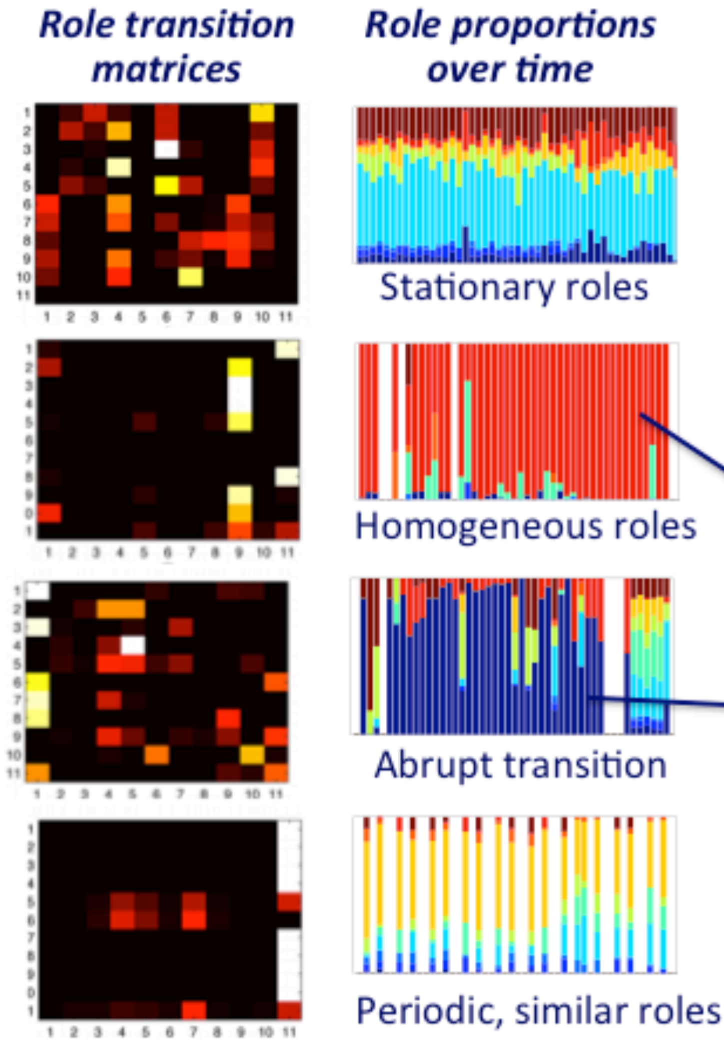
$$\mathbf{G}'_{\mathbf{t+1}} = \mathbf{G_t T}$$

**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

# Dynamic Network Analysis with Roles

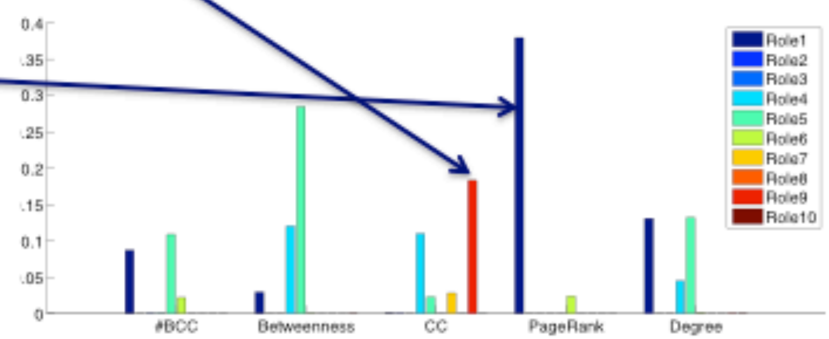



Roles exhibit many of the traditional time-series patterns

Roles are interpretable

Fit role-model to matrix of network statistics:

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

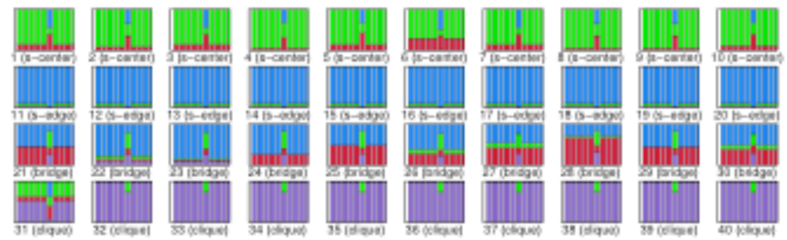


# Anomalous Structural Transitions

**Problem:** detect nodes with unusual structural transitions

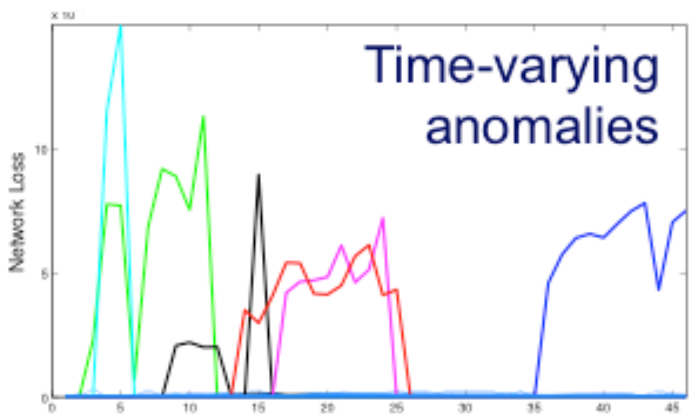
**Anomaly score:**

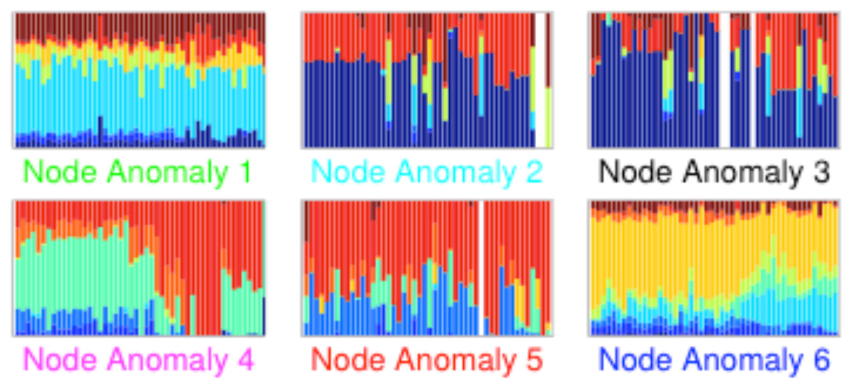
1. Estimate transition model T for *v*
2. Use it to predict *v*'s memberships
3. Take the difference from actual



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

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

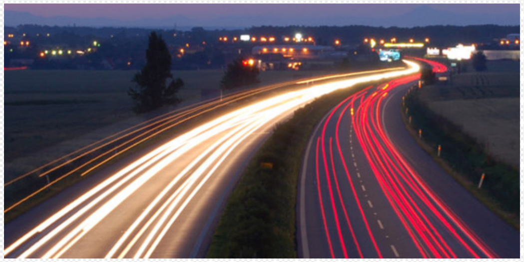


# Roles: Regular Equivalence vs. Role Discovery

| | 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 | ✓ | |

# Roadmap



- What are roles
- Roles and communities
- Roles and equivalences (from sociology)
- Roles (from data mining)
- 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*

# Acknowledgement


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

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

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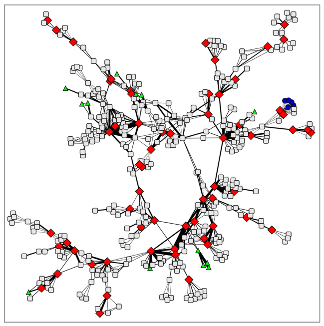
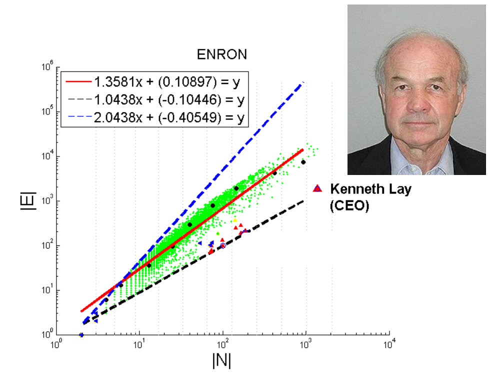
# Back to Overview






Features

Roles

Anomalies

= rare roles

Patterns