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

- Part 1: Between Nodes
  - Roles
  - Proximity
- Part 2: Between Graphs
  - Known node correspondence
  - Unknown node correspondence

Applications:
- Re-identification across Networks
- Cross-network Analytics
- Anomaly Detection in Dynamic Graphs
- Anomaly Detection in Static Graphs
- Classification
- Clustering
- Visualization
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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 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
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- Node Proximity
Roles and Communities are Complementary

Roles (similar structural properties)

Communities (well-connectedness)

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

• 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
  - Regular
  - Automorphic
- Probabilistic
  - Structural
  - Stochastic
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

\[
\sum_i \left( (n_i^1 + n_i^0) \times H(p_i^1) \right) + \sum_i \left( \text{cost of describing } n_i^1, n_i^0 \text{ and groups} \right)
\]

Code Cost

Description Cost

Binary Matrix

\[ p_i^1 = \frac{n_i^1}{n_i^1 + n_i^0} \]

(a) before

(b) after
Deterministic Equivalences

Regular

Automorphic

Structural
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 $\pi$, 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

Automorphic

Structural
Regular Equivalence

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

- Deterministic
  - Regular
  - Automorphic
  - Structural

- Probabilistic
  - Stochastic
Stochastic Equivalence

- 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
  - Parametric vs. non-parametric models
Roadmap

• Node Roles
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  - Roles (from data mining)
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• Node Proximity
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

Input

Node $\times$ Node Matrix → Recursive Feature Extraction → Node $\times$ Feature Matrix

Role Extraction

Output

Node $\times$ Role Matrix $\rightarrow$ Role $\times$ Feature Matrix
RolX: Flowchart

Input:

Node × Node Matrix → Recursive Feature Extraction → Node × Feature Matrix

Role Extraction

Node × Role Matrix → Role × Feature Matrix

Output:

Example: degree, avg weight, # of edges in egonet, mean clustering coefficient of neighbors, etc
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

Input

Recursively extract features

Features

Nodes

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 \( V \approx GF \)

\[ \begin{align*}
\begin{array}{c}
\text{features} \\
\text{nodes}
\end{array}
\approx
\begin{array}{c}
\text{roles} \\
\text{nodes}
\end{array}
\times
\begin{array}{c}
\text{features} \\
\text{roles}
\end{array}
\end{align*} \]

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

\[ \arg\min_{G, F} \| V - GF \|_{fro}, \text{s.t. } G \geq 0, \ F \geq 0 \]
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

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

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

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

Input → Recursively extract features → Features

Automatically factorize roles

Output
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

(1) RolX

(2) Learning

(3) Role Assignment

(4) Inference

Role Definitions

Role Memberships

P(class | role membership)

Target Network

External Network

Classifier

Target Network
## Data for Role Transfer

<table>
<thead>
<tr>
<th></th>
<th>IP-A1</th>
<th>IP-A2</th>
<th>IP-A3</th>
<th>IP-A4</th>
<th>IP-B</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong># Nodes</strong></td>
<td>81,450</td>
<td>57,415</td>
<td>154,103</td>
<td>206,704</td>
<td>181,267</td>
</tr>
<tr>
<td><strong>% labeled</strong></td>
<td>36.7%</td>
<td>28.1%</td>
<td>20.1%</td>
<td>32.9%</td>
<td>15.3%</td>
</tr>
<tr>
<td><strong># Links</strong></td>
<td>968,138</td>
<td>432,797</td>
<td>1,266,341</td>
<td>1,756,082</td>
<td>1,945,215</td>
</tr>
<tr>
<td>(# unique)</td>
<td>206,112</td>
<td>137,822</td>
<td>358,851</td>
<td>465,869</td>
<td>397,925</td>
</tr>
<tr>
<td><strong>Class Distribution</strong></td>
<td><img src="chart1.png" alt="Chart" /></td>
<td><img src="chart2.png" alt="Chart" /></td>
<td><img src="chart3.png" alt="Chart" /></td>
<td><img src="chart4.png" alt="Chart" /></td>
<td><img src="chart5.png" alt="Chart" /></td>
</tr>
</tbody>
</table>

- **Web**
- **DNS**
- **P2P**
Role Transfer Results

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

RolX selects high accuracy model sizes

9 roles automatically discovered by RolX
Classification accuracy is highest when RoI 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

Node Sense: \( GE \approx M \)

- Role 1
- Role 2
- Role 3
- Role 4
- Default
- cliquey
- bridge
- periphery
- isolated
Making Sense of Roles

Roles can be interpreted using topological measures & role homophily

Node Sense: $GE \approx M$

Neighbor Sense: $GQ \approx N$

- cliquey
- bridge
- periphery
- isolated

SDM’14 Tutorial  D. Koutra & T. Eliassi-Rad & C. Faloutsos
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

ReFeX

Recursive Structural Feature Extraction

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

NMF + Model Selection

RoIX

RolX: Structural Role Extraction & Mining in Large Graphs
In KDD 2012.
GLRD

Guided Learning for Role Discovery (GLRD): Framework, Algorithms, and Applications
In KDD 2013

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

RoIX
RoIX: Structural Role Extraction & Mining in Large Graphs
In KDD 2012.
Adding Constraints

Role assignment vector

Soft role assignments for individual user

Role definition / explanation
GLRD Framework

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

\[
\begin{align*}
\text{minimize} & \quad ||V - GF||_2 \\
\text{subject to} & \quad g_i(G) \leq d_{G_i}, \ i = 1, \ldots, t_G \\
& \quad f_i(F) \leq d_{F_i}, \ i = 1, \ldots, t_F \\
\text{where} & \quad g_i \text{ and } f_i \text{ are convex functions.}
\end{align*}
\]

- 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

<table>
<thead>
<tr>
<th>Guidance Type</th>
<th>Effect of increasing guidance</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>on role assignment ($G$)</td>
</tr>
<tr>
<td>Sparsity</td>
<td>Reduces the number of nodes with minority memberships in roles</td>
</tr>
<tr>
<td>Diversity</td>
<td>Limits the amount of allowable overlap in assignments</td>
</tr>
<tr>
<td>Alternative</td>
<td>Decreases the allowable similarity between the two sets of role assignments</td>
</tr>
</tbody>
</table>
### Sparsity

\[
\text{argmin}_{G, F} \quad \|V - GF\|_2 \\
\text{subject to:} \quad G \geq 0, F \geq 0 \\
\forall i \quad \|G_{\cdot i}\|_1 \leq \epsilon_G \\
\forall i \quad \|F_{i \cdot}\|_1 \leq \epsilon_F \\
\text{where} \quad \epsilon_G \text{ and } \epsilon_F \text{ define upper bounds for the sparsity constraints (amount of allowable density).}
\]
Diversity

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

\[
\arg\min_{G,F} \|V - GF\|_2
\]

subject to:

\[G \geq 0, F \geq 0\]

\[\forall i, j \quad G_{i\bullet}^T G_{\bullet j} \leq \epsilon_G \quad i \neq j\]

\[\forall i, j \quad F_{i\bullet} F_{j\bullet}^T \leq \epsilon_F \quad i \neq j\]

where \(\epsilon_G\) and \(\epsilon_F\) 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

### Experiment Details

#### Table 2: Information about DBLP co-authorship networks for each conference

| 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

Recall

<table>
<thead>
<tr>
<th>Target Graph (Overlap)</th>
<th>Percent</th>
</tr>
</thead>
<tbody>
<tr>
<td>cikm</td>
<td>13%</td>
</tr>
<tr>
<td>sdm</td>
<td>33%</td>
</tr>
<tr>
<td>icdm</td>
<td>26%</td>
</tr>
<tr>
<td>sigmod</td>
<td>10%</td>
</tr>
<tr>
<td>vldb</td>
<td>10%</td>
</tr>
</tbody>
</table>

Methods:
- ReFex
- RoI X
- GLRD(Sparse)
- GLRD(Diverse)
Alternative Roles

- Question: Do alternative sets of roles exist in graphs and can they be discovered?
Modeling Dynamic Graphs with Roles

-Introduced by Rossi et al. WSDM 2013

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

   Evolving mixed-role memberships

2. **Predict** future structural changes

   Transition from star to clique

3. **Detect** unusual transitions in behavior

   Role contributions
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

Slide from Rossi et al. WSDM 2013
Predicting Structural Behavior

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

$$f(G_t, G_{t-1}) = \frac{1}{2} \|G_t - G_{t-1} T\|_F^2$$

All models predict $G_{t+1}$ using $G_t$ as $G'_{t+1} = G_t T$

**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.
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

Time-varying anomalies

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:

\[ G_t \mathbf{E}_t \approx \mathbf{M}_t \]
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

<table>
<thead>
<tr>
<th>Name</th>
<th>Party</th>
<th>Exp</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hall, Ralph</td>
<td>R</td>
<td>16</td>
</tr>
<tr>
<td>Rodgers, Cathy</td>
<td>R</td>
<td>2</td>
</tr>
<tr>
<td>Myrick, Sue</td>
<td>R</td>
<td>12</td>
</tr>
<tr>
<td>Issa, Darrell</td>
<td>R</td>
<td>6</td>
</tr>
<tr>
<td>Drake, Thelma</td>
<td>R</td>
<td>2</td>
</tr>
<tr>
<td>Kuhl, Randy</td>
<td>R</td>
<td>2</td>
</tr>
<tr>
<td>Poe, Ted</td>
<td>R</td>
<td>2</td>
</tr>
<tr>
<td>Boozman, John</td>
<td>R</td>
<td>6</td>
</tr>
<tr>
<td>Conaway, Michael</td>
<td>R</td>
<td>2</td>
</tr>
<tr>
<td>Wamp, Zach</td>
<td>R</td>
<td>12</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Name</th>
<th>Party</th>
<th>Exp</th>
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<tbody>
<tr>
<td>Jackson-Lee, Sheila</td>
<td>D</td>
<td>12</td>
</tr>
<tr>
<td>Cohen, Steve</td>
<td>D</td>
<td>0</td>
</tr>
<tr>
<td>Hare, Phil</td>
<td>D</td>
<td>0</td>
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<tr>
<td>Grijalva, Raul</td>
<td>D</td>
<td>4</td>
</tr>
<tr>
<td>English, Phil</td>
<td>R</td>
<td>12</td>
</tr>
<tr>
<td>Honda, Michael</td>
<td>D</td>
<td>6</td>
</tr>
<tr>
<td>Mc Cotter, Thaddeus</td>
<td>R</td>
<td>4</td>
</tr>
<tr>
<td>Filner, Bob</td>
<td>D</td>
<td>14</td>
</tr>
<tr>
<td>Hinchey, Maurice</td>
<td>D</td>
<td>14</td>
</tr>
<tr>
<td>Gonzalez, Charles</td>
<td>D</td>
<td>8</td>
</tr>
</tbody>
</table>

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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
[Chen et al. CIKM’12]

RoleLearn on Yahoo! IM
[Long T. Le, TER, Hanghang Tong. under review]
$\lambda_1 - \lambda_2$ is Small (Especially in Social Graphs)

Our new problem formulation:
Learn to predict which edges to cut.
Yahoo! IM
(% Drop in $\lambda$ 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

<table>
<thead>
<tr>
<th></th>
<th>Role Discovery</th>
<th>Regular Equivalence</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mixed-membership over roles</td>
<td>✓</td>
<td></td>
</tr>
<tr>
<td>Automatically selects the best model</td>
<td>✓</td>
<td></td>
</tr>
<tr>
<td>Can incorporate arbitrary features</td>
<td>✓</td>
<td></td>
</tr>
<tr>
<td>Uses structural features</td>
<td>✓</td>
<td></td>
</tr>
<tr>
<td>Uses structure</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>Generalizes across disjoint networks</td>
<td>✓</td>
<td>?</td>
</tr>
<tr>
<td>(longitudinal &amp; cross-sectional)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Scalable (linear on # of edges)</td>
<td>✓</td>
<td></td>
</tr>
<tr>
<td>Guidance</td>
<td>✓</td>
<td></td>
</tr>
</tbody>
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Acknowledgement

- LLNL: Brian Gallagher, Keith Henderson
- CCNY: Hanghang Tong
- Google: Sugato Basu
- SUNY Stony Brook: Leman Akoglu
- 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

References

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