

# FAST KATZ AND COMMUTERS

Quadrature Rules and Sparse Linear Solvers  
for Link Prediction Heuristics

David F. Gleich  
Sandia National Labs

la/opt seminar  
October 14<sup>th</sup> 2010

With Pooya Esfandiar, Chen Grief,  
Laks V. S. Lakshmanan, and Byung-Won On

# MAIN RESULTS –SLIDE ONE

**A** – adjacency matrix

**L** – Laplacian matrix

Katz score :

$$K_{i,j} = [(\mathbf{I} - \alpha \mathbf{A})^{-1}]_{i,j}, i \neq j$$

Commute time:

$$C_{i,j} = L_{i,i}^+ + L_{j,j}^+ - 2L_{i,j}^+$$

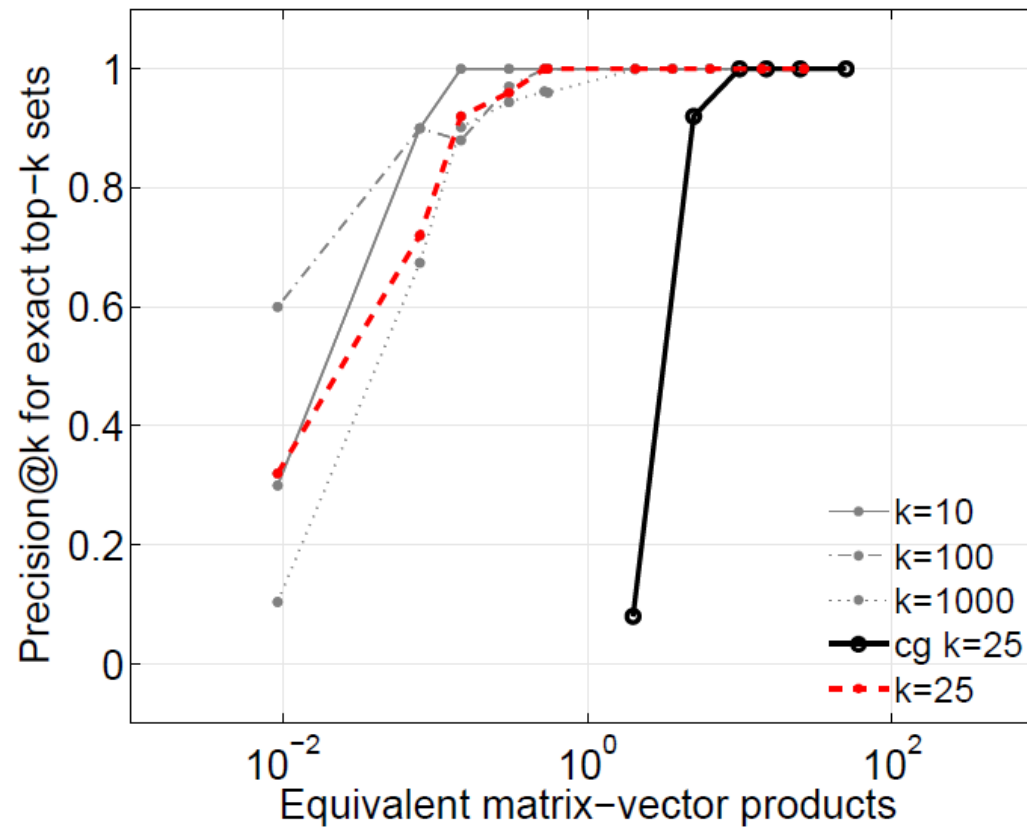
# MAIN RESULTS – SLIDE TWO

**For Katz** Compute one  $K_{i,j}$  fast  
 Compute top  $K_{i,:}$  fast

**For Commute**  
 Compute one  $C_{i,j}$  fast

**For almost commute**  
 Compute top  $F_{i,:}$  fast

# MAIN RESULTS – SLIDE THREE



# OUTLINE

Why study these measures?

Katz Rank and Commute Time

How else do people compute them?

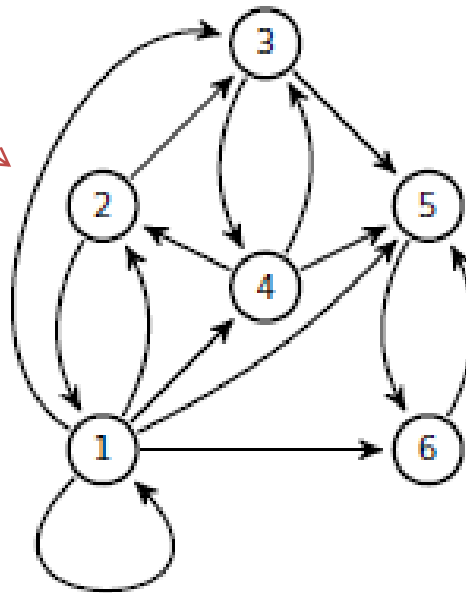
Quadrature rules for pairwise scores

Sparse linear systems solves for top-k

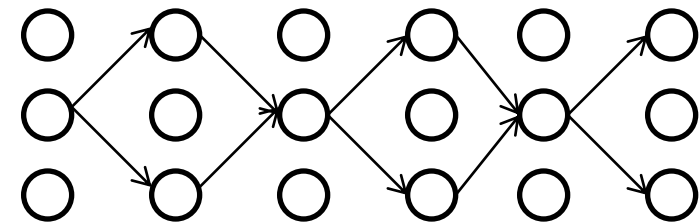
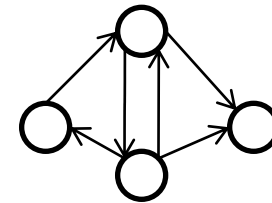
As many results as we have time for...

# WHY? LINK PREDICTION

facebook



~~Neighborhood based~~



Path based

*Liben-Nowell and Kleinberg 2003, 2006 found that path based link prediction was more efficient*

# NOTE

All graphs are undirected

All graphs are connected

# Leo Katz (statistician)

From Wikipedia, the free encyclopedia

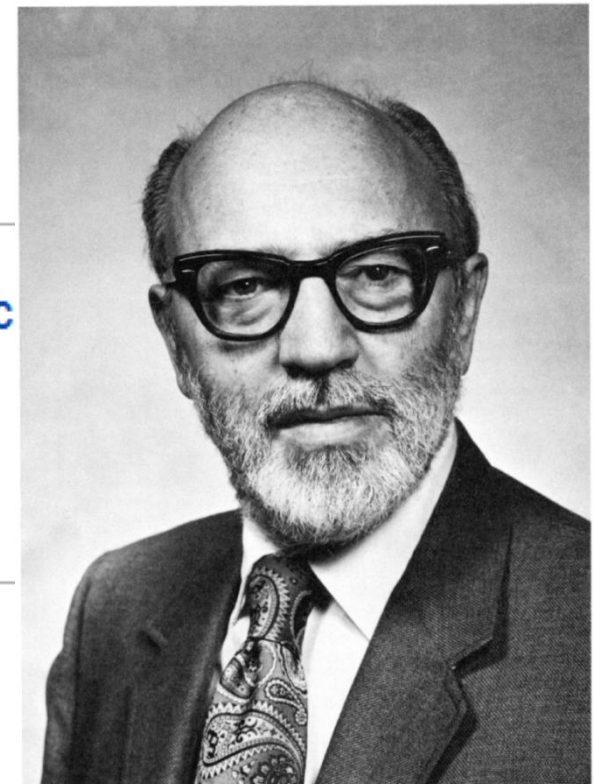
**Leo Katz** (born 29 November 1914 in Detroit - died 6 May 1976) was an American statistician. In 1953, he wrote a paper that already outlined the algorithm today known as [PageRank](#)<sup>[1]</sup>.

## References

- <sup>↑</sup> Katz, Leo. "A new status index derived from [soc Psychometrika](#), 18 (1953), 39-43

## External links

- <http://www.jstor.org/pss/3213364> [↗](#) Obituary





# NOT QUITE, WIKIPEDIA

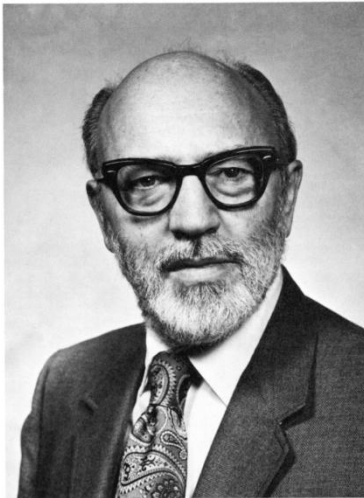
**A** : adjacency, **P** = **D**<sup>-1</sup>**A** : random walk

PageRank  $(\mathbf{I} - \alpha \mathbf{P}^T)^{-1} \mathbf{e}$

Katz  $(\mathbf{I} - \alpha \mathbf{A}^T)^{-1} \mathbf{e}$

These are equivalent if G has constant degree

# WHAT KATZ ACTUALLY SAID



“we assume that each link independently has the same probability of being effective” ...

“we conceive a constant  $\alpha$ , depending on the group and the context of the particular investigation, which has the force of a probability of effectiveness of a single link. A k-step chain then, has probability  $\alpha^k$  of being effective.”

“We wish to find the column sums of the matrix”

$$T = \alpha C + \alpha^2 C^2 + \cdots + \alpha^k C^k + \cdots = (I - \alpha C)^{-1} - I.$$

Leo Katz 1953, A New Status Index Derived from Sociometric Analysis, *Psychometria* 18(1):39-43

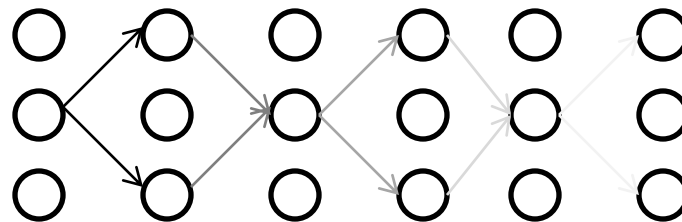
# A MODERN TAKE

The Katz score (node-based) is

$$t_i = \sum_j \sum_{k=1}^{\infty} \alpha^k \text{nwalks}_{i,j}^{(k)}$$

The Katz score (edge-based) is

$$K_{i,j} = \sum_{k=1}^{\infty} \alpha^k \text{nwalks}_{i,j}^{(k)}$$



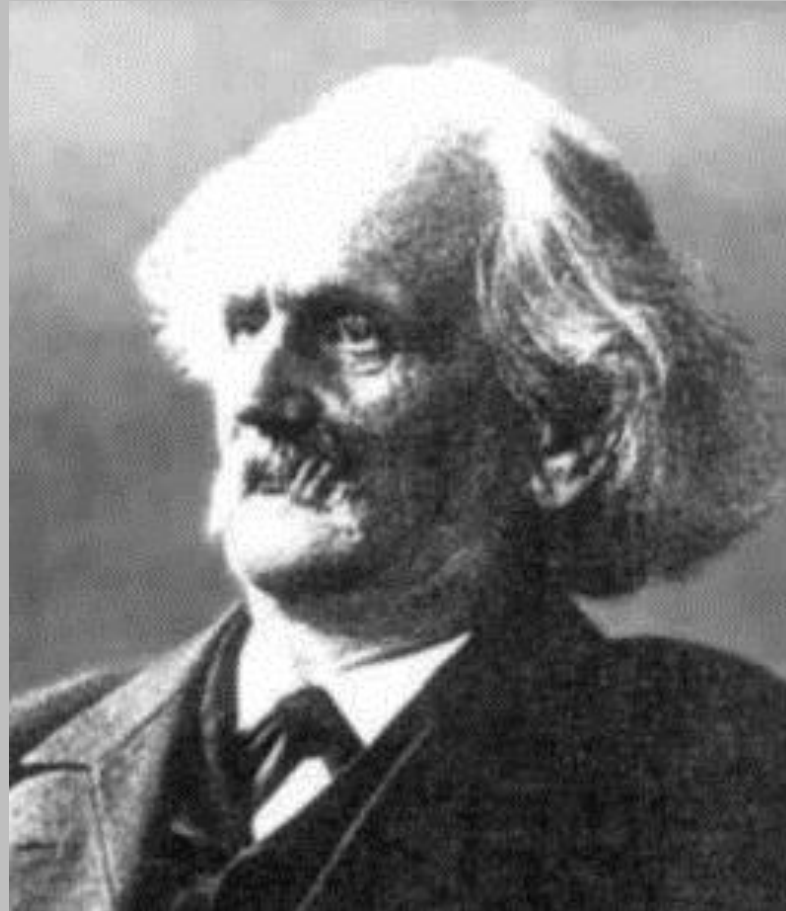
# RETURNING TO THE MATRIX

$$nwalks_{i,j}^{(k)} = A_{i,j}^k$$

$$\mathbf{K} = \alpha \mathbf{A} + \alpha^2 \mathbf{A}^2 + \alpha^3 \mathbf{A}^3 + \dots$$

Carl Neumann  $(\mathbf{I} - \mathbf{A})^{-1} = \sum_{k=0}^{\infty} \mathbf{A}^k$

$$\mathbf{K} = (\mathbf{I} - \alpha \mathbf{A})^{-1} - \mathbf{I}$$



## *Carl Neumann*

*I've heard the Neumann series called the "von Neumann" series more than I'd like! In fact, the von Neumann kernel of a graph should be named the "Neumann" kernel!*

# PROPERTIES OF KATZ'S MATRIX

**K** is symmetric

**K** exists when  $\alpha \neq 1/\lambda(\mathbf{A})$

$(\mathbf{I} - \alpha\mathbf{A})$  is sym. pos. def. when  $\alpha < 1/\|\mathbf{A}\|_2$

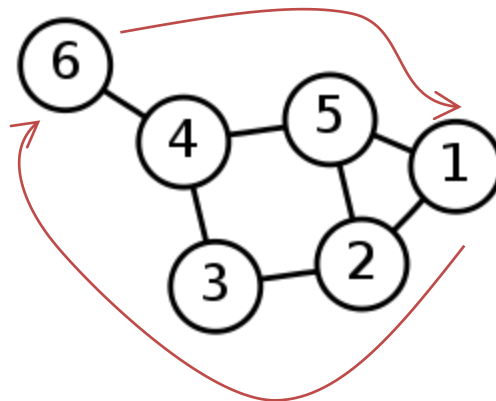
Note that  $\alpha < 1/\text{max-degree}$  suffices

# COMMUTE TIME

Consider a uniform random walk on a graph  $\mathbf{P} = \mathbf{D}^{-1}\mathbf{A}$

$$C_{i,j} = E[T \mid X_0 = i, \dots, X_T = j] + E[T \mid X_0 = j, \dots, X_T = i]$$

*Also called the hitting time from node  $i$  to  $j$ , or the first transition time*



# SKIPPING DETAILS

**$\mathbf{L} = \mathbf{D} - \mathbf{A}$**  : graph Laplacian

$$C_{i,j} = \text{Vol}(G)(\mathbf{e}_i - \mathbf{e}_j)^T \mathbf{L}^+(\mathbf{e}_i - \mathbf{e}_j)$$

**$\mathbf{L}\mathbf{e} = 0$**  is the only null-vector



# WHAT DO OTHER PEOPLE DO?

- 1) Just work with the linear algebra formulations
- 2) For Katz, Truncate the Neumann series as a few (3-5) terms *(I'm searching for this ref.)*
- 3) Use low-rank approximations from  $\text{EVD}(\mathbf{A})$  or  $\text{EVD}(\mathbf{L})$
- 4) For commute, use Johnson-Lindenstrauss inspired random sampling
- 5) Approximately decompose into smaller problems

# THE PROBLEM

All of these techniques are preprocessing based because most people's goal is to compute *all* the scores.

***We want to avoid preprocessing the graph.***

*There are a few caveats here! i.e. one could solve the system instead of looking for the matrix inverse*

# WHY NO PREPROCESSING?



The graph is constantly changing  
as I rate new movies.

# WHY NO PREPROCESSING?

Suggestions in **All Genres** ▼

---

**Suggestions to Watch Instantly**



**Cowboy Bebop: The Movie**

Because you enjoyed:

- Ghost in the Shell
- Spirited Away
- Firefly: The Complete Series

**Play**

★★★★☆

Not Interested



**The Insider**

Because you enjoyed:

- A Beautiful Mind
- Hotel Rwanda

**Play**

★★★★☆

Not Interested

**The Insider**

1999 **R** 157 minutes

Nominated for seven Oscars, this thriller from director Michael Mann tells the story of a Big Tobacco scientist who has secrets and the newsman who found out and squelched the story.

**Starring:** Al Pacino, Russell Crowe

**Director:** Michael Mann

**Genre:** Dramas Based on Real Life

**Format:** DVD and streaming

★★★★☆ 4.1 Our best

♥ Recommended based on your likes: Others, A Beautiful Mind and Hotel Rwanda

*Top-k predicted “links” are movies to watch!*



**Dr. HANK**

Long ago, far away was a girl I called “Staten Island Rita”. She treasured movies; through New York she trekked, burning through her inventory. A sweetheart! So, now I get it.  
sthenry@bellsouth

★ 121 ratings

📄 53 reviews

**Location:** Lake Worth, FL

**Reviewer Rank:** 253765

**Member Since:** January 2004

**Similarity:** 62%

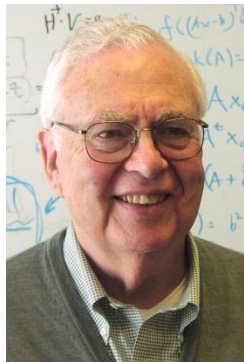


*Pairwise scores give user similarity*

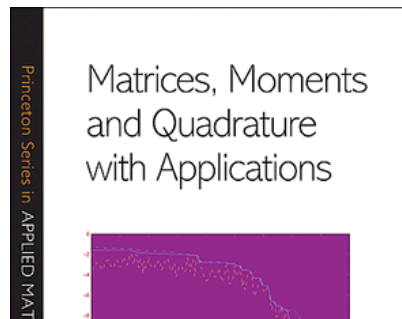
# PAIRWISE ALGORITHMS

Katz  $\mathbf{e}_i^T (\mathbf{I} - \alpha \mathbf{A})^{-1} \mathbf{e}_j$

Commute  $(\mathbf{e}_i - \mathbf{e}_j)^T \mathbf{L}^+ (\mathbf{e}_i - \mathbf{e}_j)$



*Golub and Meurant  
to the rescue!*



# MMQ - THE BIG IDEA

Quadratic form  $\mathbf{v}^T f(\mathbf{E}) \mathbf{v}$

Think  $f(x) = x^{-1}$



Weighted sum  $\sum_{i=1}^n w_i^2 f(\lambda_i)$

A is s.p.d. use EVD



Stieltjes integral  $\int_a^b f(\lambda) d\mathbf{w}(\lambda)$

“A tautology”



Quadrature approximation  $\sum_{j=1}^k f(\eta_j) \omega_j$



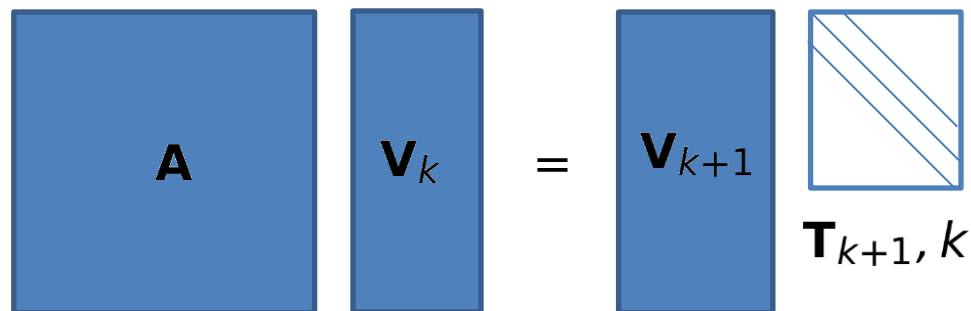
Matrix equation  $\mathbf{e}_1^T f(\mathbf{T}_k) \mathbf{e}_1$

Lanczos

# LANCZOS

**A**, **b** , \$k\$-steps of the Lanczos method produce

$$\mathbf{A}\mathbf{V}_k = \mathbf{V}_{k+1}\mathbf{T}_{k+1,k} \quad \text{and} \quad \mathbf{V}_k\mathbf{e}_1 = \rho\mathbf{b}$$



The diagram illustrates the equation  $\mathbf{A}\mathbf{V}_k = \mathbf{V}_{k+1}\mathbf{T}_{k+1,k}$ . On the left, a large blue square represents the matrix **A**, and a tall blue rectangle represents the vector **V<sub>k</sub>**. An equals sign follows. On the right, another tall blue rectangle represents the vector **V<sub>k+1</sub>**, followed by a white square with blue diagonal lines representing the tridiagonal matrix **T<sub>k+1,k</sub>**.

# PRACTICAL LANCZOS

Only need to store the last 2 vectors in  $\mathbf{V}_k$

Updating requires  $O(\text{matvec})$  work

$\mathbf{V}_k$  is not orthogonal



# MMQ PROCEDURE

Goal  $b = \mathbf{u}^T \mathbf{E}^{-1} \mathbf{u}$

Given  $l < \lambda(\mathbf{E}) < u$

1. Run  $k$ -steps of Lanczos on  $\mathbf{E}$  starting with  $\mathbf{u}$
2. Compute  $\mathbf{T}_u, \mathbf{T}$  with an additional eigenvalue at  $u$ ,  
 set  $b_u = \mathbf{e}_1^T \mathbf{T}_u^{-1} \mathbf{e}_1$ 

Correspond to a Gauss-Radau rule, with  $u$  as a prescribed node
3. Compute  $\mathbf{T}_l, \mathbf{T}$  with an additional eigenvalue at  $l$ , set  
 $b_l = \mathbf{e}_1^T \mathbf{T}_l^{-1} \mathbf{e}_1$ 

Correspond to a Gauss-Radau rule, with  $l$  as a prescribed node
4. Output  $[b_l, b_u]$  as lower and upper bounds on  $b$

# PRACTICAL MMQ

Increase  $k$  to become more accurate

Bad eigenvalue bounds yield worse results

$\mathbf{T}_u$  and  $\mathbf{T}_l$  are easy to compute

$\mathbf{T}_u^{-1}$  not required, we can iteratively update it's LU factorization

# PRACTICAL MMQ

---

## Algorithm 1 Computing Score Bounds

---

**Input:**  $E, u, a < \lambda_{\min}(E), b > \lambda_{\max}(E), k$

**Output:**  $\underline{b}_k \leq u^T E^{-1} u \leq \overline{b}_k$

- 1: **Initial step:**  $h_1 = 0, h_0 = u, \omega_1 = u^T E u, \gamma_1 = \|(E - \omega_1 I)u\|, b_1 = \omega_1^{-1}, d_1 = \omega_1, c_1 = 1,$   
 $\overline{d}_1 = \omega_1 - a, \underline{d}_1 = \omega_1 - b, h_1 = \frac{(E - \omega_1 I)u}{\gamma_1}.$
  - 2: **for**  $j = 2, \dots, k$  **do**
  - 3:    $\omega_j = h_{j-1}^T E h_{j-1}$
  - 4:    $\tilde{h}_j = (E - \omega_j I)h_{j-1} - \gamma_{j-1}h_{j-2}$
  - 5:    $\gamma_j = \|\tilde{h}_j\|$
  - 6:    $h_j = \frac{\tilde{h}_j}{\gamma_j}$
  - 7:    $b_j = b_{j-1} + \frac{\gamma_{j-1}^2 c_{j-1}^2}{d_{j-1}(\omega_j d_{j-1} - \gamma_{j-1}^2)}$
  - 8:    $d_j = \omega_j - \frac{\gamma_{j-1}^2}{d_{j-1}}; c_j = c_{j-1} \frac{\gamma_{j-1}}{d_{j-1}}$
  - 9:    $\overline{d}_j = \omega_j - a - \frac{\gamma_{j-1}^2}{d_{j-1}}; \underline{d}_j = \omega_j - b - \frac{\gamma_{j-1}^2}{d_{j-1}}$
  - 10:    $\overline{\omega}_j = a + \frac{\gamma_j^2}{\underline{d}_j}; \underline{\omega}_j = b + \frac{\gamma_j^2}{d_j}$
  - 11:    $\overline{b}_j = b_j + \frac{\gamma_j^2 c_j^2}{d_j(\overline{\omega}_j d_j - \gamma_j^2)}; \underline{b}_j = b_j + \frac{\gamma_j^2 c_j^2}{d_j(\underline{\omega}_j d_j - \gamma_j^2)}$
-

# ONE LAST STEP FOR KATZ

$$\text{Katz} \quad \mathbf{e}_i^T (\mathbf{I} - \alpha \mathbf{A})^{-1} \mathbf{e}_j$$

$$\mathbf{u} \neq \mathbf{v} \quad \text{☹}$$

$$\begin{aligned} \mathbf{u}^T f(\mathbf{E}) \mathbf{v} = & 1/4 [(\mathbf{u} + \mathbf{v})^T f(\mathbf{E})(\mathbf{u} + \mathbf{v}) \\ & - (\mathbf{u} - \mathbf{v})^T f(\mathbf{E})(\mathbf{u} - \mathbf{v})] \end{aligned}$$

# TOP-K ALGORITHM FOR KATZ

Approximate  $\mathbf{x}$

$$(\mathbf{I} - \alpha \mathbf{A})\mathbf{x} = \mathbf{e}_i$$

where  $\mathbf{A}$  is sparse

Keep  $\mathbf{x}$  sparse too

Ideally, don't “*touch*” all of  $\mathbf{A}$

# INSPIRATION - PAGERANK

Approximate  $\mathbf{x}$

$$(\mathbf{I} - \alpha \mathbf{P})\mathbf{x} = \mathbf{e}_i$$

where  $\mathbf{P}$  is sparse

Keep  $\mathbf{x}$  sparse too? YES!

Ideally, don't “*touch*” all of  $\mathbf{A}$  ? YES!

# THE ALGORITHM - MCSHERRY

For  $\mathbf{Ex} = \mathbf{b}$

Start with the Richardson iteration

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \omega(\mathbf{b} - \mathbf{Ex}^{(k)})$$

Rewrite

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \omega \mathbf{r}^{(k)}$$

Richardson converges if  $\rho(\mathbf{I} - \mathbf{A}) < 1$

# THE ALGORITHM

Note **b** is sparse.

If  $\mathbf{x}^{(0)} = 0$ , then  $\mathbf{r}^{(0)}$  is sparse.

Idea

only add one component of  $\mathbf{r}^{(k)}$  to  $\mathbf{x}^{(k)}$



# THE ALGORITHM

For  **$\mathbf{E}\mathbf{x} = \mathbf{b}$**

Init:  $\mathbf{x}^{(0)} = \mathbf{0}, \mathbf{r}^{(0)} = \mathbf{b}$

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \omega r_j^{(k)} \mathbf{e}_j$$

$$\mathbf{r}^{(k+1)} = \mathbf{r}^{(k)} + \omega r_j^{(k)} \mathbf{E} \mathbf{e}_j$$

How to pick  $j$ ?

# THE ALGORITHM FOR KATZ

For  $(\mathbf{I} - \alpha \mathbf{A})\mathbf{x} = \mathbf{e}_i$

Init:  $\mathbf{x}^{(0)} = \mathbf{0}, \mathbf{r}^{(0)} = \mathbf{e}_1$

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + r_j^{(k)} \mathbf{e}_j$$

$$\mathbf{r}^{(k+1)} = \mathbf{r}^{(k)} - r_j^{(k)} \mathbf{e}_j + \alpha r_j^{(k)} \mathbf{A} \mathbf{e}_j$$

Pick  $j$  as  $\max r_j^{(k)}$

*Storing the non-zeros of the residual in a heap makes picking the max  $\log(n)$  time. See Anderson et al. FOCS2008 for more*

# CONVERGENCE?

If you pick  $j$  as the maximum element, we can show this is convergent if Richardson converges. This proof requires  $\mathbf{E}$  to be symmetric positive definite.

# RESULTS - DATA

Graph	Nodes	Edges
dblp	93,156	178,145
arxiv	86,376	517,563
flickr	513,969	3,190,452

All unweighted, connected graphs

# RESULTS – KATZ ALPHAS

Easy  $\alpha$

$$1/(10\|\mathbf{A}\|_1 + 10)$$

Hard  $\alpha$

$$1/(\|\mathbf{A}\|_2 + 1)$$

# PAIRWISE RESULTS

Katz upper and lower bounds

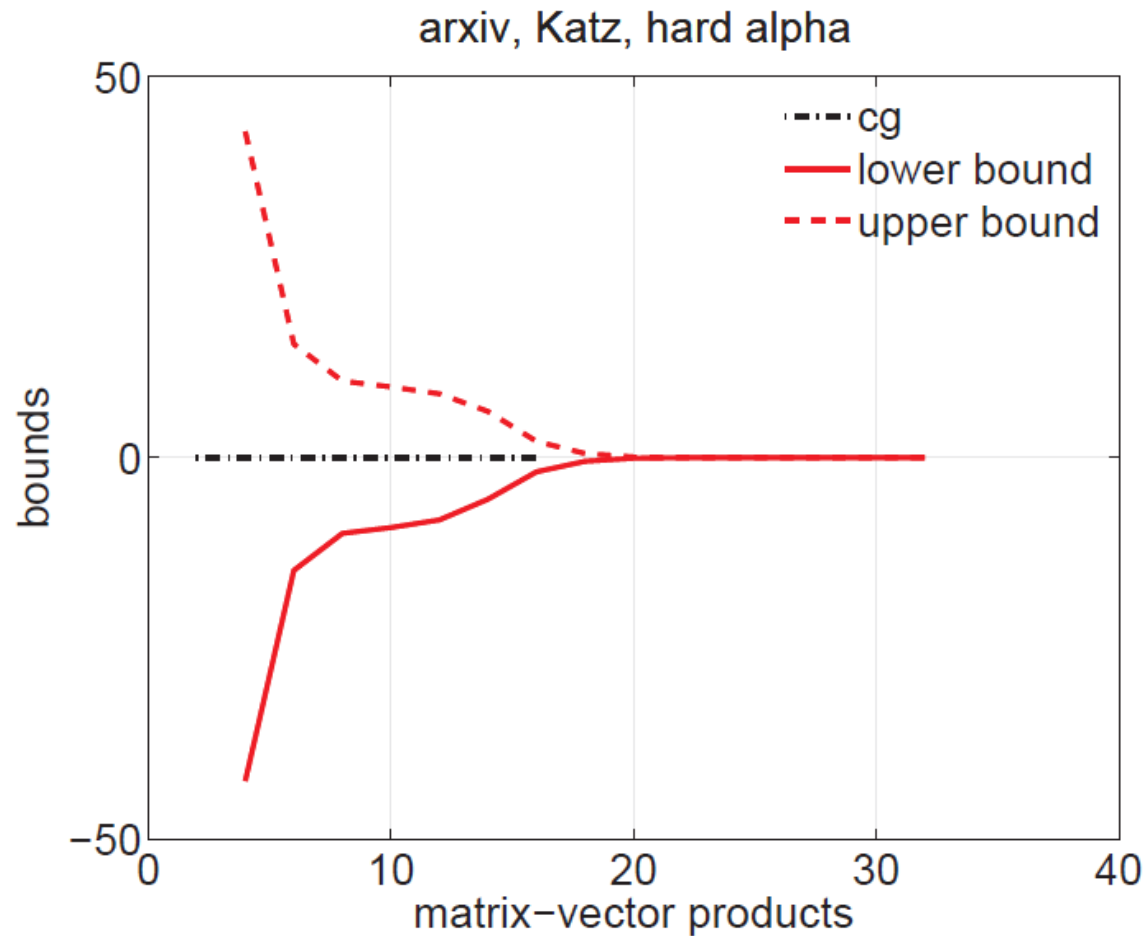
Katz error convergence

Commute-time upper and lower bounds

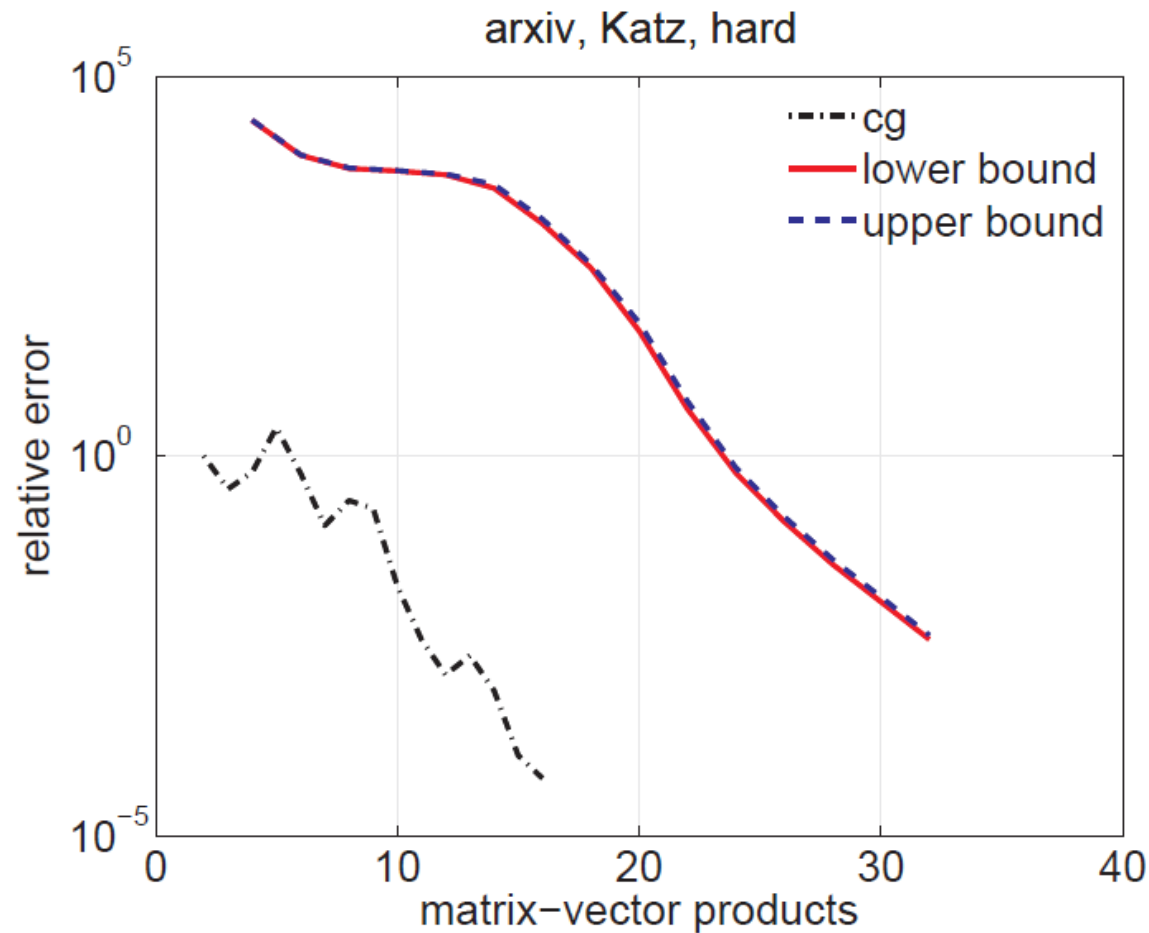
Commute-time error convergence

For the arXiv graph here

# KATZ BOUND CONVERGENCE

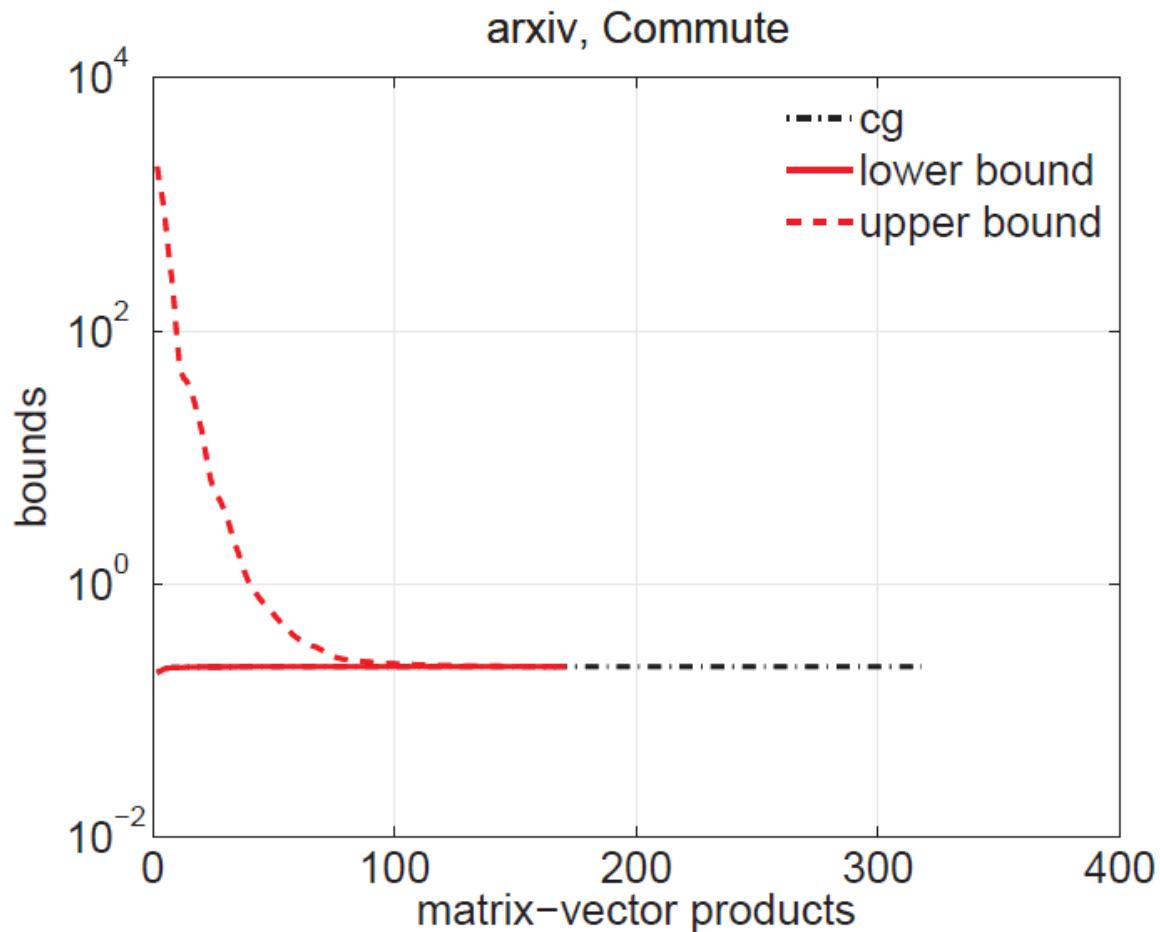


# KATZ ERROR CONVERGENCE

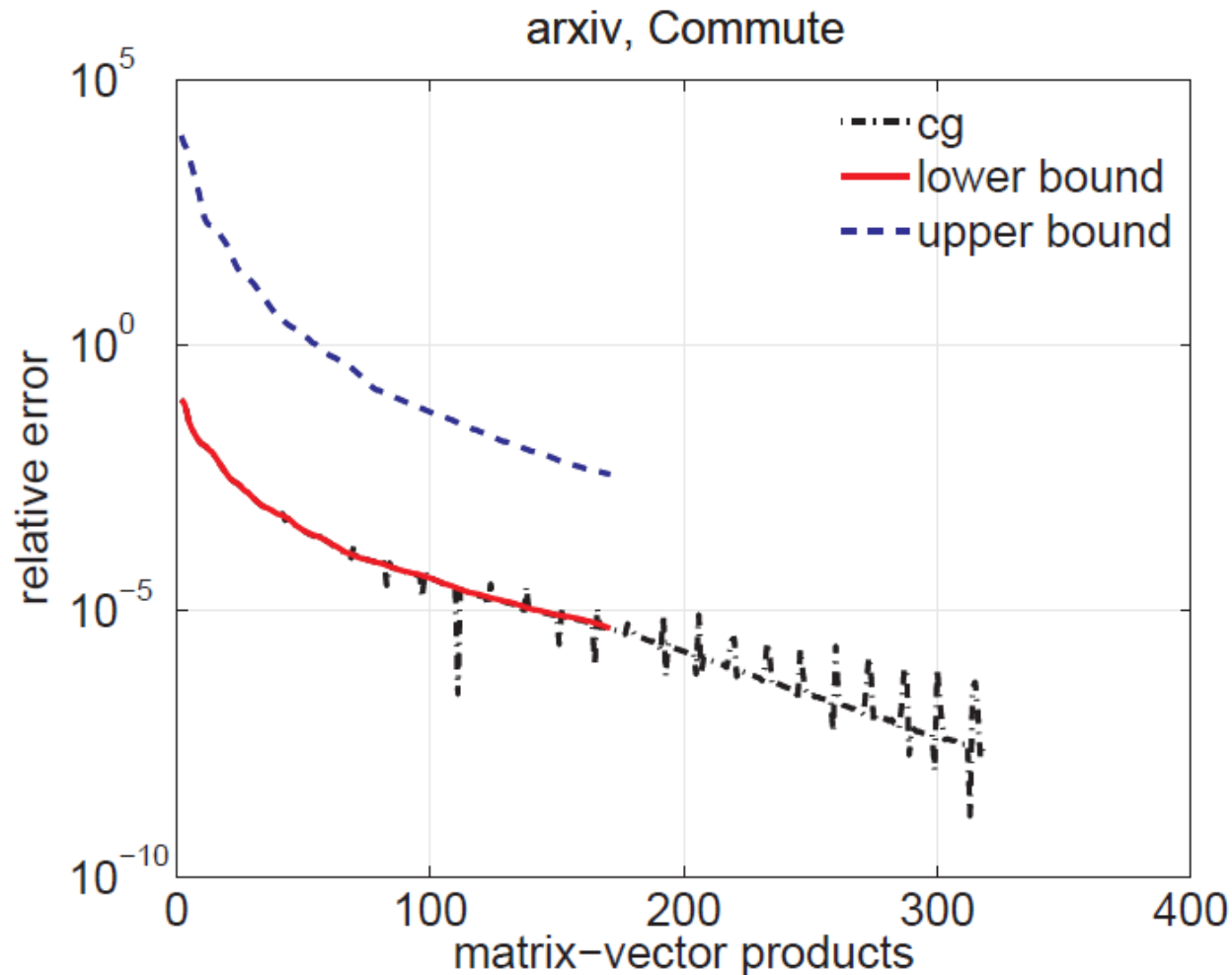




# COMMUTE BOUND CONVERG.



# COMMUTE ERROR CONVERG.



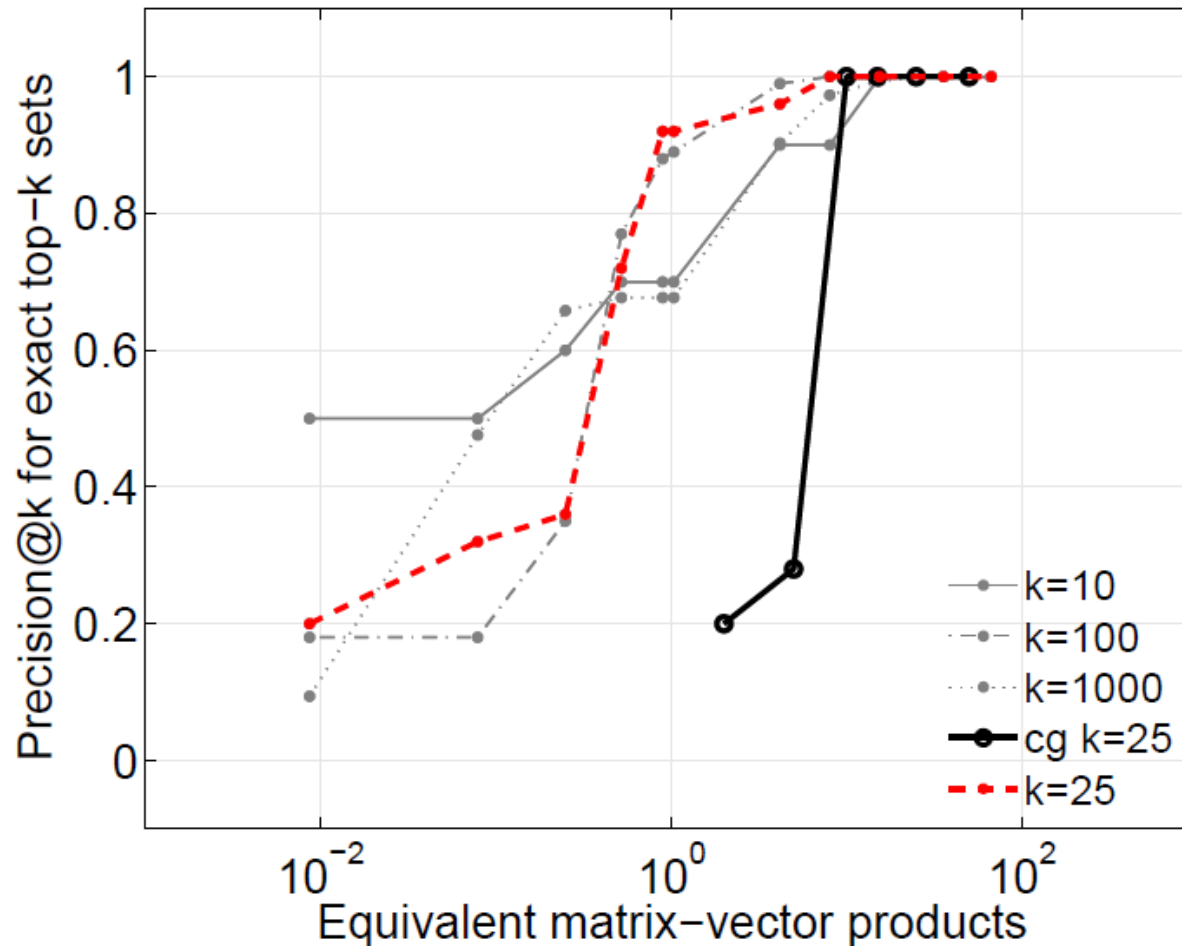
# TOP-K RESULTS

Katz set convergence

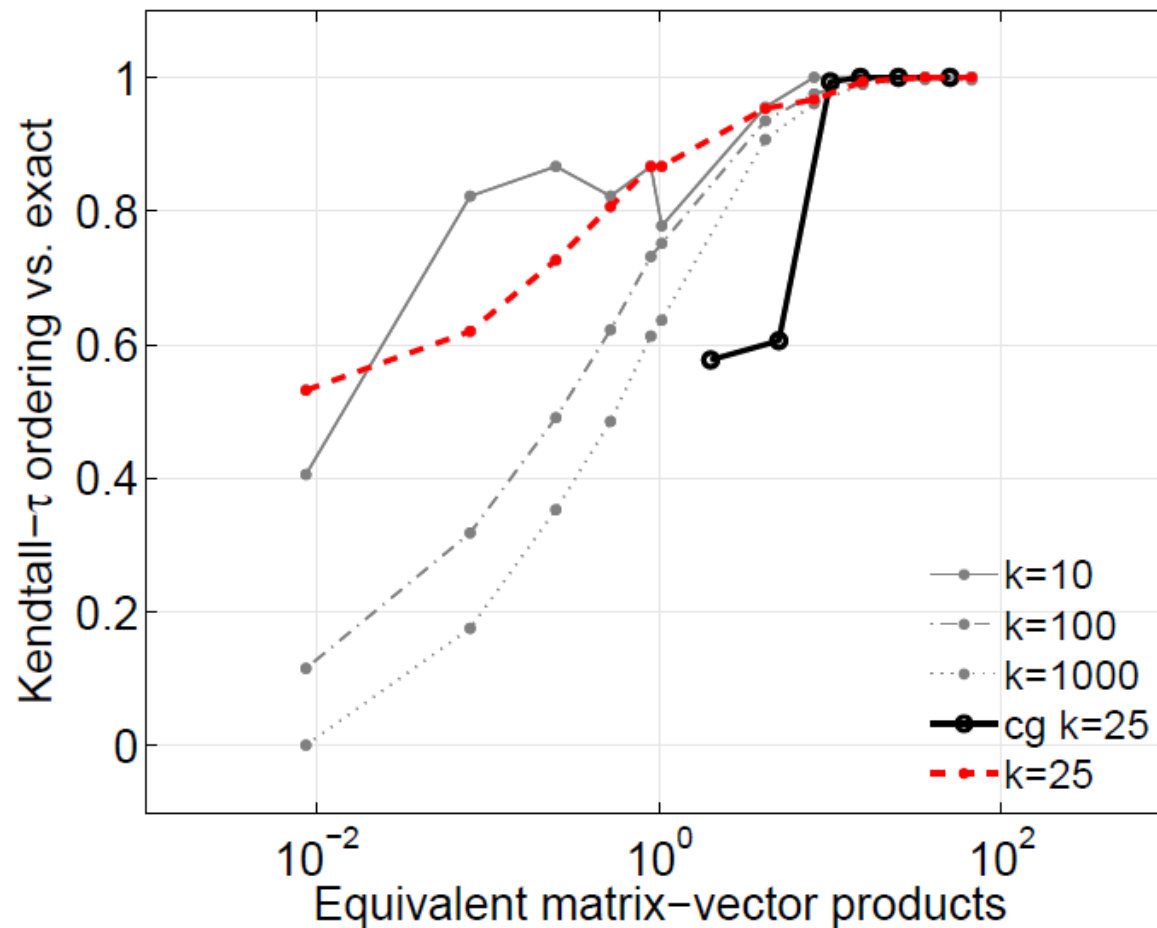
Katz order convergence

For arXiv graph

# KATZ SET CONVERGENCE



# KATZ ORDER CONVERGENCE



# CONCLUSIONS

These algorithms are faster than many alternatives.

For pairwise commute, stopping criteria are simpler

For top-k, we often need less than 1 matvec for good enough results

# WARTS

Stopping criteria on our top-k algorithm  
can be a bit hairy

The top-k approach doesn't work right for  
commute time

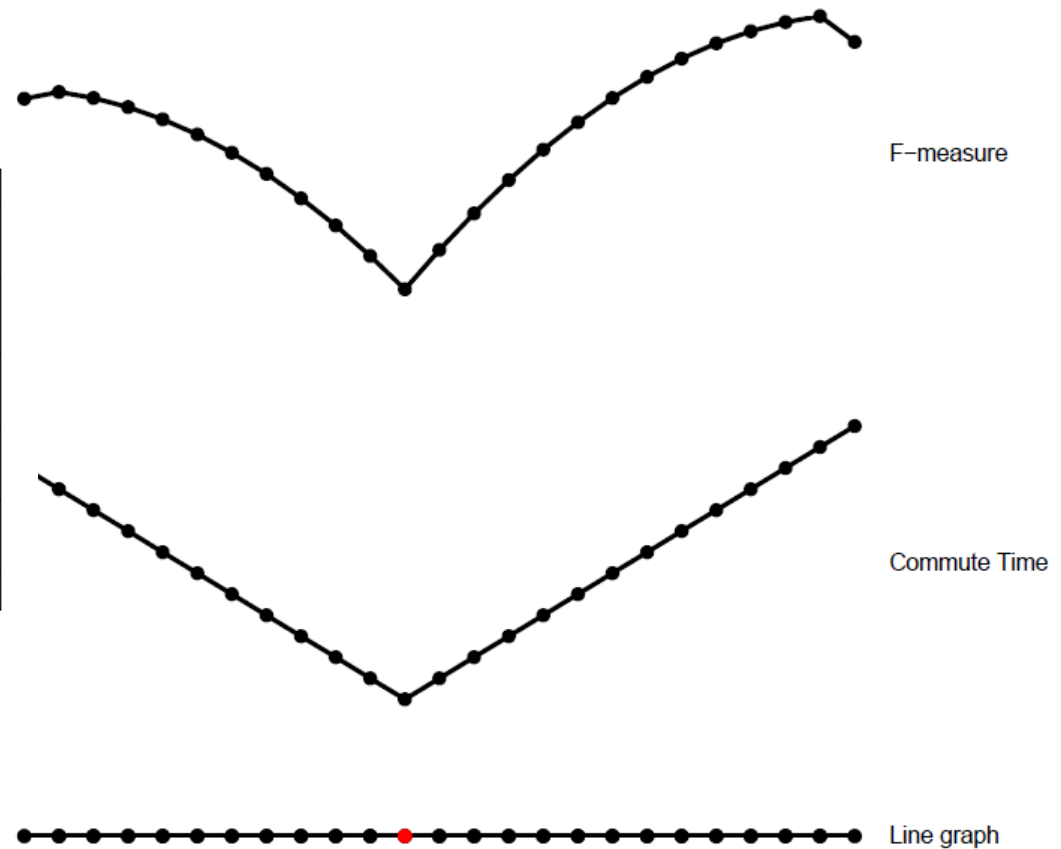
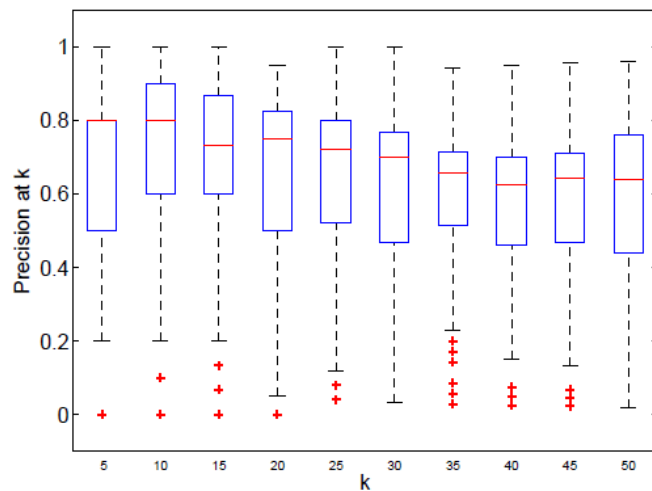
# TODO

Try on netflix data! 😊

Explore our “almost commute measure more”



# F-MEASURE





*By AngryDogDesign on DeviantArt*

Preprint available by request

Slides should be online soon

Code is online already  
[stanford.edu/~dgleich/  
publications/2010/codes/fast-katz](http://stanford.edu/~dgleich/publications/2010/codes/fast-katz)