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Large Graph Mining: Patterns, Tools and Case Studies

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CMU

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Outline

- Part 1: Patterns
- Part 2: Matrix and Tensor Tools
- ➡ Part 3: Proximity
- Part 4: Case Studies

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Part 3: Proximity on Graphs

-Definitions, Fast Solutions, and Applications

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Joint work with

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Huiming Qu

Hani Jamjoom

IBM

Tina Eliassi-Rad (LLNL)

Brian Gallagher (LLNL)

Kensuke Oonuma (Sony Corp.)

Yasushi Sakurai (NTT Labs)

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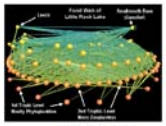
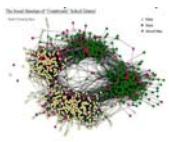
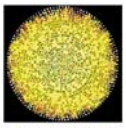
Recap: Graphs are everywhere!

Internet Map [lumeta.com]


Food Web [Martinez '91]


Friendship Network [Moody '01]


Protein Interactions [genomebiology.com]

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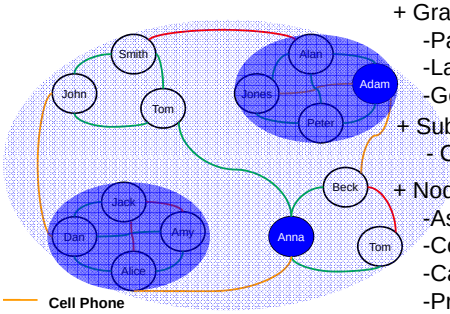
Graph Mining: Big Picture



+ Graph Level
  -Patterns
  -Laws
  -Generators
+ Subgraph Level
  - Community
+ Node Level
  -Association
  -Correlation
  -Causality
  -Proximity

We are here!

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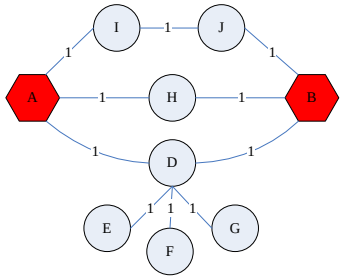
Proximity on Graph: What?



a.k.a Relevance, Closeness, 'Similarity'…

3-7

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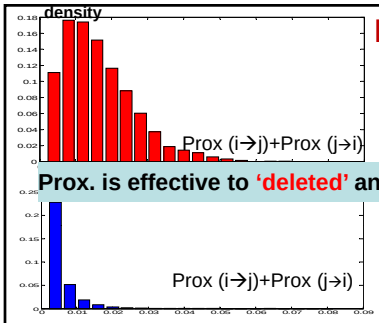
Proximity on Graphs: Why?

- Link prediction [Liben-Nowell+], [Tong+]
- Ranking [Haveliwala], [Chakrabarti+]
- Email Management [Minkov+]
- Image caption [Pan+]
- Neighborhooh Formulation [Sun+]
- Conn. subgraph [Faloutsos+], [Tong+], [Koren+]
- Pattern match [Tong+]
- Collaborative Filtering [Fouss+]
- Many more…

Will return to this later

 Copyright: Faloutsos, Tong (2008)

Link Prediction



Prox. Hist. for a set of deleted links

Prox. is effective to 'deleted' and absent edges!

Prox. Hist. for a set of absent links

Q: How to predict the existence of the link?

A: Proximity! [Liben-Nowell + 2003]

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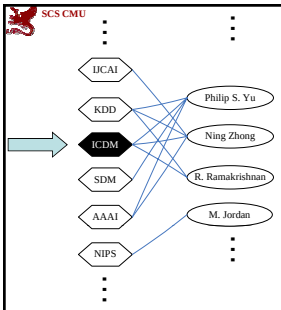
Neighborhood Search on graphs



Conference Author

Q: what is most related conference to ICDM?

A: Proximity! [Sun+ ICDM2005]

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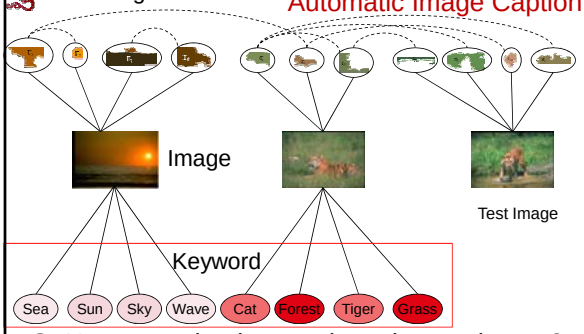
Automatic Image Caption



Q: How to assign keywords to the test image?

A: Proximity! [Pan+ 2004]

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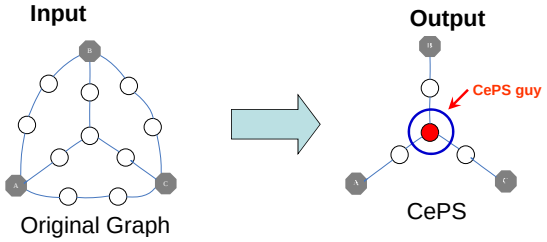
Center-Piece Subgraph(CePS)



Q: How to find hub for the black nodes?

A: Proximity! [Tong+ KDD 2006]

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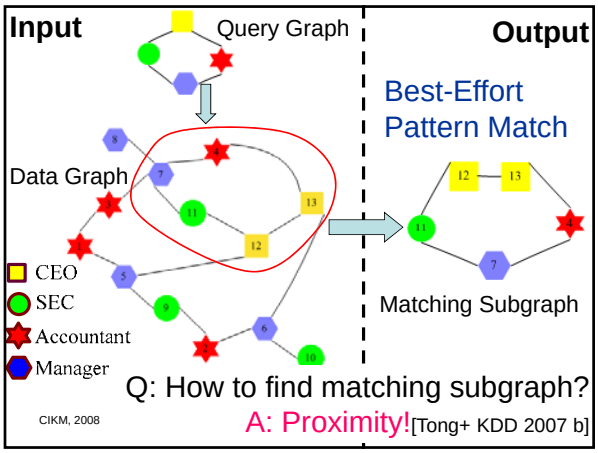

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Outline: Part 3

- Motivation
- Definitions
- Fast Solutions
- Applications
- Conclusion

- Basic: RWR
- Variants
- Properties
- Generalizations

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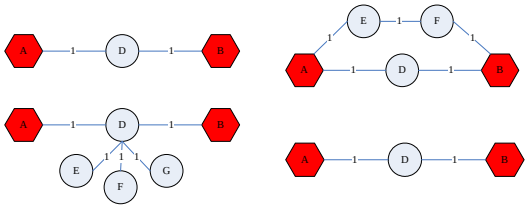
Some ``bad'' proximities

Why not shortest path?



'pizza delivery guy' problem

'multi-facet' relationship

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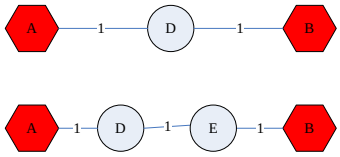
Some ``bad'' proximities

Why not max. netflow?



No punishment on long paths

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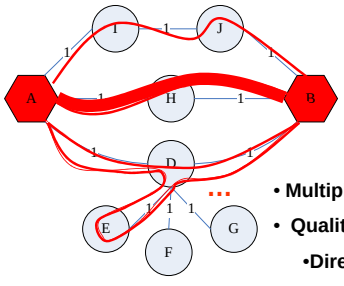
What is a ``good'' Proximity?



- **Multiple Connections**
- **Quality of connection**
  - **Direct & In-directed Conns**
  - **Length, Degree, Weight…**

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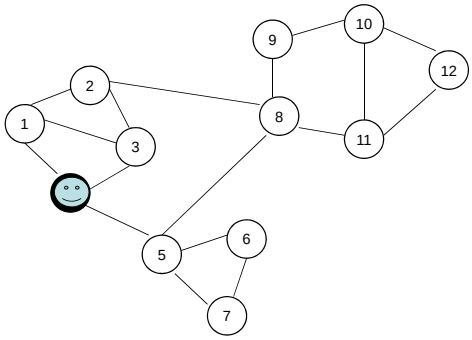
Random walk with restart



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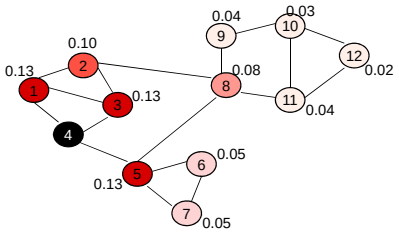
Random walk with restart



	Node 4
Node 1	0.13
Node 2	0.10
Node 3	0.13
Node 4	0.22
Node 5	0.13
Node 6	0.05
Node 7	0.05
Node 8	0.08
Node 9	0.04
Node 10	0.03
Node 11	0.04
Node 12	0.02

Nearby nodes, higher scores
More red, more relevant

Ranking vector $\vec{r}_4$

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Why RWR is a good score?

$$Q = (I - c\tilde{W})^{-1} = \; Q(i,j) \propto r_{i,j}$$

$\tilde{W}$: adjacency matrix.
c: damping factor

$$Q = c\,\tilde{W} + c^2\,\tilde{W}^2 + c^3\,\tilde{W}^3 + \cdots$$

all paths from i to j with length 1 | all paths from i to j with length 2 | all paths from i to j with length 3

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→ Variants

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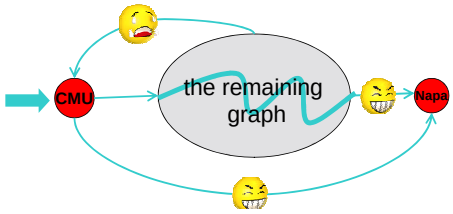
Variant: escape probability

- Define Random Walk (RW) on the graph
- Esc_Prob(CMU→Napa)
  - Prob (starting at CMU, reaches Napa before returning to CMU)



Esc_Prob = Pr (smile before cry)

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Other Variants

- Other measure by RWs
  - Community Time/Hitting Time [Fouss+]
  - SimRank [Jeh+]
  - **All are "related to" or "similar to" random walk with restart!**
  - String Systems
- Katz [Katz], [Huang+], [Scholkopf+]
- Matrix-Forest-based Alg [Chobotarev+]

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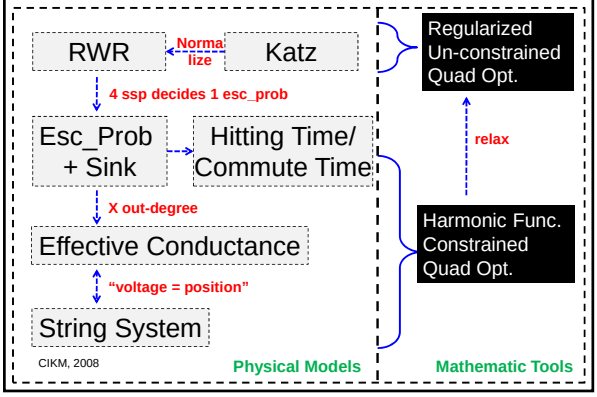
Chaptering different measurements



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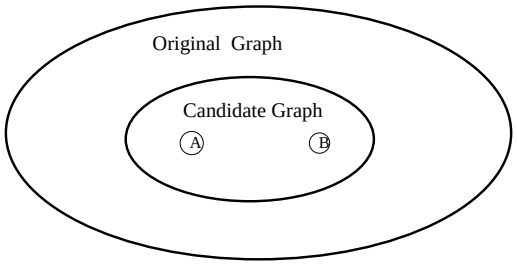
Property: Monotonicity



We want: $\text{Prox}^{candi}(a \to b) \leq \text{Prox}^{origianl}(a \to b)$

A: degree preserving! [Koren+ KDD06][Tong+ KDD07a][Tong+ SDM08]

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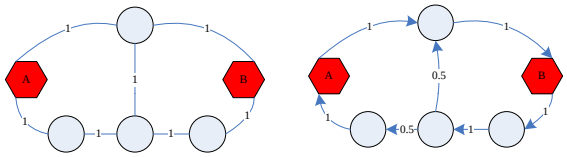
Property: Asymmetry [Tong+ KDD07 a]



What is Prox between A and B?

What is Prox from A to B?
What is Prox from B to A?

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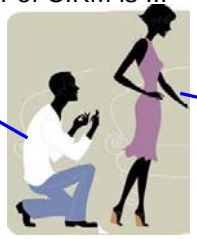
Asymmetry in un-directed graphs

- Hanghang's # 1 Conf. is CIKM
- The #1 author of CIKM is ...

Hanghang



CIKM

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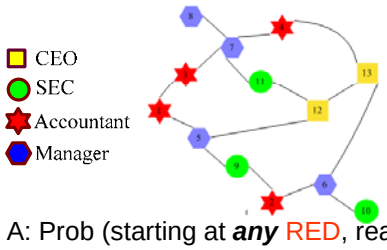
Group Proximity [Tong+ KDD07 a]

- Q: *How close are Accountants to SECs?*



- A: Prob (starting at ***any*** RED, reaches ***any*** GREEN before touching ***any*** RED again)

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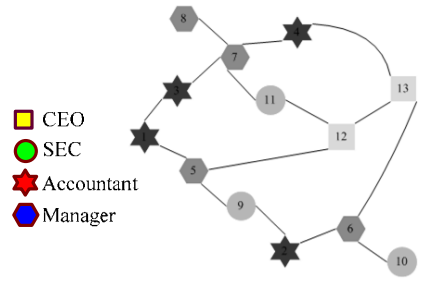
Proximity on Attributed Graphs [Tong+ KDD07 b]



What is the proximity from node 7 to 10?

If we know that…

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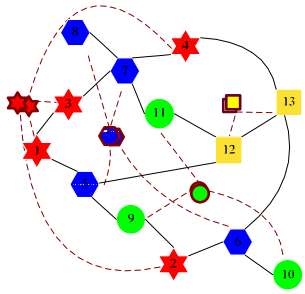
A: Augmented graphs [Tong+ KDD07 b]



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More on Generalizations

- Attributed on edges [Chakrabarti+ KDD 06]
- Proximity w/ Time
  - [Minkov+], [Tong+ SDM 2008], [Tong+ CIKM 2008]
- Proximity w/ Side Information [Tong+ 2008]
- …

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Summary of Proximity Definitions

- Goal: Summarize multiple … relationship
- Solutions
  - Basic: Random Walk with Restart
    - [Pan+ 2004][Sun+ 2006][Tong+ 2006]
  - Properties: Asymmetry, monotonicity
    - [Koren+ 2006][Tong+ 2007] [Tong+ 2008]
  - Variants: Esc_Prob and many others.
    - [Faloutsos+ 2004] [Koren+ 2006][Tong+ 2007]
  - Generalizations: Group Prox, w/ Attr., w/ Time, w/ Side Information
    - [Charkrabarti+ 2006][Tong+ 2007] [Tong+ 2008]

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Outline: Part 3

- Motivation
- Definitions
- Fast Solutions
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Outline: Part 3

- Motivation
- Definitions
- Fast Solutions
  - B_Lin: RWR
  - BB_Lin: Skewed BGs
  - FastUpdate: Time-Evolving
- Applications
- Conclusion

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Preliminary: Sherman–Morrison Lemma

If:

$$\tilde{A} = A + u \times v^T$$

Then:

$$\tilde{A}^{-1} = (A + u \cdot v^T)^{-1} = A^{-1} - \frac{A^{-1} \cdot u \cdot v^T A^{-1}}{1 + v^T \cdot A^{-1} \cdot u}$$

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SM: The block-form

A	B
C	D

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix}^{-1} = \begin{bmatrix} A^{-1} + A^{-1}B(D-CA^{-1}B)^{-1}CA^{-1} & -A^{-1}B(D-CA^{-1}B)^{-1} \\ -(D-CA^{-1}B)^{-1}CA^{-1} & (D-CA^{-1}B)^{-1} \end{bmatrix}$$

Or…

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix}^{-1} = \begin{bmatrix} (A-BD^{-1}C)^{-1} & -A^{-1}B(D-CA^{-1}B)^{-1} \\ -D^{-1}C(A-BD^{-1}C)^{-1} & (D-CA^{-1}B)^{-1} \end{bmatrix}$$

And many other variants…
Also known as Woodburg Identity

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SM Lemma: Applications

- RLS (Recursive least square)
  - and almost any algorithm in time series!
- Leave-one-out cross validation for LSR
- Kalman filtering
- Incremental matrix decomposition
- …
- … and all the fast sol.s we will introduce!

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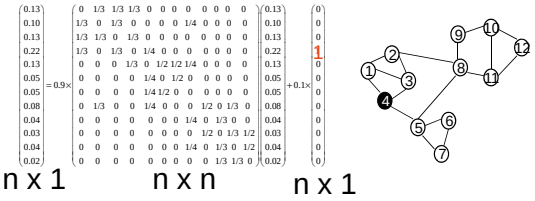
Computing RWR

$$\vec{r}_i = c\tilde{W}\vec{r}_i + (1-c)\vec{e}_i$$

Ranking vector — Adjacency matrix — Restart p — Starting vector



n x 1 n x n n x 1

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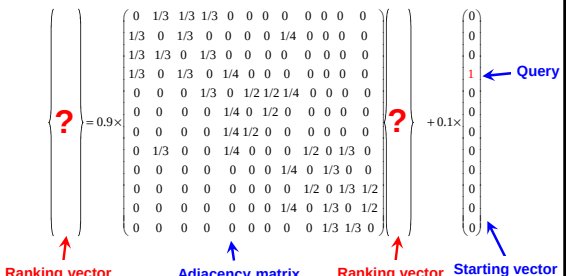
Q: Given query *i*, how to solve it?



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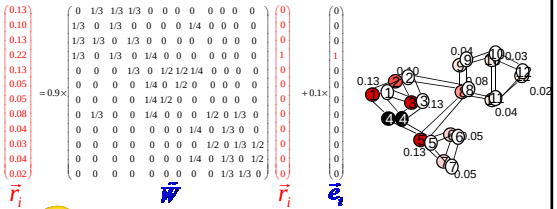
OntheFly: $\vec{r}_i[t+1] = c\tilde{W}\vec{r}_i[t] + (1-c)\vec{e}_i$



No pre-computation/ light storage

Slow on-line response O(mE)

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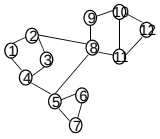
PreCompute

R:

	r_1	r_2	r_3	r_4	r_5	r_6	r_7	r_8	r_9	r_{10}	r_{11}	r_{12}
	0.20	0.13	0.14	0.13	0.68	0.56	0.56	0.63	0.44	0.35	0.39	0.34
	0.28	0.20	0.13	0.96	0.64	0.53	0.53	0.85	0.60	0.48	0.53	0.45
	0.14	0.13	0.20	1.29	0.68	0.56	0.56	0.63	0.44	0.35	0.39	0.33
	0.13	0.10	0.13	2.06	0.95	0.78	0.78	0.61	0.43	0.34	0.38	0.32
	0.09	0.09	0.09	1.27	2.41	1.97	1.97	1.05	0.73	0.58	0.66	0.56
	0.03	0.04	0.04	0.52	0.98	2.06	1.37	0.43	0.30	0.24	0.27	0.22
	0.03	0.04	0.04	0.52	0.98	1.37	2.06	0.43	0.30	0.24	0.27	0.22
	0.08	0.11	0.04	0.82	1.05	0.86	0.86	2.13	1.49	1.19	1.33	1.13
	0.03	0.04	0.03	0.28	0.36	0.30	0.30	0.74	1.78	1.00	0.76	0.79
	0.04	0.04	0.04	0.34	0.44	0.36	0.36	0.89	1.50	2.45	1.54	1.80
	0.04	0.05	0.04	0.38	0.49	0.40	0.40	1.00	1.14	1.54	2.28	1.72
	0.02	0.03	0.02	0.21	0.28	0.22	0.22	0.56	0.79	1.20	1.14	2.05



$R = c \times Q$

$Q = (I - c\tilde{W})^{-1}$ [Haveliwala+ 2002]

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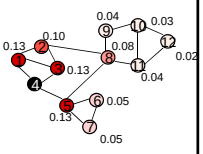
PreCompute: $Q = (I - c\tilde{W})^{-1}$

$Q = (I - c\tilde{W})^{-1}$

2.20	1.28	1.43	1.29	0.68	0.56	0.56	0.63	0.44	0.35	0.39	0.34
1.28	2.02	1.28	0.96	0.64	0.53	0.53	0.85	0.60	0.48	0.53	0.45
1.43	1.28	2.20	1.29	0.68	0.56	0.56	0.63	0.44	0.35	0.39	0.33
1.29	0.96	1.29	2.06	0.95	0.78	0.78	0.61	0.43	0.34	0.38	0.32
0.91	0.86	0.91	1.27	2.41	1.97	1.97	1.05	0.73	0.58	0.66	0.56
0.37	0.35	0.37	0.52	0.98	2.06	1.37	0.43	0.30	0.24	0.27	0.22
0.37	0.35	0.37	0.52	0.98	1.37	2.06	0.43	0.30	0.24	0.27	0.22
0.84	1.14	0.84	0.82	1.05	0.86	0.86	2.13	1.49	1.19	1.33	1.13
0.29	0.40	0.29	0.28	0.36	0.30	0.30	0.74	1.78	1.00	0.76	0.79
0.35	0.48	0.35	0.34	0.44	0.36	0.36	0.89	1.50	2.45	1.54	1.80
0.39	0.53	0.39	0.38	0.49	0.40	0.40	1.00	1.14	1.54	2.28	1.72
0.22	0.30	0.22	0.21	0.28	0.22	0.22	0.56	0.79	1.20	1.14	2.05



Fast on-line response

Heavy pre-computation/storage cost

$O(n^3)$ $O(n^2)$

SCS CMU

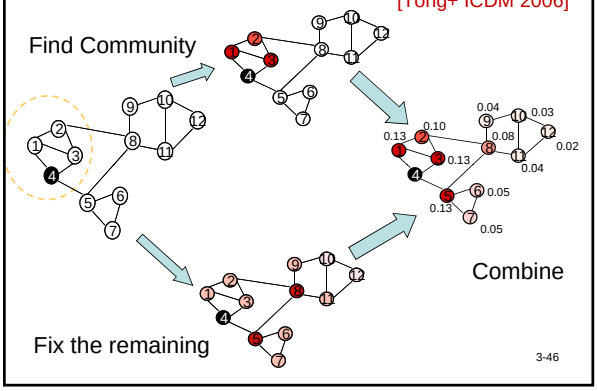
Q: How to Balance?

 Copyright: Faloutsos, Tong (2008)

SCS CMU

B_Lin: Basic Idea

[Tong+ ICDM 2006]



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B_Lin: details

details

$\tilde{W} \simeq$ + U S V

$\tilde{W}_1$: within community

Cross-community

 Copyright: Faloutsos, Tong (2008)

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B_Lin: details

details

$$\left(I - c\tilde{W}\right)^{-1} \approx \left[I - c\tilde{W}_1 - U\,S\,V\right]^{-1}$$

Easy to be inverted

LRA difference

SM Lemma!

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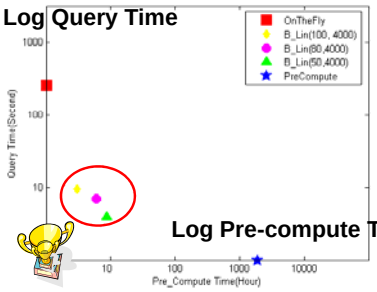
B_Lin: summary

- Pre-Computational Stage
  - Q: Efficiently compute and store Q
  - A: A few small, instead of ONE BIG, matrices inversions
- On-Line Stage
  - Q: Efficiently recover one column of Q
  - A: A few, instead of MANY, matrix-vector multiplications

SCS CMU

Query Time vs. Pre-Compute Time



- **Quality: 90%+**
- **On-line:**
  - **Up to 150x speedup**
- **Pre-computation:**
  - **Two orders saving**

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Outline: Part 3

- Motivation
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- Conclusion

- B_Lin: RWR
- BB_Lin: Skewed BGs
- FastUpdate: Time-Evolving

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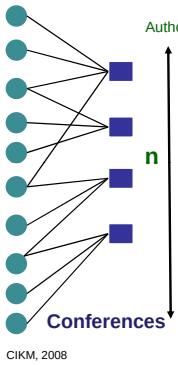
authors RWR on Bipartite Graph



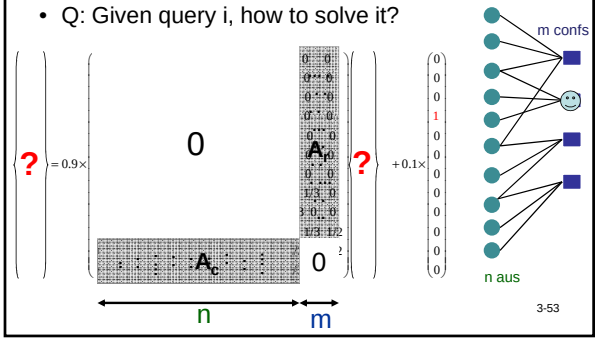
Observation: n >> m!

Examples:
1. DBLP: 400k aus, 3.5k confs
2. NetFlix: 2.7M usrs,18k mvs

SCS CMU

RWR on Skewed bipartite graphs

- Q: Given query i, how to solve it?



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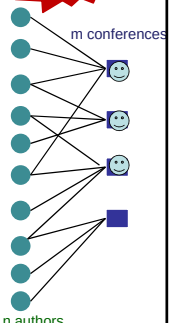
BB_Lin: Pre-Computation

2-step RWR for Conferences

[Tong+ ICDM 06]

details

- Step 1: $M = A_c \times A_r$



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BB_Lin: Pre-Computation [Tong+ ICDM 06]

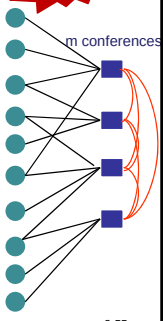
2-step RWR for Conferences

details

- Step 1: M = A_c x A_r

All Conf-Conf Prox. Scores

- Step 2: $\Lambda = (I - 0.9 \times M)^{-1}$



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BB_Lin: Pre-Computation [Tong+ ICDM 06]

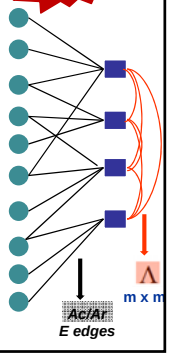
2-step RWR for Conferences

details

- Step 1: M = A_c x A_r

All Conf-Conf Prox. Scores

- Step 2: $\Lambda = (I - 0.9 \times M)^{-1}$
- Cost: $O(m^3 + m \cdot E)$
- Examples
  - NetFlix: 1.5hr for pre-computation;
  - DBLP: 1 few minutes



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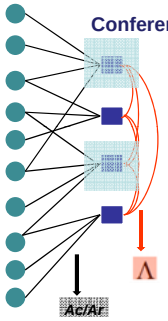
BB_Lin: On-Line Stage

authors

Conferences

(Base) Case 1:
- Conf - Conf

Read out !



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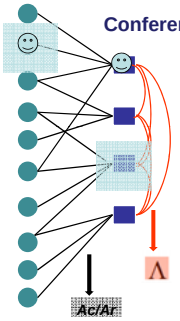
BB_Lin: On-Line Stage

authors

Conferences

Case 2:
- Au - Conf

1 matrix-vec!



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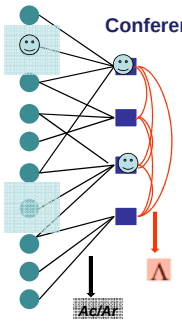
BB_Lin: On-Line Stage

authors

Conferences

Case 3:
- Au - Au

2 matrix-vec!



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BB_Lin: Examples

Dataset	Off-Line Cost	On-Line Cost
DBLP	a few minutes	frac. of sec.
NetFlix	1.5 hours	<0.01 sec.

400k authors x 3.5k conf.s

2.7m user x 18k movies

 Copyright: Faloutsos, Tong (2008)

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Outline: Part 3

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  - B_Lin: RWR
  - BB_Lin: Skewed BGs
  - FastUpdate: Time-Evolving
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Challenges

- BB_Lin is good for skewed bipartite graphs
  - for NetFlix (2.7M nodes and 100M edges)
  - **On-line cost** for query: fraction of seconds
    - w/ 1.5 hr pre-computation for m x m core matrix
- But…what if the graph is ***evolving*** over time
  - New edges/nodes arrive; edge weights increase…
  - **On-line cost:** 1.5hr itself becomes a part of this!

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Q: How to update the core matrix?

t=0 $\Lambda = (I - 0.9 \times M)^{-1}$ $O(m^3 + m \cdot E)$

t=1 $\tilde{\Lambda} = (I - 0.9 \times \tilde{M})^{-1}$ $O(m^3 + m \cdot E)$?

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details

Update the core matrix Λ

- Step 1:

$\tilde{M}$ = A_c x A_r = M + x

Rank 2 update

- Step 2:

$\tilde{\Lambda} = (I - 0.9 \times \tilde{M})^{-1}$

= Λ + x

$O(m^2)$ $O(m^3 + m \cdot E)$

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details

Update Λ: General Case

$\tilde{M}$ = A_c x A_r

n authors

m Conferences

- E' edges changed
- Involves n' authors, m' confs.

SCS CMU

details

Update Λ: General Case

- Observation: $\min(n', m') \ll E'$
  - the rank of update is small!
  - Real Example (DBLP Post)
    - 1258 time steps
    - E' up to ~20,000!
    - $\min(n', m')$ <=132
- Our Algorithm

$O(\min(n', m')m^2 + E')$

$O(m^3 + m \cdot E)$

n authors

m Conferences

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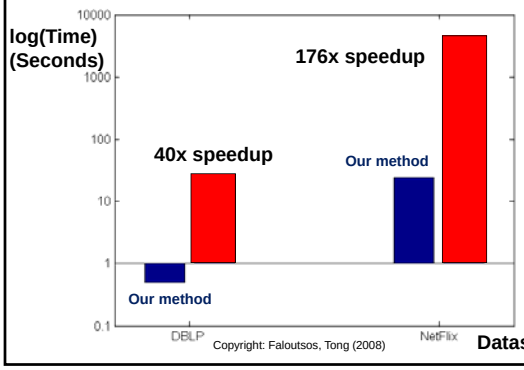
Fast-Single-Update



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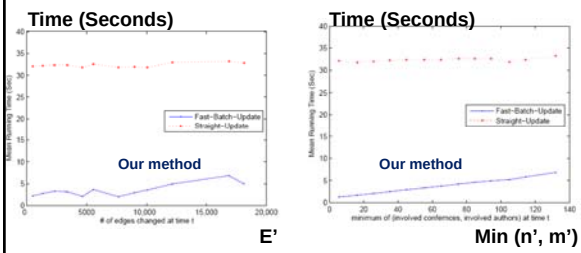
Fast-Batch-Update



15x speed-up on average!

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More on "Fast Solutions"

- FastAllDAP
  - Simultaneously solve multiple linear systems
  - [Tong+ KDD 2007 a]
- MT3
  - Multiple-Resolution Analysis on Time [Tong+ CIKM 2008]
- Fast-ProSIN
  - On-Line response for users' feedback [Tong+ ICDM 2008]

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Summary of Fast Solutions

- Goal: Efficiently Solve Linear System(s)
- Sols.
  - B_Lin: one large linear system [Tong+ ICDM06]
  - BB_Lin: the intrinsic complexity is small [Tong+ ICDM06]
  - FastUpdate: dynamic linear system [Tong+ SDM08]
  - FastAllDAP: multiple linear systems [Tong+ KDD07 a]
  - MT3: [Tong+ CIKM 2008]
  - Fast-ProSIN: [Tong+ 2008]

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Outline: Part 3

- Motivation
- Definitions
- Fast Solutions
- Applications
- Conclusion

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Outline: Part 3

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→ Link Prediction & +
- Ranking Related Tasks
- User Specific Patterns
- Time Related Tasks

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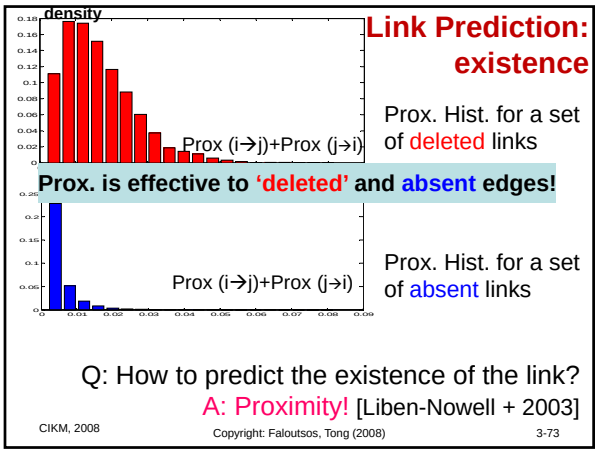

Link Prediction: existence

Prox. Hist. for a set of deleted links

Prox. is effective to 'deleted' and absent edges!

Prox. Hist. for a set of absent links

Q: How to predict the existence of the link?

A: Proximity! [Liben-Nowell + 2003]

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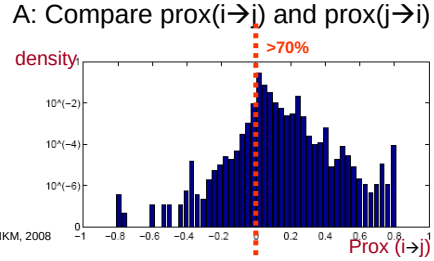
Link Prediction: direction [Tong+ KDD 07 a]

- Q: Given the existence of the link, what is the direction of the link?
- A: Compare prox(i→j) and prox(j→i)



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Beyond Link Prediction

- Collaborative Filtering [Fouss+]
- Name Disambiguation
  - [Minkov+ SIGIR 06]
- Anomaly Nodes/Edges
  - 'a' is abnormal if the neighborhood of 'a' is so different
  - [Sun+ ICDM 2005]

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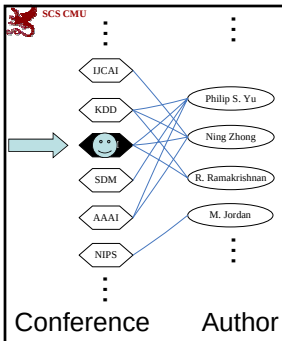
Neighborhood Search on graphs



Conference Author

Q: what is most related conference to ICDM?

A: Proximity! [Sun+ ICDM2005]

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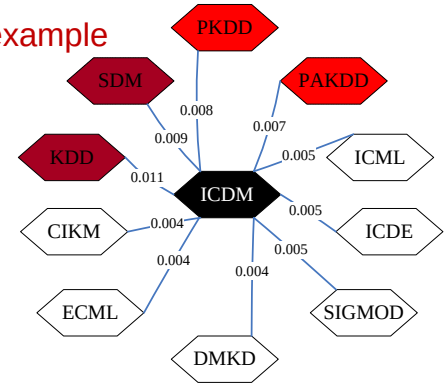
NF: example



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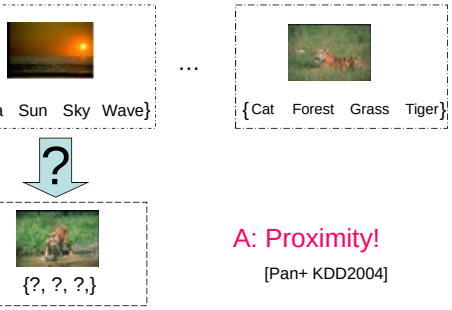
gCaP: Automatic Image Caption

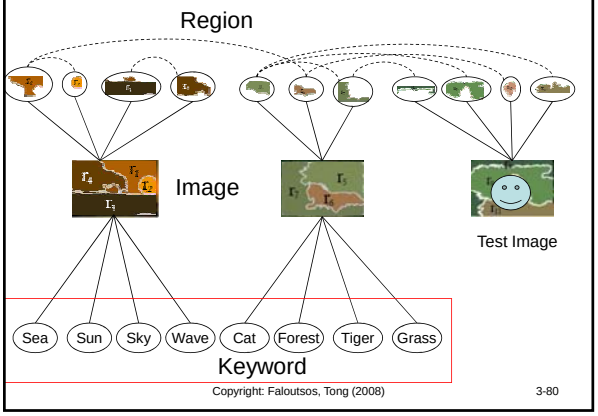
- Q



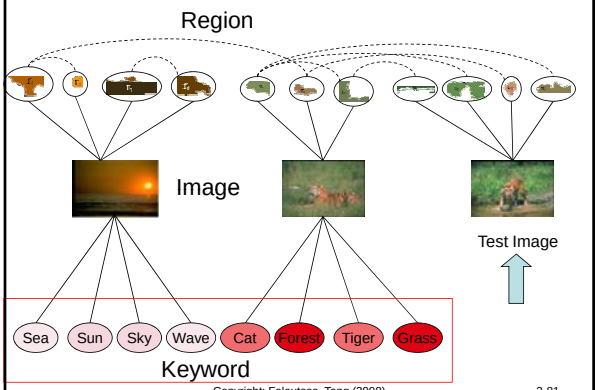
A: Proximity!

[Pan+ KDD2004]

SCS CMU

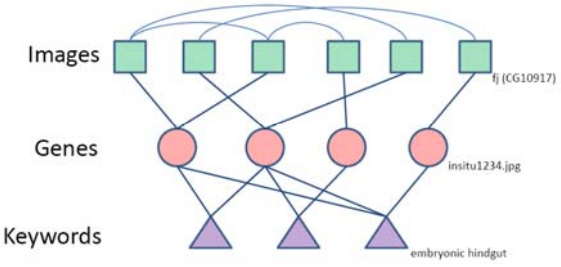


SCS CMU

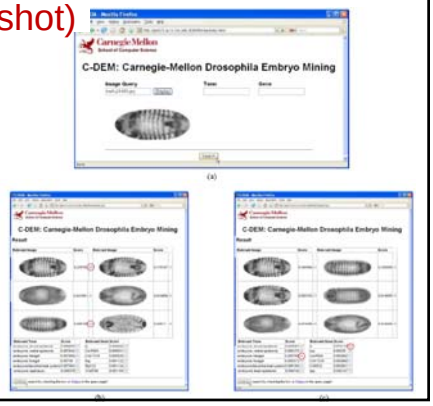


SCS CMU

C-DEM: Multi-Modal Query System for Drosophila Embryo Databases [Fan+ VLDB 2008]



C-DEM (Screen-shot)



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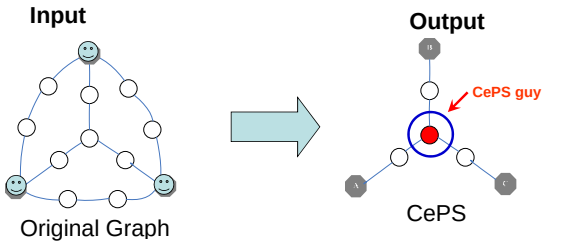
SCS CMU

Center-Piece Subgraph(CePS)



Q: How to find hub for the black nodes?

A: Proximity! [Tong+ KDD 2006]

Red: **Max** (Prox(A, Red) x Prox(B, Red) x Prox(C, Red))

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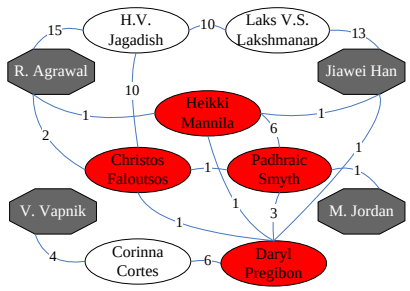
CePS: Example



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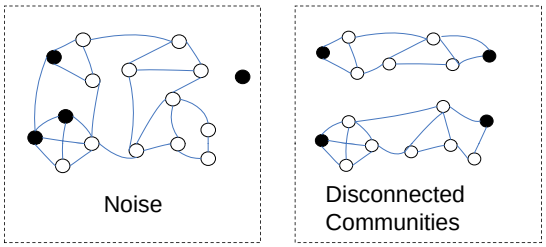
K_SoftAnd: Relaxation of AND



Asking AND query? ➔ No Answer!

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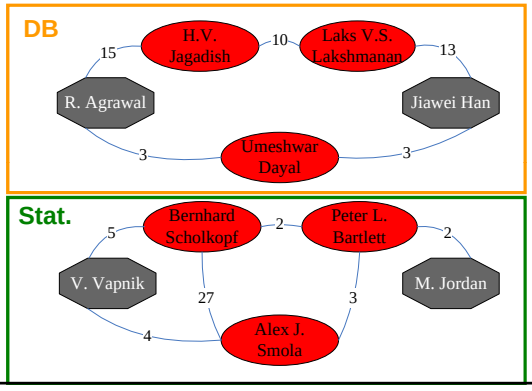
CePS: 2 SoftAND



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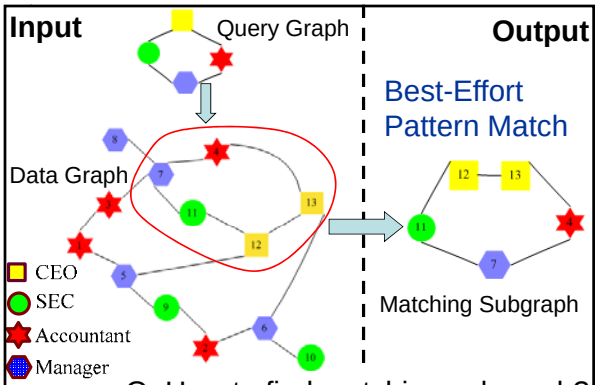
Input / Output



Q: How to find matching subgraph?

A: Proximity! [Tong+ KDD 2007 b]

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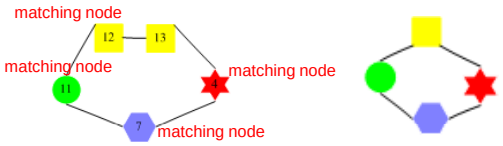
G-Ray: How to?

details



Goodness = Prox (12, 4) x Prox (4, 12) x
Prox (7, 4) x Prox (4, 7) x
Prox (11, 7) x Prox (7, 11) x
Prox (12, 11) x Prox (11, 12)

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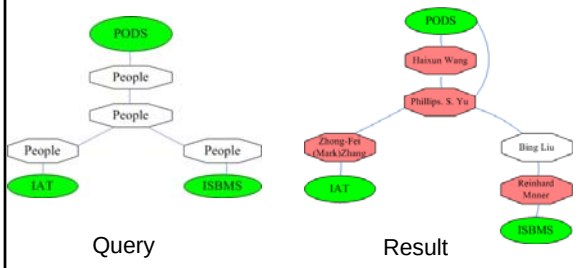
Effectiveness: star-query



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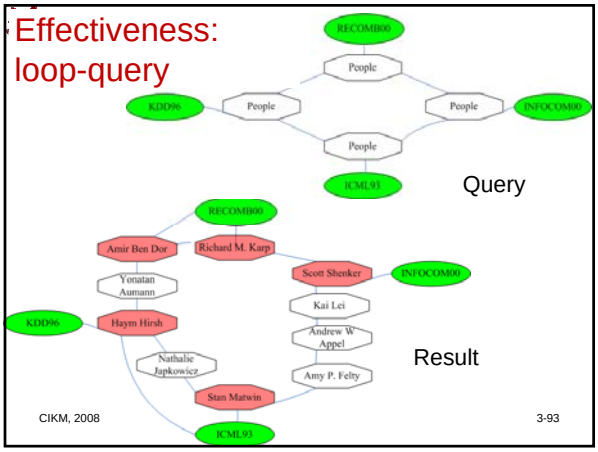
Effectiveness: line-query

Effectiveness: loop-query



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Challenge

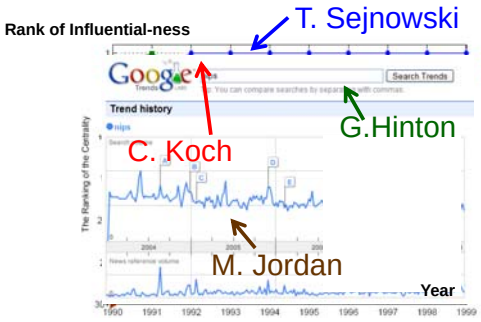
- Graphs are evolving over time!
  - –New nodes/edges show up;
  - –Existing nodes/edges die out;
  - –Edge weights change…

Q: How to generalize everything?

A: Track Proximity! [Tong+ SDM 2008]

SCS CMU

pTrack/cTrack: Trend analysis on graph level



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pTrack: Problem Definition

- **[Given]**
  - (1) a large, skewed time-evolving bipartite graphs,
  - (2) the query nodes of interest
- **[Track]**
  - (1) top-k most related nodes for each query node at each time step t;
  - (2) the proximity score (or rank of proximity) between any two query nodes at each time step t

SCS CMU

pTrack: Philip S. Yu's Top-5 conferences up to each year

ICDE ICDCS SIGMETRICS PDIS VLDB	CIKM ICDCS ICDE SIGMETRICS ICMCS	KDD SIGMOD ICDM CIKM ICDCS	ICDM KDD ICDE SDM VLDB
1992	1997	2002	2007

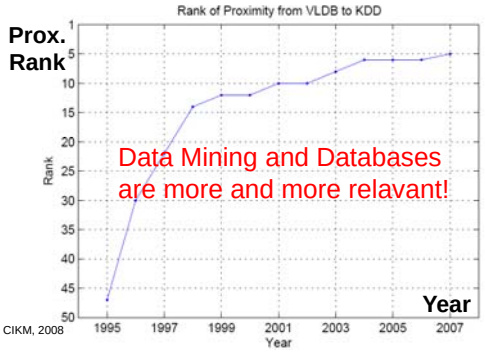
Databases
Performance
Distributed Sys.

DBLP: (Au. x Conf.)
- 400k aus,
- 3.5k confs
- 20 yrs

Databases
Data Mining

SCS CMU

KDD's Rank wrt. VLDB over years



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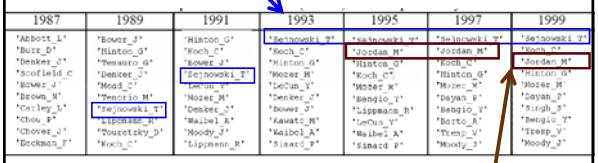
cTrack:10 most influential authors in NIPS community up to each year

T. Sejnowski



M. Jordan

Author-paper bipartite graph from NIPS 1987-1999.
3k. 1740 papers, 2037 authors,
spreading over 13 years

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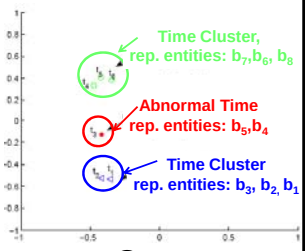
T3: Understand Time in Complex Context

[Tong+ CIKM 2008]

Time	Event	Entity
t_1	e_1	b_1, b_2
	e_2	b_2, b_3
t_2	e_3	b_2, b_3
	e_4	b_3, b_4
t_3	e_5	b_4, b_5
t_4	e_6	b_5, b_6
	e_7	b_6, b_7
t_5	e_8	b_6, b_7
t_6	e_9	b_7, b_8

Input



Output

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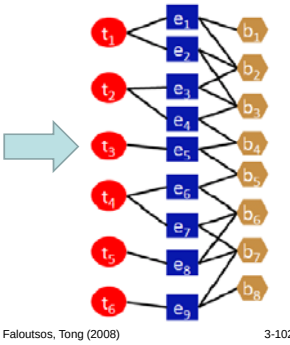
T3: Time-to-Time Proximity Matrix

Time	Event	Entity
t_1	e_1	b_1, b_2
	e_2	b_2, b_3
t_2	e_3	b_2, b_3
	e_4	b_3, b_4
t_3	e_5	b_4, b_5
t_4	e_6	b_5, b_6
	e_7	b_6, b_7
t_5	e_8	b_6, b_7
t_6	e_9	b_7, b_8



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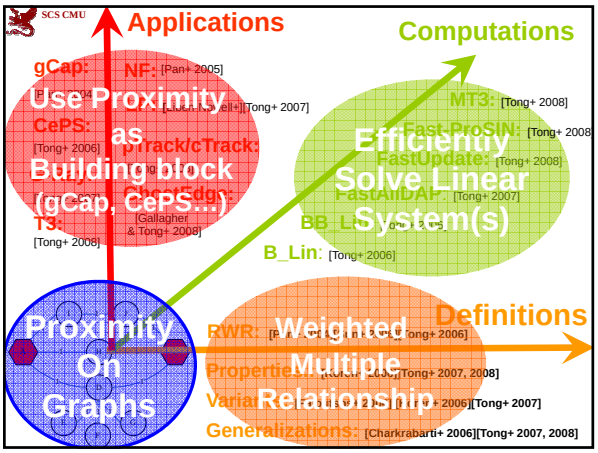
More Applications

- Clustering
  - Proximity as input [Ding+ KDD 2007]
- Email management [Minkov+ CEAS 06].
- Business Process Management [Qu+ 2008]
- ProSIN
  - Listen to clients' comments [Tong+ 2008]
- Ghost Edge
  - Within Network Classification [Gallagher & Tong+ KDD08 b]
- …



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Take-home messages

- Proximity Definitions
  - RWR $\vec{r}_i = c\tilde{W}\vec{r}_i + (1-c)\vec{e}_i$
  - and a lot of variants
- Computations
  - Sherman–Morrison Lemma
  - Fast Incremental Computation
- Applications
  - Proximity as a building block

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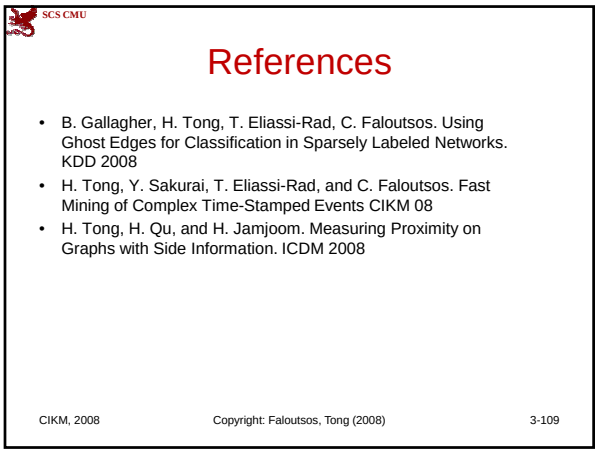
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