

## Spectrum and eigenstates of Google matrix

## Klaus Frahm

Quantware MIPS Center
Université Paul Sabatier
Laboratoire de Physique Théorique, UMR 5152, IRSAMC, CNRS
supported by EC FET Open project NADINE

NADINE project REVIEW 2013, Toulouse, 14 November 2013

## Google matrix structure


top $200 \times 200$
(in PageRank order)
coarse-grained
$500 \times 500$
(in PageRank order)

Wikipedia 2009
Twitter 2009

Density of non-zero elements $N_{G}$ of the adjacency matrix among top PageRank nodes:


## Diagonalization of Google matrices

Arnoldi method to (partly) diagonalize large sparse matrices:

- choose an initial normalized vector $\xi_{0}$ (random or "otherwise")
- determine the Krylov space of dimension $n_{A}$ (typically: $\left.1 \ll n_{A} \ll d\right)$ spanned by the vectors: $\xi_{0}, G \xi_{0}, \ldots, G^{n_{A}-1} \xi_{0}$
- determine by Gram-Schmidt orthogonalization an orthonormal basis $\left\{\xi_{0}, \ldots, \xi_{n_{A}-1}\right\}$ and the representation of $G$ in this basis:

$$
G \xi_{k}=\sum_{j=0}^{k+1} H_{j k} \xi_{j}
$$

- diagonalize the Arnoldi matrix $H$ which has Hessenberg form:
$H=\left(\begin{array}{ccccc}* & * & \cdots & * & * \\ * & * & \cdots & * & * \\ 0 & * & \cdots & * & * \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & * & * \\ \hline 0 & 0 & \cdots & 0 & *\end{array}\right)$ which provides the Ritz eigenvalues that are
very good aproximations to the "largest" eigenvalues of $A$.


## Invariant subspaces

Problem: (possibly) large degeneracy of $\lambda_{1}=1$.
$\Rightarrow$ Determine the invariant subspaces defined as subsets of nodes such that for any node in a subspace each outgoing link stays in the subspace.
$\Rightarrow$ Decomposition of the network in many separate subspaces with $N_{s}$ nodes and a "big" core space of the remaining $N-N_{s}$ nodes.
$\Rightarrow$ block structure:

$$
S=\left(\begin{array}{cc}
S_{s s} & S_{s c} \\
0 & S_{c c}
\end{array}\right)
$$

$$
S_{s s}=\left(\begin{array}{ccc}
S_{1} & 0 & \ldots \\
0 & S_{2} & \\
\vdots & & \ddots
\end{array}\right)
$$

- Exact (or Arnoldi) diagonalization for each subspace with at least one unit eigenvalue per subspace ( $\Rightarrow$ degeneracy).
- Arnoldi method for $S_{c c}$ to determine the largest core space eigenvalues $\lambda_{j}$ (note: $\left|\lambda_{j}\right|<1$ ).


## University networks

KMF, B. Georgeot and D.L. Shepelyansky, J. Phys. A: Math. Theor. 44, 465101 (2011)


Cambridge 2006 (Oxford 2006), $N=212710$ (200823), $N_{\ell}=2015265$ (1831542),
$N_{s}=48239$ (30579), Number of subspaces $=1543$ (1889), $n_{A}=20000$, max. dim. $=4656$ (1545), degeneracy of $\lambda_{1}=1: 1832$ (2360).

## core sorce arg



(Blue crosses shifted up by $10^{9}$ )

## Small gap:

$\Rightarrow$ exponential localization of eigenvectors
$\Rightarrow$ quasi-subspace

## Spectrum of Twitter

KMF and D.L. Shepelyansky, Eur. Phys. J. B 85, 355 (2012)
Twitter 2010 : $N=41652230$ nodes, $N_{\ell}=1468365182$ network links.


$n_{A}=640$ for both cases

## Spectrum of Wikipedia

L. Ermann, KMF and D.L. Shepelyansky, Eur. Phys. J. B 86, 193 (2013) Wikipedia 2009 : $N=3282257$ nodes, $N_{\ell}=71012307$ network links.


$n_{A}=6000$ for both cases

## Spectra of other networks




## Some Eigenvectors:









left (right): PageRank (CheiRank)
$\xi_{\text {IPR }} \sim 10-100 \ll N$
black: PageRank (CheiRank) at $\alpha=0.85$
grey: PageRank (CheiRank) at $\alpha=1-10^{-8}$
red and green: first two core space eigenvectors
blue and pink: two eigenvectors with large imaginary part in the eigenvalue

## "Themes" of certain eigenvectors (Wikipedia 2009):



|  | $\lambda_{1481}=0.1699+i 0.3325$ ("Bible") | $\left\|\psi_{i}\right\|$ |
| :--- | :---: | :---: |
| 1 | Portal:Bible | 0.02311 |
| 2 | Portal:Bible/Featured chapter/archives | 0.02201 |
| 3 | Portal:Bible/Featured article | 0.02063 |
| 4 | Bible | 0.01684 |
| 5 | Portal:Bible/Featured chapter | 0.01644 |
| 6 | Books of Samuel | 0.00852 |
| 7 | Books of Kings | 0.00849 |
| 8 | Books of Chronicles | 0.00840 |
| 9 | Book of Leviticus | 0.00426 |
| 10 | Book of Ezra | 0.00425 |
| 11 | Book of Ruth | 0.00420 |
| 12 | Book of Deuteronomy | 0.00417 |
| 13 | Book of Joshua | 0.00400 |
| 14 | Book of Exodus | 0.00397 |
| 15 | Book of Judges | 0.00395 |
| 16 | Book of Genesis | 0.00394 |
| 17 | Book of Numbers | 0.00389 |
| 18 | Portal:Bible/Featured chapter/1 Kings | 0.00347 |
| 19 | Portal:Bible/Featured chapter/Numbers | 0.00347 |
| 20 | Portal:Bible/Featured chapter/2 Samuel | 0.00347 |

## Physical Review network

KMF, Young-Ho Eom, D. Shepelyansky, arXiv:1310.5624
$N=463347$ nodes and $N_{\ell}=4691015$ links.
Coarse-grained matrix structure ( $500 \times 500$ cells):

left: time ordered
right: journal and then time ordered
"11" Journals of Physical Review: (Phys. Rev. Series I), Phys. Rev., Phys. Rev. Lett., (Rev. Mod. Phys.), Phys. Rev. A, B, C, D, E, (Phys. Rev. STAB and Phys. Rev. STPER).
$\Rightarrow$ nearly triangular matrix structure of adjancy matrix: most citations links $t \rightarrow t^{\prime}$ are for $t>t^{\prime}$ ("past citations") but there is small number (12126 $=2.6 \times 10^{-3} N_{\ell}$ ) of links $t \rightarrow t^{\prime}$ with $t \leq t^{\prime}$ corresponding to

## future citations.

Spectrum by "double-precision" Arnoldi method with $n_{A}=8000$ :


Numerical problem: eigenvalues with $|\lambda|<0.3-0.4$ are not reliable! Reason: large Jordan subspaces associated to the eigenvalue $\lambda=0$.
"very bad" Jordan perturbation theory:
Consider a "perturbed" Jordan block of size $D$ :

$$
\left(\begin{array}{ccccc}
0 & 1 & \cdots & 0 & 0 \\
0 & 0 & \cdots & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \cdots & 0 & 1 \\
\varepsilon & 0 & \cdots & 0 & 0
\end{array}\right)
$$

characteristic polynomial: $\lambda^{D}-(-1)^{D} \varepsilon$
$\varepsilon=0 \quad \Rightarrow \quad \lambda=0$
$\varepsilon \neq 0 \quad \Rightarrow \quad \lambda_{j}=-\varepsilon^{1 / D} \exp (2 \pi i j / D)$
for $D \approx 10^{2}$ and $\varepsilon=10^{-16} \Rightarrow$ "Jordan-cloud" of artifical eigenvalues due to rounding errors in the region $|\lambda|<0.3-0.4$.

## Triangular approximation

Remove the small number of links due to "future citations".
Semi-analytical diagonalization is possible:

$$
S=S_{0}+e d^{T} / N
$$

where $e_{n}=1$ for all nodes $n, d_{n}=1$ for dangling nodes $n$ and $d_{n}=0$ otherwise. $S_{0}$ is the pure link matrix which is nil-potent:

$$
S_{0}^{l}=0 \text { with } l=352
$$

Let $\psi$ be an eigenvector of $S$ with eigenvalue $\lambda$ and $C=d^{T} \psi$.

- If $C=0 \Rightarrow \psi$ eigenvector of $S_{0} \Rightarrow \lambda=0$ since $S_{0}$ nil-potent. These eigenvectors belong to large Jordan blocks and are responsible for the numerical problems.
Note: Similar situation as in network of integer numbers where $l=\left[\log _{2}(N)\right]$ and numerical instability for $|\lambda|<0.01$.
- If $C \neq 0 \Rightarrow \lambda \neq 0$ since the equation $S_{0} \psi=-C e / N$ does not have a solution $\Rightarrow \lambda 1-S_{0}$ invertible.

$$
\begin{gathered}
\Rightarrow \psi=C\left(\lambda \mathbf{1}-S_{0}\right)^{-1} e / N=\frac{C}{\lambda} \sum_{j=0}^{l-1}\left(\frac{S_{0}}{\lambda}\right)^{j} e / N . \\
\text { From } \lambda^{l}=\left(d^{T} \psi / C\right) \lambda^{l} \Rightarrow \mathcal{P}_{r}(\lambda)=0
\end{gathered}
$$

with the reduced polynomial of degree $l=352$ :

$$
\mathcal{P}_{r}(\lambda)=\lambda^{l}-\sum_{j=0}^{l-1} \lambda^{l-1-j} c_{j}=0 \quad, \quad c_{j}=d^{T} S_{0}^{j} e / N
$$

$\Rightarrow$ at most $l=352$ eigenvalues $\lambda \neq 0$ which can be numerically determined as the zeros of $\mathcal{P}_{r}(\lambda)$.
However: still numerical problems:

- $c_{l-1} \approx 3.6 \times 10^{-352}$
- alternate sign problem with a strong loss of significance.
- big sensitivity of eigenvalues on $c_{j}$


## Solution:

Using the multi precision library GMP with 256 binary digits the zeros of $\mathcal{P}_{r}(\lambda)$ can be determined with accuracy $\sim$ $10^{-18}$.
Furthermore the Arnoldi method can also be implemented with higher precision.
red crosses: zeros of $\mathcal{P}_{r}(\lambda)$ from 256 binary digits calculation
blue squares: eigenvalues from Arnoldi method with $52,256,512,1280$ binary digits. In the last case: $\Rightarrow$ break off at $n_{A}=352$ with vanishing coupling element.


## Full Physical Review network

High precision Arnoldi method for full Physical Review network (including the "future citations") for 52, 256, 512, 768 binary digits and $n_{A}=2000$ :


## Degeneracies



High precision in Arnoldi method is "bad" to count the degeneracy of certain degenerate eigenvalues.

In theory the Arnoldi method cannot find several eigenvectors for degenerate eigenvalues, a shortcoming which is (partly) "repaired" by rounding errors.

Q: How are highly degenerate core space eigenvalues possible?

## Semi-analytical argument for the full PR network:

$S=S_{0}+e d^{T} / N \Rightarrow$ two groups of eigenvectors $\psi$

1. Those with $d^{T} \psi=0 \quad \Rightarrow \quad \psi$ is also an eigenvector of $S_{0}$.

Determine degenerate subspace eigenvalues of $S_{0}$ of the form: $\lambda= \pm 1 / \sqrt{n}$ with $n=1,2,3, \ldots$
2. Those with $d^{T} \psi \neq 0 \quad \Rightarrow \mathcal{R}(\lambda)=0$ with the rational function:

$$
\mathcal{R}(\lambda)=1-d^{T} \frac{\mathbf{1}}{\lambda \mathbf{1}-S_{0}} e / N=1-\sum_{j=0}^{\infty} c_{j} \lambda^{-1-j} \approx \frac{P_{n_{R}}(\lambda)}{Q_{n_{R}}(\lambda)}
$$

Determine $\mathcal{R}(\lambda)$ for $2 n_{R}+1$ values with $|\lambda|=1$ where the series converges: $\Rightarrow$ Rational interpolation method The zeros of $P_{n_{R}}(\lambda)$ are approximations of the eigenvalues of $S$. The maximal value of $n_{R}$ for reliable eigenvalues depends on the precision $p$ of binary digits: e. g. $p=1024 \Rightarrow n_{R}=300$.

## Examples:

Some "artificial zeros" for $n_{R}=340$ and $p=1024$ (left top and middle pane/s) where both variants of the method differ.

For $n_{R}=300$ and $p=1024$ most zeros coincide with HP Arnoldi method (right top and middle panels) and both variants of the method coincide.

Lower panels: comparison for $n_{R}=$ 2000, $p=12288$ (left) or for $n_{R}=$ $2500, p=16384$ with HP Arnoldi method.


Accurate eigenvalue spectrum for the full Physical Review network by the rational interpolation method (left) and the HP Arnoldi method (right):




## Random Perron-Frobenius

## matrices

Construct random matrix ensembles $G_{i j}$ such that:

- $G_{i j} \geq 0$
- $G_{i j}$ are (approximately) non-correlated and distributed with the same distribution $P\left(G_{i j}\right)$ (of finite variance $\sigma^{2}$ ).
- $\sum_{j} G_{i j}=1 \quad \Rightarrow \quad\left\langle G_{i j}\right\rangle=1 / N$
- $\Rightarrow$ average of $G$ has one eigenvalue $\lambda_{1}=1$ ( $\Rightarrow$ "flat" PageRank) and other eigenvalues $\lambda_{j}=0$ (for $j \neq 1$ ).
- degenerate perturbation theory for the fluctuations $\Rightarrow$ circular eigenvalue density with $R=\sqrt{N} \sigma$ and one unit eigenvalue.


## Different variants of the model:

- uniform full: $P(G)=N / 2$ for $0 \leq G \leq 2 / N$
$\Rightarrow \quad R=1 / \sqrt{3 N}$
- uniform sparse with $Q$ non-zero elements per column: $P(G)=Q / 2$ for $0 \leq G \leq 2 / Q$ with probability $Q / N$ and $G=0$ with probability $1-Q / N$
$\Rightarrow \quad R=2 / \sqrt{3 Q}$
- constant sparse with $Q$ non-zero elements per column: $G=1 / Q$ with probability $Q / N$ and $G=0$ with probability $1-Q / N$

$$
\Rightarrow \quad R=1 / \sqrt{Q}
$$

- powerlaw with $p(G)=D(1+a G)^{-b}$ for $0 \leq G \leq 1$ and $2<b<3$ :

$$
\Rightarrow \quad R=C(b) N^{1-b / 2} \quad, \quad C(b)=(b-2)^{(b-1) / 2} \sqrt{\frac{b-1}{3-b}}
$$

## Numerical verification:

uniform full:
$N=400$
uniform sparse:
$N=400$,
$Q=20$
power law:
$b=2.5$


triangular random and average
constant sparse:
$N=400$,
$Q=20$
power law case:
$R_{\mathrm{th}} \sim N^{-0.25}$

## Conclusion

- Accurate eigenvalue computation requires determination of invariant subspaces.
- Eigenvalue spectra for many different network examples.
- Mainly localized eigenvectors for the Wikipedia network: identification of themes or communities.
- Subtle numerical problems for the eigenvalue problem of the Physical Review citation network which can be solved by a semi-analytical method and a high precision implementation of the Arnoldi method.
- Random Perron-Frobenius matrices with nearly uniform circular eigenvalue density: $R \sim 1 / \sqrt{Q}$ for $Q$ non-zero elements per column.
- Understanding of the degeneracies of core space eigenvalues and a decompostion of the core space eigenvalues in two groups. Important role of subspaces of $S_{0}$ (very different from the subspaces of $S$ !).
- New rational interpolation method to determine accurately the eigenvalues of a network matrix. Well suited for nearly triangular matrices but works in principle also for other case (e. g. Wikipedia but less efficient here).
- Drastic effect of the triangular approximation on the eigenvalue spectrum. Strong reduction of non-vanishing eigenvalues, from about $\sim 8000-10000$ to 352 and only very few eigenvalues on the real axis. This implies a very strong effect of the few future citations on the spectrum.
- Very useful applications of the GNU high precision library GMP: http://gmplib.org/ for different numerical methods: determination of zeros of the reduced polynomial, rational interpolation method, Arnoldi method.


## Appendix:

The subspace of $\lambda \neq 0$ is represented by the vectors $v^{(j)}=S_{0}^{j-1} e / N$ for $j=1, \ldots, l$

$$
\Rightarrow \quad S v^{(j)}=c_{j-1} v^{(1)}+v^{(j+1)}=\sum_{k=0}^{l-1} \bar{S}_{k, j} v^{(k)}
$$

"Small" $l \times l$-representation matrix :

$$
\bar{S}=\left(\begin{array}{ccccc}
c_{0} & c_{1} & \cdots & c_{l-2} & c_{l-1} \\
1 & 0 & \cdots & 0 & 0 \\
0 & 1 & \cdots & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \cdots & 1 & 0
\end{array}\right) \quad, \quad \bar{P}=C\left(\begin{array}{c}
1 \\
1 \\
1 \\
\vdots \\
1
\end{array}\right)
$$

with $P=\sum_{j} \bar{P}_{j} v^{(j)}=C \sum_{j} v^{(j)}$ and due to sum rule: $\sum_{j} c_{j}=1$.

