# A Nearly Sublinear Approximation to $\exp \{\mathbf{P}\} \mathbf{e}_{\boldsymbol{i}}$ for Large Sparse Matrices from Social Networks 

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- $\exp \{\mathbf{A}\}$ is common, but other $f(\mathbf{A})$ can be used: pagerank and heatkernel PR
- Assume column stochastic, $\mathbf{P}=\mathbf{G D}^{-1}$ (more on this later)


## Difficulties with current methods: Sidje, TOMS 1998; Al-Mohy and Higham, SISC 2011

■ Leading methods for $\exp \{\mathbf{A}\} \mathbf{b}$ use Krylov or Taylor methods: "basically" repeated mat-vecs
■ "Small world" property: graph diameter $\leq 4 \Rightarrow$ repeated mat-vecs fill in rapidly (see picture)
■ Not designed specifically for sparse networks.

## Fill-in from repeated matvecs



Vectors $\mathbf{P}^{k} \mathbf{e}_{i}$ for $k=1,2,3,4 . n=1133$

## Local Method

New method: avoid mat-vecs! $\rightarrow$ use a local method.

Local algorithms run in time proportional to size of output: sparse solution vector $=$ small runtime

Instead of matvecs, we do specially-selected vector adds using a relaxation method.

## $\exp \{\mathbf{P}\} \mathbf{e}_{i}$ is a localized vector


$x$-axis: vector index, $y$-axis: magnitude of entry the column of $\exp \{\mathbf{P}\}$ produced by previous slide's matvecs

## Overview

Outline of Nexpokit method

1. Express $\exp \{\mathbf{A}\} \mathbf{e}_{i}$ via a Taylor polynomial
2. Form large linear system out of Taylor terms
3. Use sparse solver to approximate each terms' largest entries
4. Combine approximated terms into a solution

## In terms of Taylor terms

Taylor polynomial:

$$
\exp \{\mathbf{A}\} \mathbf{e}_{i} \approx\left(\mathbf{I}+\mathbf{A}+\frac{1}{2} \mathbf{A}^{2}+\frac{1}{3!} \mathbf{A}^{3}+\cdots+\frac{1}{N!} \mathbf{A}^{N}\right) \mathbf{e}_{i}
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Compute terms recursively: $\mathbf{v}_{k}=\frac{1}{k!} \mathbf{A}^{k} \mathbf{e}_{i}=\frac{1}{k} \mathbf{A}\left(\frac{1}{(k-1)!} \mathbf{A}^{k-1}\right) \mathbf{e}_{i}$

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Then $\exp \{\mathbf{A}\} \mathbf{e}_{i} \approx \mathbf{v}_{0}+\mathbf{v}_{1}+\cdots+\mathbf{v}_{N-1}+\mathbf{v}_{N}$ (But we want to avoid computing $\mathbf{v}_{j}$ in full...)

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$$
\left[\begin{array}{ccccc}
\mathbf{l} & & & & \\
-\mathbf{A} / 1 & \mathbf{I} & & & \\
& -\mathbf{A} / 2 & \ddots & & \\
& & \ddots & \mathbf{I} & \\
& & & -\mathbf{A} / N & \mathbf{I}
\end{array}\right]\left[\begin{array}{c}
\mathbf{v}_{0} \\
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\vdots \\
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From
$\mathbf{v}_{k}=\frac{1}{k} \mathbf{A} \mathbf{v}_{k-1}$
$\exp \{\mathbf{A}\} \mathbf{e}_{i} \approx \mathbf{v}_{0}+\mathbf{v}_{1}+\cdots+\mathbf{v}_{N-1}+\mathbf{v}_{N}$ (never formed explicitly)

## Sparse solver: Gauss Southwell

Basic idea of Gauss Southwell (GS): solving $\mathbf{M x}=\mathbf{b}$ when $\mathbf{x}$ is "effectively sparse" (i.e. a localized vector)

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3. Add corresponding column of $\mathbf{M}$ to residual:

$$
\mathbf{r}^{k+1}=\left(\mathbf{r}^{k}-r_{i}^{k} \cdot \mathbf{e}_{i}\right)+r_{i}^{k} \cdot \mathbf{M}(:, i)
$$

## NEXPOKIT

Apply GS to our linear system, $\mathbf{M} \overline{\mathbf{v}}=\overline{\mathbf{e}}_{i}$ :

$$
\left[\begin{array}{ccccc}
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Now residual has index and block section: $r(i, j)$. Iteration reduces to: (1) adding $r(i, j)^{k}$ to a single entry of $\mathbf{x}$, our approximation; (2) adding scaled column, $\frac{r(i, j)^{k}}{j} \mathbf{A}(:, i)$, to section $j$ of the residual.

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Scaling $\frac{r(i, j)^{k}}{j} \mathbf{A}(:, i)$ guarantees $\left\|\mathbf{r}^{k}\right\|_{1}$ decreases, for column stochastic $\mathbf{A}$ :

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Largest entry, $r(i, j)$ is bounded below by average, $r(i, j)>\|\mathbf{r}\|_{1} /(\#$ non zeros in $\mathbf{r}$ ).

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Largest entry, $r(i, j)$ is bounded below by average, $r(i, j)>\|\mathbf{r}\|_{1} /(\#$ non zeros in $\mathbf{r}$ ).
No component of large linear system formed explicitly:

- residual vector stored in a heap (alternative: queue with threshold)
- matrix $\mathbf{M}$ not formed at all
- blocks $\mathbf{v}_{j}$ not stored separately


## "A Nearly Sublinear Approximation ...

- Converges for stochastic matrices

■ "Nearly sublinear" - if $d_{\max }=O(\log \log n)$ (unrealistic)

- In practice, sublinear if NNZ $=O(n)$
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- In practice, sublinear if NNZ $=O(n)$
- Less work than a single mat-vec
- New: for power-law degree distributed networks, the runtime for an error of $\varepsilon$ is

$$
\log (1 / \varepsilon)(1 / \varepsilon)^{3 / 2} d_{\max } \log \left(d_{\max }\right)^{2}
$$

- Social networks tend to have $d_{\max }=O\left(n^{r}\right)$ for $r<1$, so this is sublinear in $n$.


## Power-law degree distribution


[Laboratory for Web Algorithms, http://law.di.unimi.it/index.php]

## Intuition for Proof

Our sublinear runtime proof depends on the degree distribution:
■ decrease in $\|\mathbf{r}\|$ depends on largest value in $\mathbf{r}, r_{i}$
■ lowerbound $r_{i}$ using the average value of $\mathbf{r}$
■ average value $=\|\mathbf{r}\| /(\#$ of nonzeros in $\mathbf{r})$
(\# of nonzeros in $\mathbf{r}$ ) upper bounded by $d_{\max } *$ (\#iterations)

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(\# of nonzeros in $\mathbf{r}$ ) upper bounded by $d_{\max } *$ (\#iterations)
Power-law network: \# of nonzeros in $\mathbf{r}$ after $t$ iterations grows like $O(t)$ instead of $d_{\text {max }} * t . \Rightarrow$ average value can't decay too fast. Hence, $\|\mathbf{r}\|$ is guaranteed to decrease "fast enough": $\left\|\mathbf{r}^{t}\right\|<O\left(t^{-2 / 3}\right)$

## Runtime v. Graph Size


"GSQ" is a version of our Gauss-Southwell method that stores the residual vector in a queue instead of a heap.

## Runtime on larger networks



For ljournal-2008, $n=5,363,260$, ave degree $=14.7$.

## Runtime on larger networks



For webbase-2001, $n=118,142,155$, ave degree $=8.6$.

## Accuracy of algorithm



For $\mathrm{pgp}-\mathrm{cc} n=10,680$, but this is representative of dataset.

## Number of operations performed



Effective matrix-vector products
For dblp-cc, $n=226,413$. Again, this is representative.

## Future Work

- Adapt the method to other functions: $\cosh (x), x^{\frac{1}{p}}, \log (x)$.
- Allow for scaling, $f(t \mathbf{A}) \mathbf{e}_{i}$.

■ Allow for $f(\mathbf{A})$ times a vector $\mathbf{v}$ (other than $\mathbf{e}_{i}$ ).

- Improve domain of convergence, $\rho(\mathbf{A}) \in(0,1]$.


## Code and Further Details

Code available at
http://www.cs.purdue.edu/homes/dgleich/codes/nexpokit
For details and references, see our paper at

$$
\text { http://arxiv.org/abs/1310. } 3423
$$

