Graph Analysis in the Wild: Theory to Practice

C. Seshadhri
(Seshadhri Comandur)

Dept of Computer Science

Theory and practice

There and back again

Theory

(CS Theory)

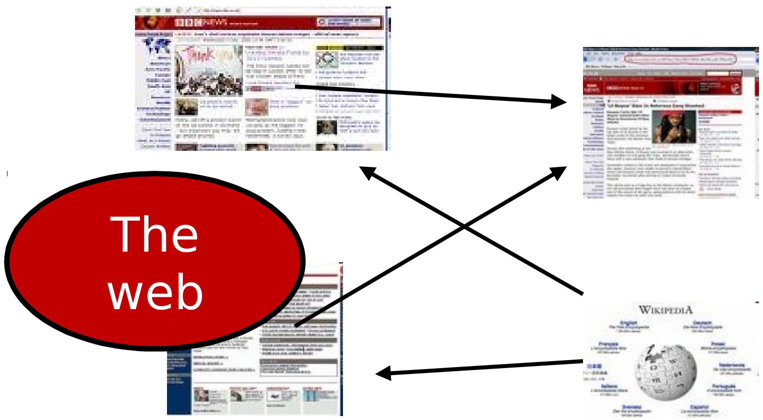
Algorithms
Graph theory
Probability theory
Combinatorics

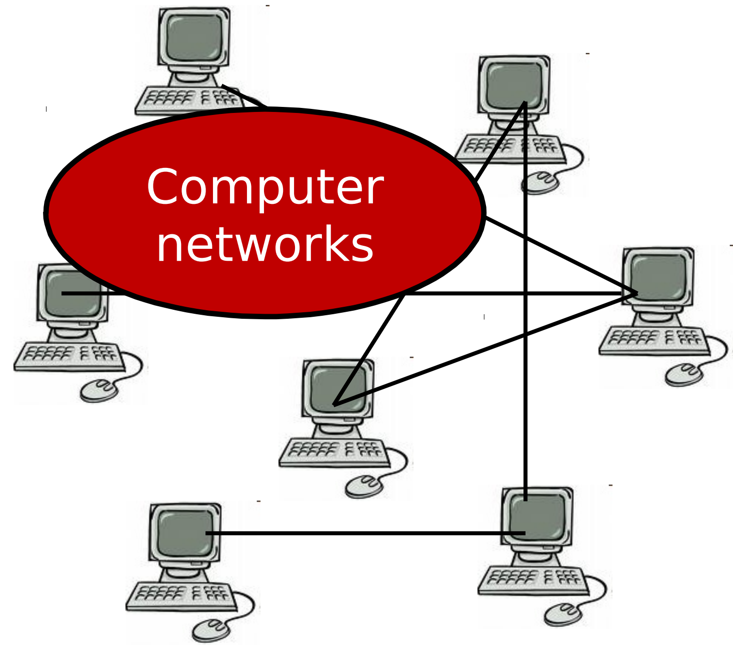
Practice

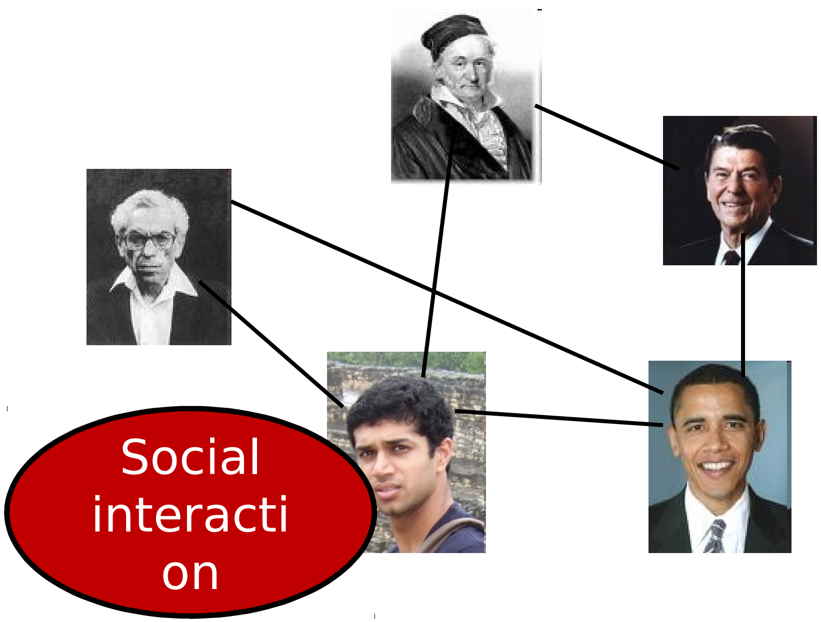
(Graph analysis)

Graph modeling
Clustering
Pattern counting
Scalable algorithms

Large graphs



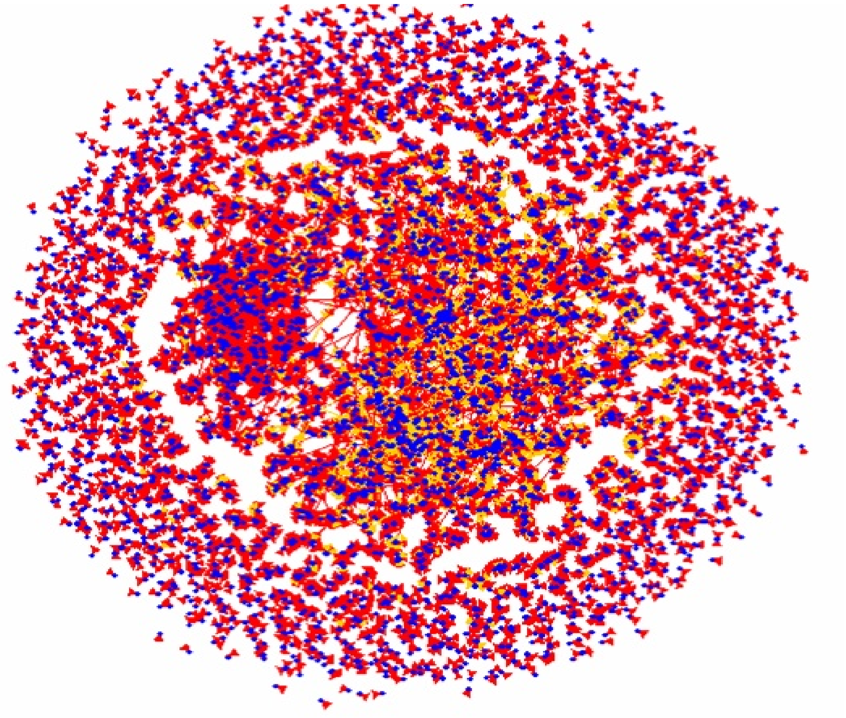




- Convenient representation
- Vertices and edges connecting them
- Big, millions, billions,…

So what about them?

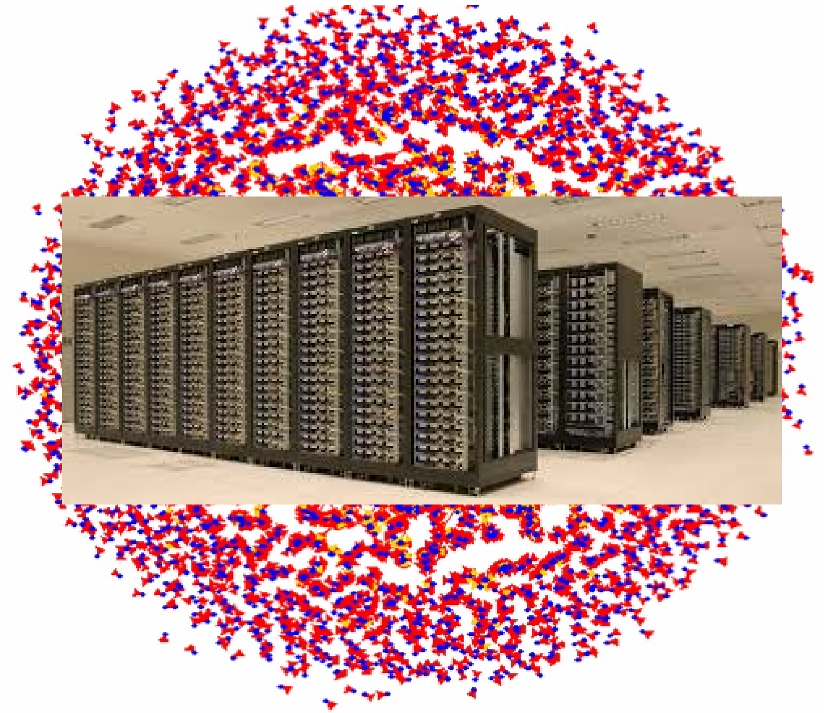
- Are there common patterns?
- Can you find "interesting" activity?
- Is this graph "special"?
- Which regions should I "care" about?



Often reduces to some algorithmic question (via graph theory)

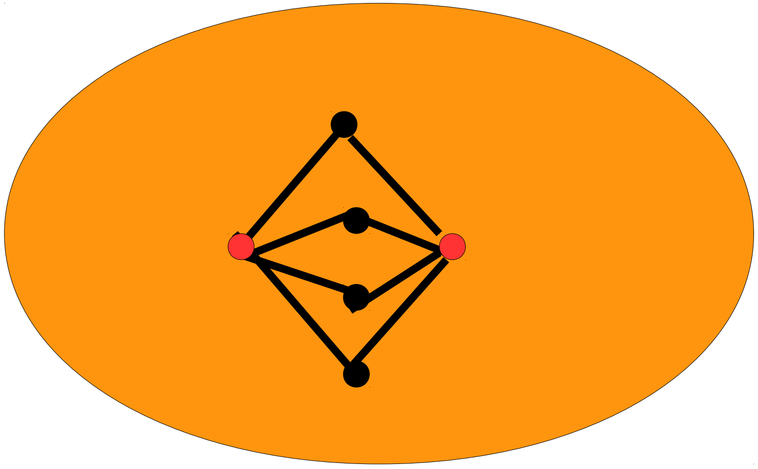
The size problem

- Graph is massive (millions to billions)
- Distributed
- Noisy
- Probably can't see of all it
- Maybe only one pass of data



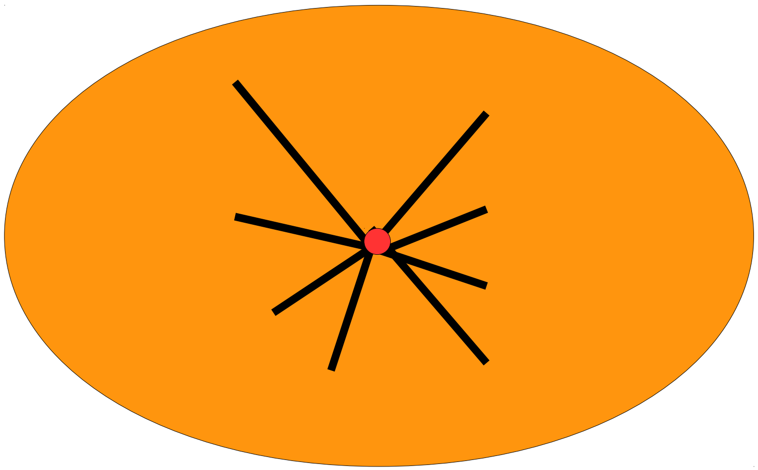
We need to rethink the past 50 years of graph algorithmics.

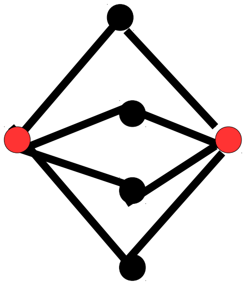
Most common neighbors



- G is undirected, simple graph
- Find top k pairs with most nearest neighbors

Some naïve algorithms

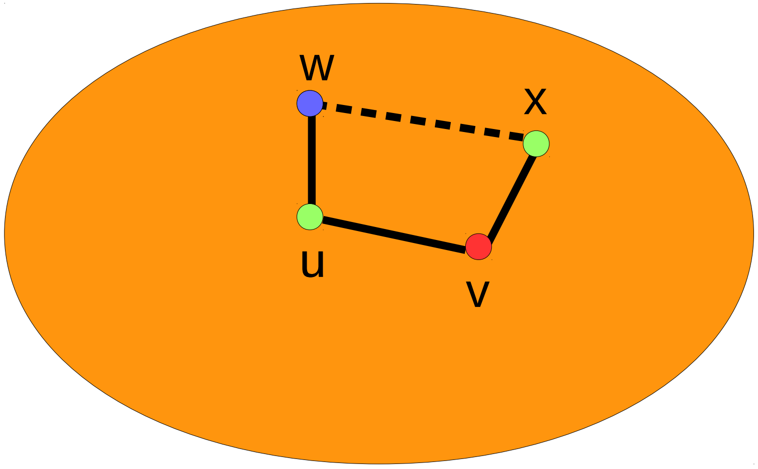




- Try all pairs
  - Complexity $n^2 \sim 10^{12}$
- Do 2-step BFS from each node
  - Complexity superlinear $\sim 10^9$

What we did

[Ballard Pinar Kolda S ICDM15]



Repeat 10,000 times

Output pairs that are frequently reported

- Pick e = (u,v) with probability prop. to $d_u d_v$
- Pick random neighbor w of u, and x of v
- Check if (w,x) exists
- If so, output u,x as candidate

Why would you do that?

- Works well (68M edge graph, top 1000 pairs in a second) where we assume $t' \ll mn$. We let Ω_s denote the indices of all the nonzeros in X and $\Omega_{t'}$ denote the top-t' entries in X; this requires a sort in Line 1 of at most s items (and generally many fewer, depending on the proportion of three-paths that close into diamonds). We compute the t' dot products in Lines 3 to 5 at a cost of $O(t'd)$. Finally, we let Ω_t denote the top-t dot products from $\Omega_{t'}$ in Line 6, requiring a sort of t' items.

Algorithm 2 Postprocessing

Given $\Omega_s = \{(i,j) \mid x_{ij} > 0\}$. Let t be the number of top dot products, and $t' \geq t$ be the budget of dot products.

```
1: Extract top-t' entries of X, i.e., |Ω_t'| ≤ t' and
   Ω_t' ← { (i,j) ∈ Ω_s | x_ij ≥ x_i'j' ∀(i',j') ∈ Ω_s \ Ω_t' }
2: C ← all-zero matrix of size m × n
3: for (i,j) ∈ Ω_t' do
4:     c_ij ← a_i^T b_j
5: end for
6: Extract top-t entries of C, i.e., |Ω_t| ≤ t and
   Ω_t ← { (i,j) ∈ Ω_t' | c_ij ≥ c_i'j' ∀(i',j') ∈ Ω_t' \ Ω_t }
```

B. General inputs

We present the binary version as general motivation, but our implementation and analysis are based on the diamond sampling algorithm for general real-valued A and B in Algorithm 3. In this case, we define the matrix of weights $W \in \mathbb{R}^{d \times n}$ such that

$$w_{ki} = |a_{ki}| \, \|a_{*i}\|_1 \|b_{k*}\|_1 \quad \text{for all} \quad k \in [d],\ i \in [m].$$

The weight w_{ki} correspond to the weight of all three paths with edge (i,k) at its center. This is computed in Line 2. The sampling in Line 6 has the same complexity as in the binary case, but the sampling in Lines 7 and 8 now has a nonuniform distribution and so has higher complexity than in the binary case. The postprocessing is unchanged.

Algorithm 3 Diamond sampling with general inputs

Given matrices $A \in \mathbb{R}^{m \times d}$ and $B \in \mathbb{R}^{n \times d}$.
Let s be the number of samples.

```
1: for all a_ki ≠ 0 do
2:     w_ki ← |a_ki| ||a_*i||_1 ||b_k*||_1
3: end for
4: X ← all-zero matrix of size m × n
5: for ℓ = 1, ..., s do
6:     Sample (k,i) with probability w_ki / ||W||_1
7:     Sample j with probability |b_kj| / ||b_k*||_1
8:     Sample k' with probability |a_k'i| / ||a_*i||_1
9:     x_ij ← x_ij + sgn(a_ki b_kj a_k'i) b_k'j
10: end for
11: Postprocessing (see Algorithm 2)
```

1) Nonnegative inputs: If A and B are nonnegative, the only change is that the sign computations can be ignored in computing the sample increment in Line 9 in Algorithm 3. This avoids potentially expensive random memory accesses.

2) Equal inputs (Gram matrix): If $B = A$, then $C =$ is symmetric. The matrix X is not symmetric, although is. Hence, we modify X before by inserting the followin before the postprocessing in Line 11 in Algorithm 3:

$$X \leftarrow (X + X^T)/2.$$

Now X is symmetric, and the forthcoming analysis is fected.

3) Equal symmetric inputs (squared matrix): If $B =$ A is symmetric, then $C = A^2$ and we can replace Line Algorithm 3 with the following two lines:

$$x_{ij} \leftarrow x_{ij} + \mathrm{sgn}(a_{ki} b_{kj} a_{k'i})\, b_{k'j}/2,$$
$$x_{kk'} \leftarrow x_{kk'} + \mathrm{sgn}(a_{ki} b_{kj} a_{k'i})\, b_{k'j}/2.$$

This exploits the fact that we can swap the role of k an the initial edge sample. Again, X may not be symmetr we insert (2) before the postprocessing in Line 11.

C. Complexity and space

Let $\alpha = \mathrm{nnz}(A)$ and $\beta = \mathrm{nnz}(B)$. In the dense case, md and $\beta = nd$. The total work is

$$O(\alpha + \beta + s\log(s\alpha\beta)).$$

The total storage (not counting the inputs A and B) is

$$2\,\mathrm{storage}(A) + \mathrm{storage}(B) + 5s + 3t' + 3t.$$

We give detailed arguments below and in the implemen discussion in Section V.

Preprocessing. For the sampling in Lines 7 and 8 precompute cumulative, normalized column sums for B the same for rows of A, requiring storage of storage(storage(B) and computation of $O(\alpha + \beta)$. The matrix W the same nonzero pattern as A, so the cost to store it is to storage(A) and to compute it is $O(\alpha)$.

Sampling. For a straightforward implementation, the per sample in Line 6 is $O(\log(\alpha))$. For Line 7, the co sample is $O(\log(\beta/d))$; here, we have used the approxim $\mathrm{nnz}(b_{k*}) \approx \beta/d$. A similar analysis applied for A and Li So, the cost per sample is $O(\log(\alpha) + \log(\beta/d) + \log(\alpha$ Without loss of generality, we assume that we need to the three-paths and the summand in Line 9 for a total st of $5s$.

Postprocessing. Conservatively, we require $3t'$ storag the $(i, j, x_{ij}$ or $c_{ij})$ triples in $\Omega_{t'}$ and $3t$ storage fo (i, j, c_{ij}) triples in Ω_t. The sorting requires at most $O(s$ time, and usually much less since $\mathrm{nnz}(X)$ may be much than s due to only some three-paths forming diamond concentration, i.e., picking the same (i, j) pair multiple t

IV. Analysis of Diamond Sampling

This section provides a theoretical analysis of dia sampling. We first prove that the expected value of $c_{ij}^2/\|W\|_1$, and then we prove error bounds on our estim a function of the number of samples. Unless stated other our analysis applies to the general version of the dian sampling algorithm (Algorithm 3).

A. Expectation

For a single instance of Lines 6 to 8 of Algorithm 3, we define the event

$$\mathcal{E}_{k'ikj} = \text{choosing three-path } (k', i, k, j).$$

LEMMA 1. $\Pr(\mathcal{E}_{k'ikj}) = |a_{ki} b_{kj} a_{k'i}| / \|W\|_1$.

Proof: The probability of choosing three-path (k', i, k, j) is (by independence of these choices) the product of the following probabilities: that of choosing the center edge (i, k), then picking j, and then picking k'.

$$\begin{aligned}\Pr(\mathcal{E}_{k'ijk}) &= \Pr(\text{ctr } (i,k)) \cdot \Pr(\text{endpts } j \text{ and } k' | \text{ctr } (i,k)) \\ &= \frac{w_{ki}}{\|W\|_1} \cdot \frac{|b_{kj}|}{\|b_{k*}\|_1} \cdot \frac{|a_{k'i}|}{\|a_{*i}\|_1} \\ &= \frac{|a_{ki}| \, \|a_{*i}\|_1 \|b_{k*}\|_1}{\|W\|_1} \cdot \frac{|b_{kj}|}{\|b_{k*}\|_1} \cdot \frac{|a_{k'i}|}{\|a_{*i}\|_1} \\ &= \frac{|a_{ki} b_{kj} a_{k'i}|}{\|W\|_1}.\end{aligned}$$

■

In what follows, we use $X_{i,j,\ell}$ to be the following random variable: if i, j are the respective indices updated in the ℓth iteration, $X_{i,j,\ell} = \mathrm{sgn}(a_{ki} b_{ki} a_{k'i}) b_{k'j}$. Otherwise, $X_{i,j,\ell} = 0$. Observe that $x_{ij} = \sum_{\ell=1}^{s} X_{i,j,\ell}$.

LEMMA 2. *For diamond sampling,* $\mathbb{E}[x_{ij}/s] = c_{ij}^2/\|W\|_1$.

Proof: We note that $\mathbb{E}[x_{ij}/s] = \mathbb{E}[\sum_\ell X_{i,j,\ell}]/s = \mathbb{E}[X_{i,j,1}]$. (We use linearity of expectation and the fact that the $X_{i,j,\ell}$ are i.i.d. for fixed i, j and varying ℓ.)

$$\begin{aligned}\mathbb{E}[X_{i,j,1}] &= \sum_k \sum_{k'} \Pr(\mathcal{E}_{k'ikj}) \cdot \mathrm{sgn}(a_{ki} b_{ki} a_{k'j})\, b_{k'j} \\ &= \sum_k \sum_{k'} \frac{|a_{ki} b_{kj} a_{k'i}|}{\|W\|_1} \cdot \mathrm{sgn}(a_{ki} b_{kj} a_{k'i})\, b_{k'j} \\ &= \frac{1}{\|W\|_1} \sum_k \sum_{k'} a_{ki} b_{kj} a_{k'i} b_{k'j} \\ &= \frac{1}{\|W\|_1} \Big(\sum_k a_{ki} b_{kj}\Big)\Big(\sum_{k'} a_{k'i} b_{k'j}\Big) \\ &= \frac{1}{\|W\|_1} \Big(\sum_k a_{ki} b_{kj}\Big)^2 = \frac{c_{ij}^2}{\|W\|_1}.\end{aligned}$$

■

B. Concentration bounds

We now provide some concentration bounds when all entries in A and B are nonnegative.

LEMMA 3. *Fix $\varepsilon > 0$ and error probability $\delta \in (0,1)$. Assume all entries in A and B are nonnegative and at most K. If the number of samples*

$$s \geq 3K\|W\|_1 \log(2/\delta)/(\varepsilon^2 c_{ij}^2),$$

then

$$\Pr[|x_{ij}\|W\|_1/s - c_{ij}^2| > \varepsilon c_{ij}^2] \leq \delta.$$

Proof: Observe that $X_{i,j,\ell}$ is in the range $[0, K]$. Thus, $Y_{i,j,\ell} = X_{i,j,\ell}/K$ is in $[0,1]$. Set $y_{ij} = \sum_\ell Y_{i,j,\ell}$. Since y_{ij} is the sum of random variables in $[0,1]$, we can apply the standard multiplicative Chernoff bound (Theorem 1.1 of [32]). This yields $\Pr[y_{ij} \geq (1+\varepsilon)\mathbb{E}[y_{ij}]] < \exp(-\varepsilon^2 \mathbb{E}[y_{ij}]/3)$. By Lemma 2, $\mathbb{E}[y_{ij}] = (s/K)(c_{ij}^2/\|W\|_1)$, which is at least $3\log(2/\delta)/\varepsilon^2$ by choice of s. Hence, $\Pr[y_{ij} \geq (1+\varepsilon)\mathbb{E}[y_{ij}]] < \delta/2$. Note that $y_{ij} = x_{ij}/K$. We multiply the expression inside the $\Pr[\cdot]$ by $K\|W\|_1/s$ to get the event $x_{ij}\|W\|_1/s \geq (1+\varepsilon)c_{ij}^2$.

Using the Chernoff lower tail bound and identical reasoning, we get $\Pr[x_{ij}\|W\|_1/s \leq (1-\varepsilon)c_{ij}^2] \leq \delta/2$. A union bound completes the proof. ■

The following theorem gives a bound on the number of samples required to distinguish "large" dot products from "small" ones. The constant 4 that appears is mostly out of convenience; it can be replaced with anything > 1 with appropriate modifications to s.

THEOREM 4. *Fix some threshold τ and error probability $\delta \in (0,1)$. Assume all entries in A and B are nonnegative and at most K. Suppose $s \geq 12K\|W\|_1 \log(2mn/\delta)/\tau^2$. Then with probability at least $1-\delta$, the following holds for all indices i, j and i', j': if $c_{ij} > \tau$ and $c_{i'j'} < \tau/4$, then $x_{ij} > x_{i'j'}$.*

Proof: First consider some dot product c_{ij} with value at least τ. We can apply Lemma 3 with $\varepsilon = 1/2$ and error probability δ/mn, so with probability at least $1 - \delta/mn$, $x_{ij}\|W\|_1/s \geq c_{ij}^2/2 \geq \tau^2/2$. Now consider dot product $c_{i'j'} < \tau/3$. Define $y_{i'j'}$ and $Y_{i',j',\ell}$ as in the proof of Lemma 3. We can apply the lower tail bound of Theorem 1.1 (third part) of [32]: for any $b > 2e\mathbb{E}[y_{i'j'}]$, $\Pr[y_{i'j'} > b] < 2^{-b}$.

We set $b = s\tau^2/2K\|W\|_1$. From Lemma 2 and the assumption that $c_{i'j'} < \tau/3$ and $\mathbb{E}[y_{i'j'}] = \mathbb{E}[x_{i'j'}]/K = sc_{i'j'}^2/K\|W\|_1 \leq s\tau^2/(16K\|W\|_1) < b/2e$. Plugging in our bound for s, $b \geq (12K\|W\|_1 \log(2mn/\delta)/\tau^2) \cdot \tau^2/(2K\|W\|_1) = 6\log(2mn/\delta)$. Hence, $\Pr[y_{i'j'} > b] < \delta/(2mn)$. Equivalently, $\Pr[x_{i'j'}\|W\|_1/s > \tau^2/2] < \delta/(2mn)$. We take a union bound over all the error probabilities (there are at most mn pairs i, j or i', j').

In conclusion, with probability at least $1-\delta$, for any pair of indices i, j: if $c_{ij} > \tau$, then $x_{ij}\|W\|_1/s \geq \tau^2/2$. If $c_{ij} < \tau/4$, then $x_{ij}\|W\|_1/s < \tau^2/2$. This completes the proof. ■

To get a useful interpretation of Lemma 3 and Theorem 4, we ignore the parameters ε and δ. Let us also assume that $K = 1$, which is a reasonable assumption for most of our experiments. Basically, to get a reasonable estimate of c_{ij}, we require $\|W\|_1/c_{ij}^2$ samples. If the value of the t-th largest entry in C is τ, we require $\|W\|_1/\tau^2$ samples to find the t-largest entries. For instance, on a graph, if we want to identify pairs of vertices with at least 200 common neighbors, we can set $\tau = 200$, and $\|W\|_1$ will be the number of (non-induced) 3-paths in the graph. The square in the denominator is what makes this approach work. In Table I of Section VI, we show some of the values of $\|W\|_1/\tau^2$ for particular datasets, where τ is the magnitude of the largest entry.

Industrial scale

- [Sharma-S-Goel 16] Solving similar problems on Twitter's network
  - Distributed computing
  - The problems of scale
  - New math

PhD Zen

Your advantage over your advisor is **time**

Don't just read it. Fight it

- P. R. Halmos

Books are for reading, maps are for getting somewhere

A paper is a map

Everyone has slumps

As some point, the learning stops and the pain begins

- S. Rao Kosaraju

Learn to present

Go back to the big picture

Ask questions