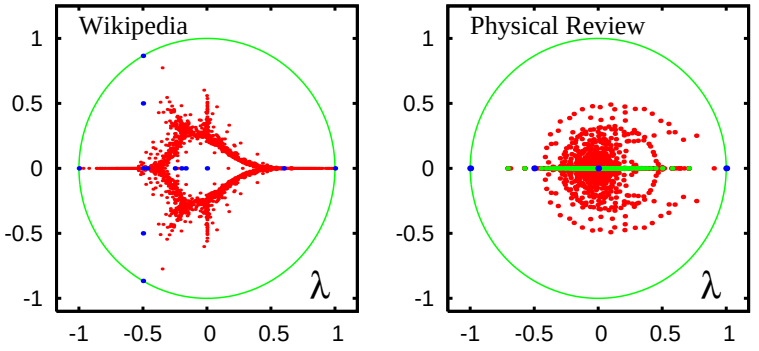

Spectral properties of Google matrix

Lecture 1

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Contents

Perron-Frobenius operators

Consider a physical system with N states $i = 1, \ldots, N$ and probabilities $p_i(t) \geq 0$ evolving by a discrete ***Markov process***:

$$p_i(t+1) = \sum_j G_{ij}\, p_j(t)$$

The transition probabilities G_{ij} provide a ***Perron-Frobenius*** matrix G such that:

$$\sum_i G_{ij} = 1 \quad , \quad G_{ij} \geq 0 \, .$$

Conservation of probability:

$\|G\,v\|_1 = \|v\|_1$ if $v_i \in \mathbb{R}$ and $v_i \geq 0 \;\Rightarrow\; \|p(t+1)\|_1 = \|p(t)\|_1 = 1.$

$\|G\,v\|_1 \leq \|v\|_1$ for any other (complex) vector

where $\|v\|_1 = \sum_i |v_i|$ is the usual 1-norm.

In general $G^T \neq G$ and eigenvalues λ may be complex.

If v is a (right) eigenvector of G: $\quad G\,v = \lambda\,v \quad \Rightarrow \quad |\lambda| \leq 1.$

The vector $e^T = (1,\,\ldots,\,1)$ is left eigenvector with $\lambda = 1$:

$$e^T\,G = 1\;e^T$$

$\Rightarrow$ existence of (at least) one right eigenvector P for $\lambda = 1$ also called ***PageRank*** in the context of Google matrices:

$$\boxed{G\,P = 1\;P}$$

Biorthogonality between left and right eigenvectors:

$G\,v = \lambda\,v$ and $w^T\,G = \tilde{\lambda}\,w^T \quad \Rightarrow \quad \boxed{w^T\,v = 0 \quad \text{if} \quad \lambda \neq \tilde{\lambda}\;.}$

Expansion in terms of eigenvectors:

$$p(0) = \sum_j C_j \, v^{(j)} \quad \Rightarrow \quad p(t) = \sum_j C_j \, \lambda_j^t \, v^{(j)}$$

with $\lambda_1 = 1$ and $v^{(1)} = P$. If $C_1 \neq 0$ and $|\lambda_j| < 1$ for $j \geq 2$

$$\Rightarrow \qquad \lim_{t \to \infty} p(t) = P \, .$$

$\Rightarrow$ ***Powermethod*** to compute P

Rate of convergence:

$$\sim |\lambda_2|^t = e^{t \, \ln(1-(1-|\lambda_2|))} \approx e^{-t(1-|\lambda_2|)}$$

$\Rightarrow$ Problem if $1 - |\lambda_2| \ll 1$ of even if $|\lambda_2| = 1$.

Complications if G is not diagonalizable

The eigenvectors do not constitute a full basis and further ***generalized eigenvectors*** are required:

$$\begin{aligned}(\lambda_j \mathbf{1} - G)\, v^{(j,0)} &= 0 \\ (\lambda_j \mathbf{1} - G)\, v^{(j,1)} &= v^{(j,0)} \\ (\lambda_j \mathbf{1} - G)\, v^{(j,2)} &= v^{(j,1)} \\ &\vdots\end{aligned}$$

$\Rightarrow$ Contributions $\sim t^l\, \lambda_j^t$ with $l = 0,\, 1,\, \ldots$ in $p(t)$ expansion.

However, for $\lambda_1 = 1$ only $l = 0$ is possible since otherwise:

$$\|p(t)\|_1 \approx \text{const.}\, t^l \quad \rightarrow \quad \infty\,.$$

“Analogy” with hamiltonian quantum systems

$$i\hbar \frac{\partial}{\partial t}\,\psi(t) = H\,\psi(t)$$

where $\psi(t)$ quantum state and $H = H^\dagger$ is a hermitian (or real symmetric) operator.

Expansion in terms of eigenvectors: $H\,\varphi^{(j)} = E_j\,\varphi^{(j)}$

$$\boxed{\psi(t) = \sum_j C_j\, e^{-i\,E_j\,t/\hbar}\,\varphi^{(j)}}$$

- H is always diagonalizable with $E_j \in \mathbb{R}$ and $(\varphi^{(k)})^T\,\varphi^{(j)} = \delta_{kj}$.
- Eigenvectors $\varphi^{(j)}$ are valid *physical states* while for PF operators only real vectors with positive entries are physical states and most eigenvectors are complex.

Example hamilontian operators:

- Disorder Anderson model in 1 dimension:

$$H_{jk} = -(\delta_{j,k+1} + \delta_{j,k-1}) + \varepsilon_j \, \delta_{j,k}$$

with random on-site energies $\varepsilon_j \in [-W/2, W/2] \quad \Rightarrow$ localized eigenvectors $\varphi_l \sim e^{-|l-l_0|/\xi}$ with localization length $\xi \sim W^{-2}$. General mesure of localization length by ***inverse participation ratio*** :

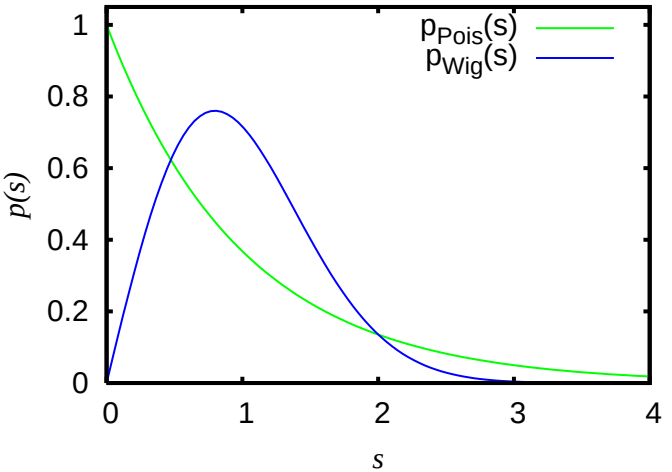
$$\frac{1}{\xi_{\mathrm{IPR}}} = \frac{\sum_l \varphi_l^4}{(\sum_l \varphi_l^2)^2} \sim \frac{1}{\xi}$$

- Gaussian Orthogonal Ensemble (GOE): $H_{jk} = H_{kj} \in \mathbb{R}$ and H_{jk} independent random gaussian variables with:

$$\langle H_{jk} \rangle = 0 \quad , \quad \langle H_{jk}^2 \rangle = (1 + \delta_{jk})\sigma^2.$$

Universal level statistics

Distribution of rescaled nearest level spacing $s = (E_{j+1} - E_j)/\Delta$ with average level spacing Δ:



- ***Poisson statistics:*** $P_{\rm Pois}(s) = \exp(-s)$

  Anderson model with $\xi \ll L$ ($L =$ system size), integrable systems, . . .

- ***Wigner surmise:*** $P_{\rm Wig} = (\pi s/2)\exp(-\pi s^2/4)$

  GOE, Anderson model with $\xi \gtrsim L$, generic (classically) chaotic systems, . . .

PF Operators for directed networks

Consider a directed network with N nodes $1, \ldots, N$ and N_ℓ links.

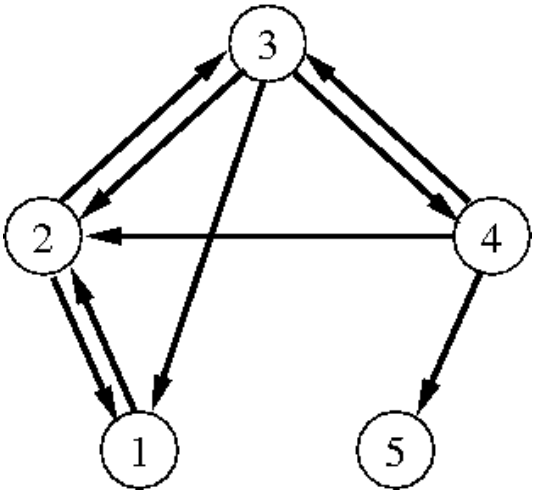
- Define the adjacency matrix by $A_{jk} = 1$ if there is a link $k \to j$ and $A_{jk} = 0$ otherwise. In certain cases, when explicitely considering multiple links, one may have $A_{jk} = m$ where $m =$ multiplicity of a a link (e. g. Network for integer numbers).

- Define a matrix S_0 from A by sum-normalizing each non-zero column to one and keeping zero columns.

- Define a matrix S from S_0 by replacing each zero column with $1/N$ entries.

- Same procedure for inverted network: $A^* \equiv A^T$ and S^* is obtained in the same way from A^*. Note: in general: $S^* \neq S^T$. Leading (right) eigenvector of S^* is called ***CheiRank***.

Example:



$$A = \begin{pmatrix} 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

$$S_0 = \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{3} & 0 & 0 \\ 1 & 0 & \frac{1}{3} & \frac{1}{3} & 0 \\ 0 & \frac{1}{2} & 0 & \frac{1}{3} & 0 \\ 0 & 0 & \frac{1}{3} & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{3} & 0 \end{pmatrix} \quad , \quad S = \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{3} & 0 & \frac{1}{5} \\ 1 & 0 & \frac{1}{3} & \frac{1}{3} & \frac{1}{5} \\ 0 & \frac{1}{2} & 0 & \frac{1}{3} & \frac{1}{5} \\ 0 & 0 & \frac{1}{3} & 0 & \frac{1}{5} \\ 0 & 0 & 0 & \frac{1}{3} & \frac{1}{5} \end{pmatrix}$$

The nodes with no out-going links, associated to zero columns in A, are called ***dangling nodes***. On can formally write:

$$S = S_0 + \frac{1}{N}\, e\, d^T$$

with $d =$ dangling vector with $d_j = 1$ for dangling nodes and $d_j = 0$ for other nodes and $e =$ uniform unit vector with $e_j = 1$ for all nodes.

Damping factor

Define for $0 < \alpha < 1$, typically $\alpha = 0.85$, the matrix:

$$G(\alpha) = \alpha S + (1 - \alpha)\, \frac{1}{N}\, e e^T$$

- G is also PF operator with columns sum normalized.
- G has the eigenvalue $\lambda_1 = 1$ with multiplicity $m_1 = 1$ and other eigenvalues are $\alpha\lambda_j$ (for $j \geq 2$) with $\lambda_j =$ eigenvalues of S. The right eigenvectors for $\lambda_j \neq 1$ are not modified (since they are orthogonal to the left eigenvector e^T for $\lambda_1 = 1$).
- Similar expression for $G^*(\alpha)$ using S^*.

Numerical diagonalization

- Powermethod to obtain P: rate of convergence for $G(\alpha)$ is better than $\sim \alpha^t$.

- Full "exact" diagonalization: possible for $N \lesssim 10^4$:
  memory usage $\sim N^2$ and computation time $\sim N^3$.

- Arnoldi method to determine largest $n_A \sim 10^2 - 10^4$ eigenvalues:
  memory usage $\sim N\, n_A + C_1\, N_\ell + C_2\, n_A^2$ and
  computation time $\sim N\, n_A^2 + C_3\, N_\ell\, n_A + C_4\, n_A^3$.

- Strange numerical problems to determine accurately "small" eigenvalues, in particular for (nearly) triangular network structure due to large Jordan-blocks ($\Rightarrow$ $3^{\rm rd}$ *lecture*).

Arnoldi method

to (partly) diagonalize large sparse non-symmetric $N \times N$ matrices G such that the product "$G\times$vecteur" can be computed efficiently (G may contain some constant columns $\sim e$):

- choose an initial normalized vector ξ_0 (random or "otherwise")
- determine the ***Krylov space*** of dimension n_A (typically: $1 \ll n_A \ll N$) spanned by the vectors: $\xi_0,\, G\,\xi_0,\, \ldots,\, G^{n_A-1}\xi_0$
- determine by ***Gram-Schmidt*** orthogonalization an orthonormal basis $\{\xi_0,\, \ldots,\, \xi_{n-1}\}$ and the representation of G in this basis:

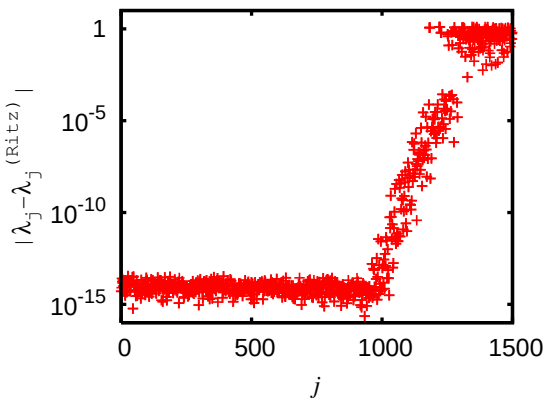
$$G\,\xi_k = \sum_{j=0}^{k+1} H_{jk}\,\xi_j$$

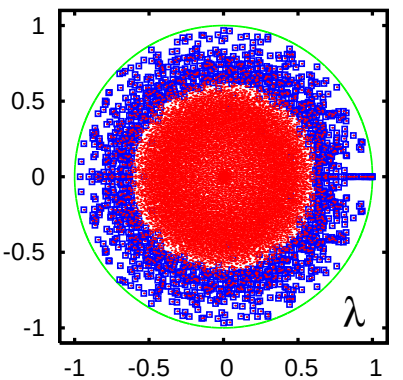
Note: if $G = G^T \;\Rightarrow\; H =$ tridiagonal symmetric and the ***Arnoldi method*** is identical to the ***Lanczos method***.

- 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 G.





Example: PF Operator for Ulam-Map ($\Rightarrow$ 2^{nd} *lecture*)

$N = 16609,\ N_\ell = 76058,\ n_A = 1500$

Invariant subspaces

In realistic WWW networks invariant subspaces of nodes create large degeneracies of λ_1 (or λ_2 if $\alpha < 1$) which is very problematic for the Arnoldi method.

Therefore determine the ***invariant subspaces*** as follows:

Let $N_c = bN$ a certain fraction of the network size N (e.g. $b = 0.1$).

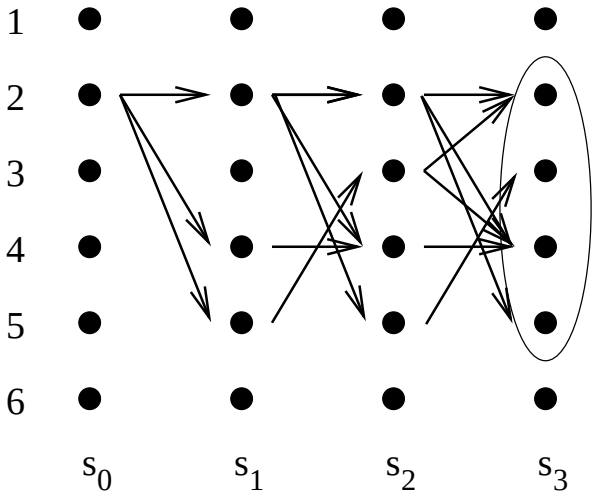
- For a given initial node i_0 determine a sequence of node sets s_n by $s_0 = \{i_0\}$ and s_{n+1} is the set containing all nodes of s_n and those which can be reached by a link from a node in s_n.

- If $s_n = s_{n+1}$ with at most N_c elements for some $n \Rightarrow s_n$ is an ***invariant subspace***.

- If for some n the set s_n contains a dangling node (connected by construction to any other node) or if s_n contains more than N_c elements $\Rightarrow i_0$ is identified as a node belonging to the ***core space*** (space of nodes not belonging to an invariant subspace).
- Repeat the procedure for every network node as potential initial node except for those nodes which are already identified as subspace nodes. If for some n the set s_n contains a previously found core space node $\Rightarrow i_0$ also belongs to the core space.
- Merge all subspaces with common members. In this way one obtains a decomposition of the network in many ***separate subspaces*** with N_s nodes and a "big" ***core space***.

This procedure can be efficiently implemented as a computer program. It turns out that for most networks the exact choice of b is not important (e.g. $b = 0.1$ or $b = 0.9$) as long as $b = \mathcal{O}(1)$. Note that a core space node may have a link to an invariant subspace but a subspace node may not have a link to another subspace or the core space.

Example:



$s_0 = \{2\}$

$s_1 = \{2, 4, 5\}$

$s_2 = \{2, 3, 4, 5\} = s_3 =$ invariant subspace

The decomposition in subspaces and a core space implies a block structure of the matrix S:

$$S = \begin{pmatrix} S_{ss} & S_{sc} \\ 0 & S_{cc} \end{pmatrix}$$

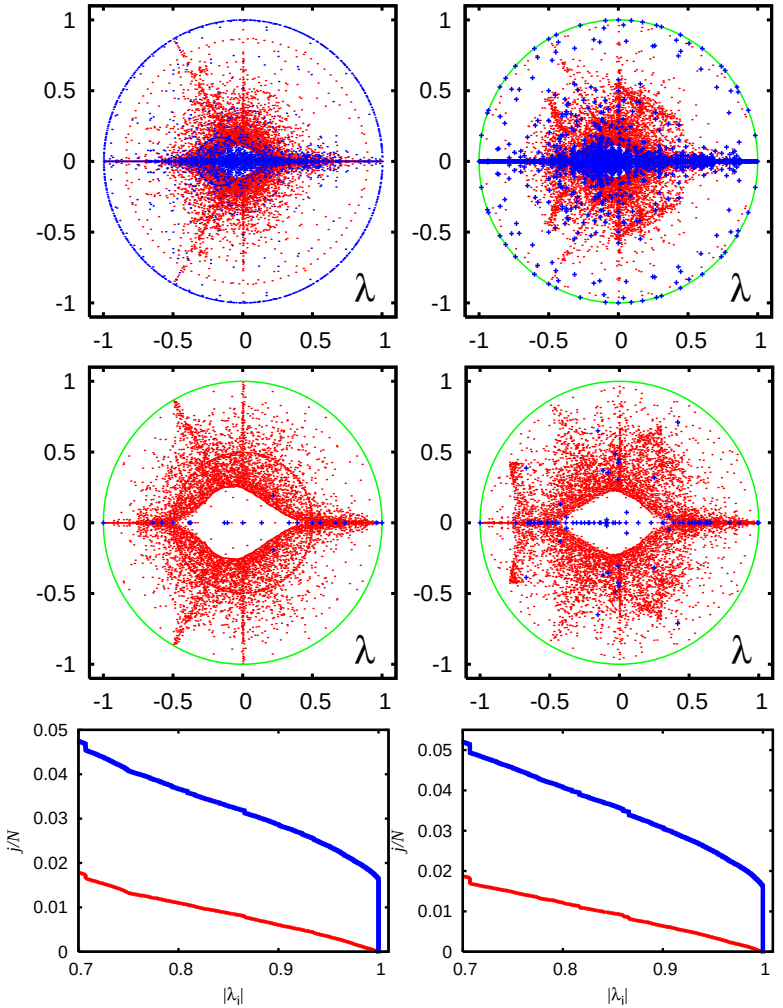
where S_{ss} is block diagonal according to the subspaces. The subspace blocks of S_{ss} are all matrices of PF type with at least one eigenvalue $\lambda_1 = 1$ explaining the high degeneracies.

To determine the spectrum of S apply:

- Exact (or Arnoldi) diagonalization on each subspace.

- The Arnoldi method to S_{cc} to determine the largest core space eigenvalues λ_j (note: $|\lambda_j| < 1$). The largest eigenvalues of S_{cc} are no longer degenerate but other degeneracies are possible (e.g. $\lambda_j = 0.9$ for Wikipedia).

University Networks



Cambridge 2006 (left),
$N = 212710$, $N_s = 48239$

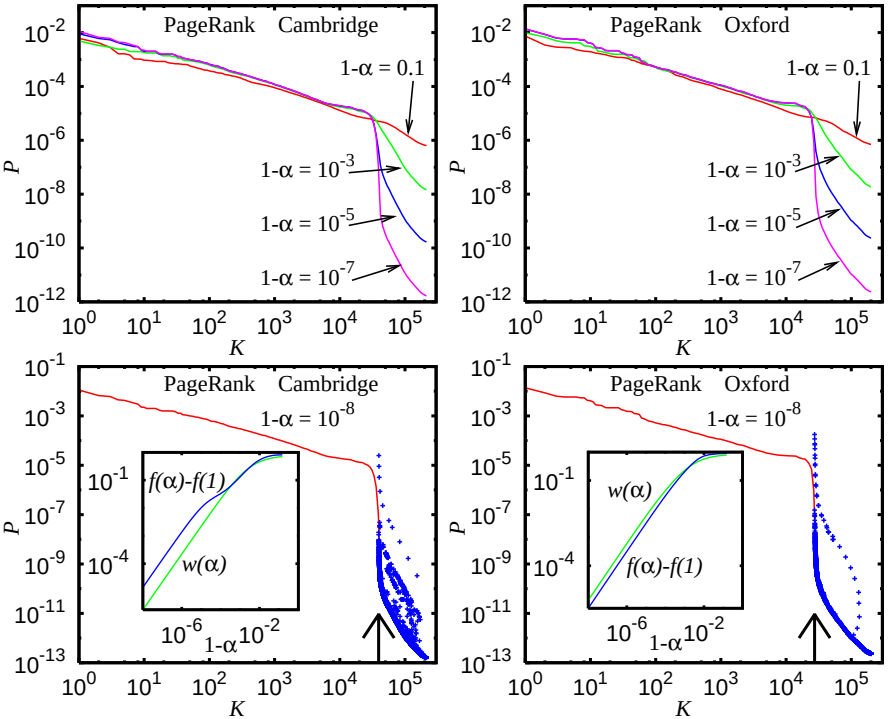
Oxford 2006 (right),
$N = 200823$, $N_s = 30579$

Spectrum of S (upper panels), S^* (middle panels) and dependence of rescaled level number on $|\lambda_j|$ (lower panels).

Blue: subspace eigenvalues

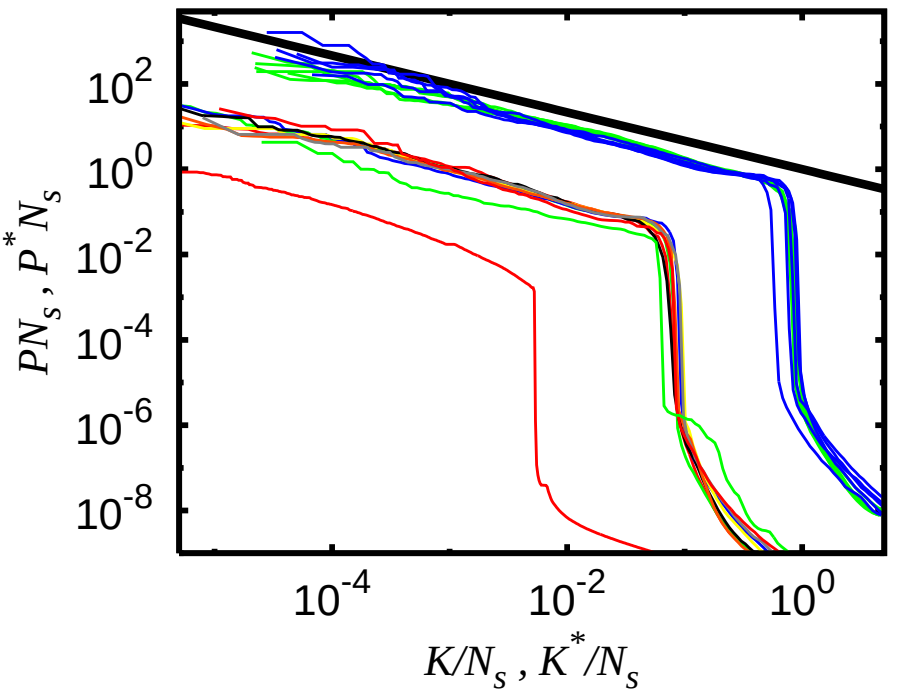
Red: core space eigenvalues (with Arnoldi dimension $n_A = 20000$)

PageRank for $\alpha \to 1$:



$$P = \underbrace{\sum_{\lambda_j=1} c_j \, \psi_j}_{\text{subspace contributions}} + \sum_{\lambda_j \neq 1} \frac{1-\alpha}{(1-\alpha)+\alpha(1-\lambda_j)} \, c_j \, \psi_j \; .$$

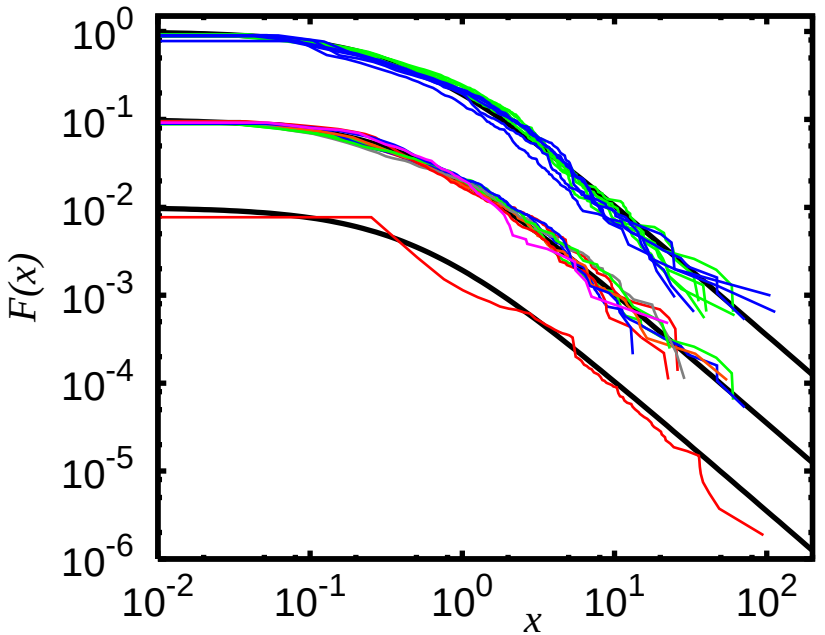
Rescaled PageRank at $\alpha = 1 - 10^{-8}$:



Top: Cambridge, Oxford 2002-2006; middle: other universities; bottom: Wikipedia*; black line $\propto K^{-2/3}$; $N_s =$ sum of all subspace dimensions.

Distribution of dimensions of invariant subspaces

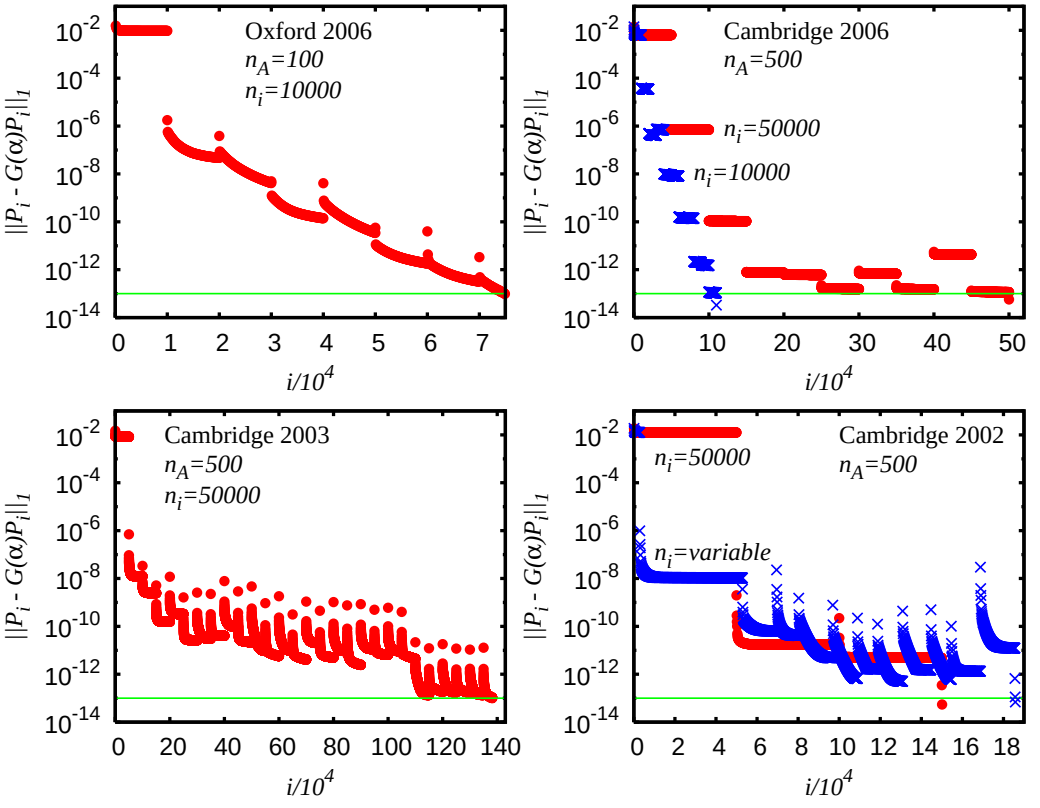
$F(x) =$ fraction of invariant subspaces with dimension larger than $x\langle d\rangle$ where $\langle d\rangle =$ average subspace dimension.



Top: Cambridge, Oxford 2002-2006; middle: other universities; bottom: Wikipedia*; black line: $F(x) = 1/(1+2x)^{3/2}$.

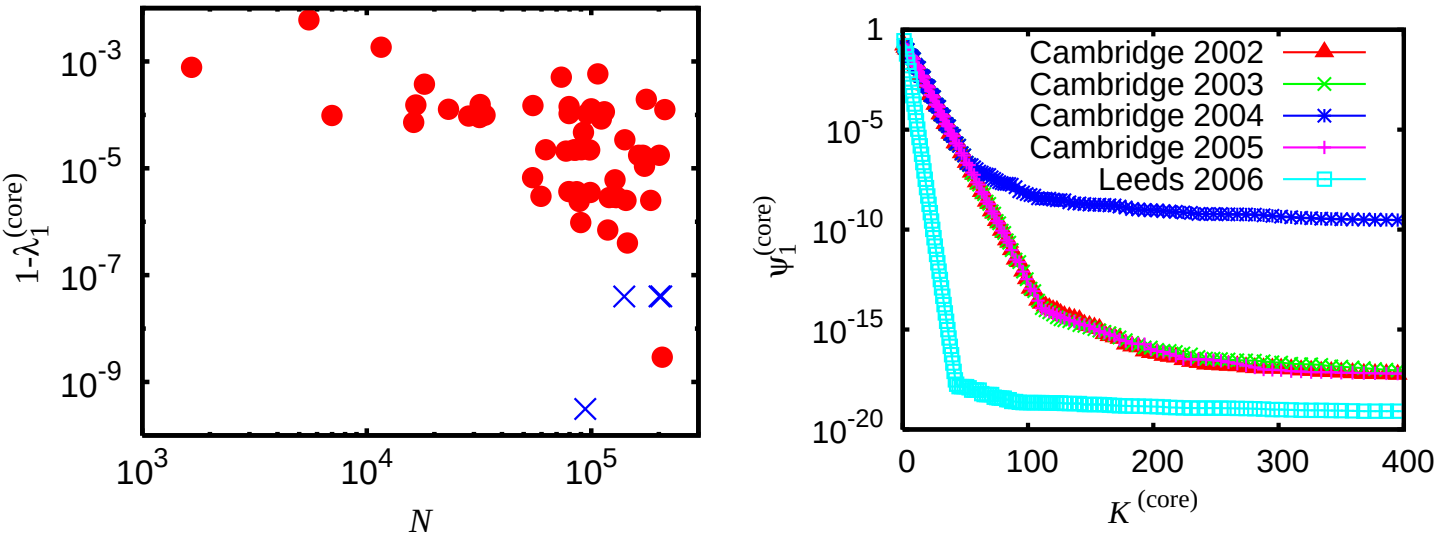
Numerical PageRank method for $\alpha \to 1$

Combination of power method and Arnoldi diagonalization :



Here: $\alpha = 1 - 10^{-8}$

Core space gap and quasi-subspaces



Left: Core space gap $1 - \lambda_1^{(\mathrm{core})}$ vs N for certain british universities.

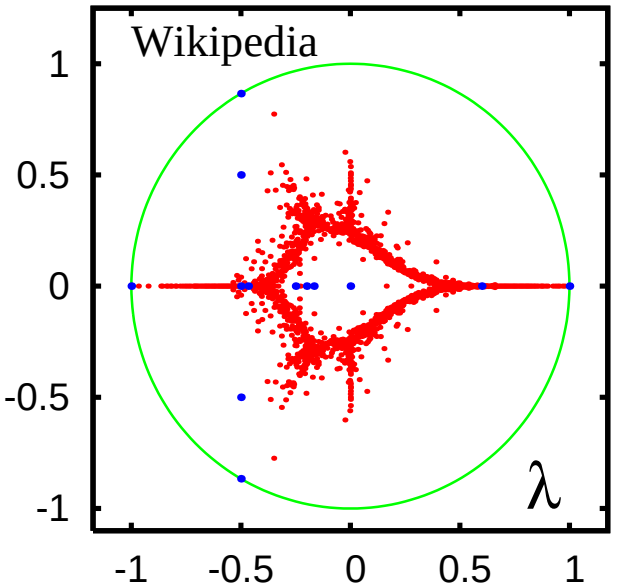
Red dots for gap $> 10^{-9}$; blue crosses (moved up by 10^9) for gap $< 10^{-16}$.

Right: first core space eigenvecteur for universities with gap $< 10^{-16}$ or gap $= 2.91 \times 10^{-9}$ for Cambridge 2004.

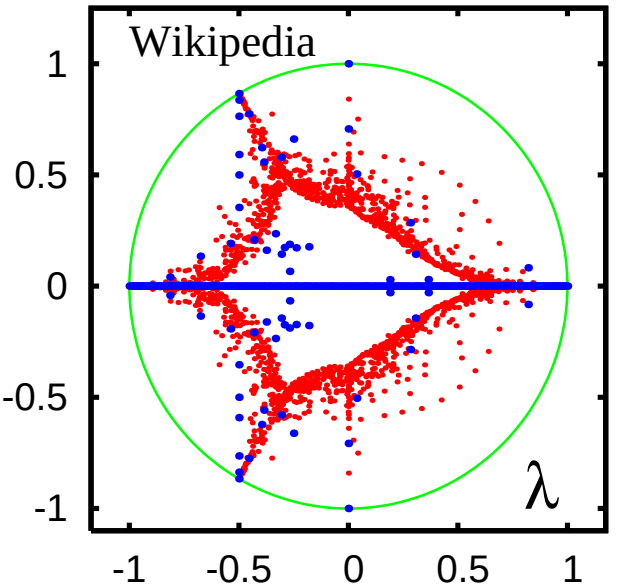
Core space gaps $< 10^{-16}$ correspond to ***quasi-subspaces*** where it takes quite many “iterations” to reach a dangling node.

Spectrum Wikipedia

Wikipedia 2009 : $N = 3282257$ nodes, $N_\ell = 71012307$ network links.



spectrum of S, $N_s = 515$

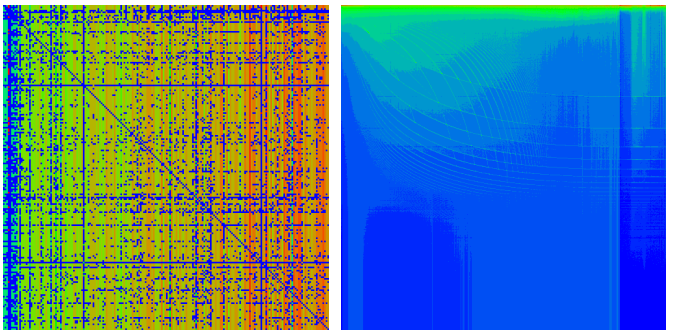


spectrum of S^*, $N_s = 21198$

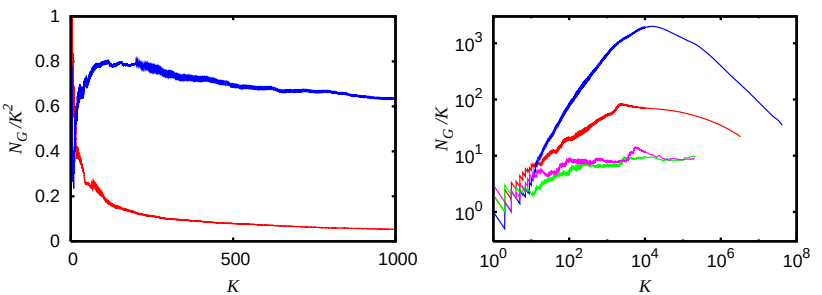
Twitter network

Twitter 2009 : $N = 41652230$ nodes, $N_\ell = 1468365182$ network links.

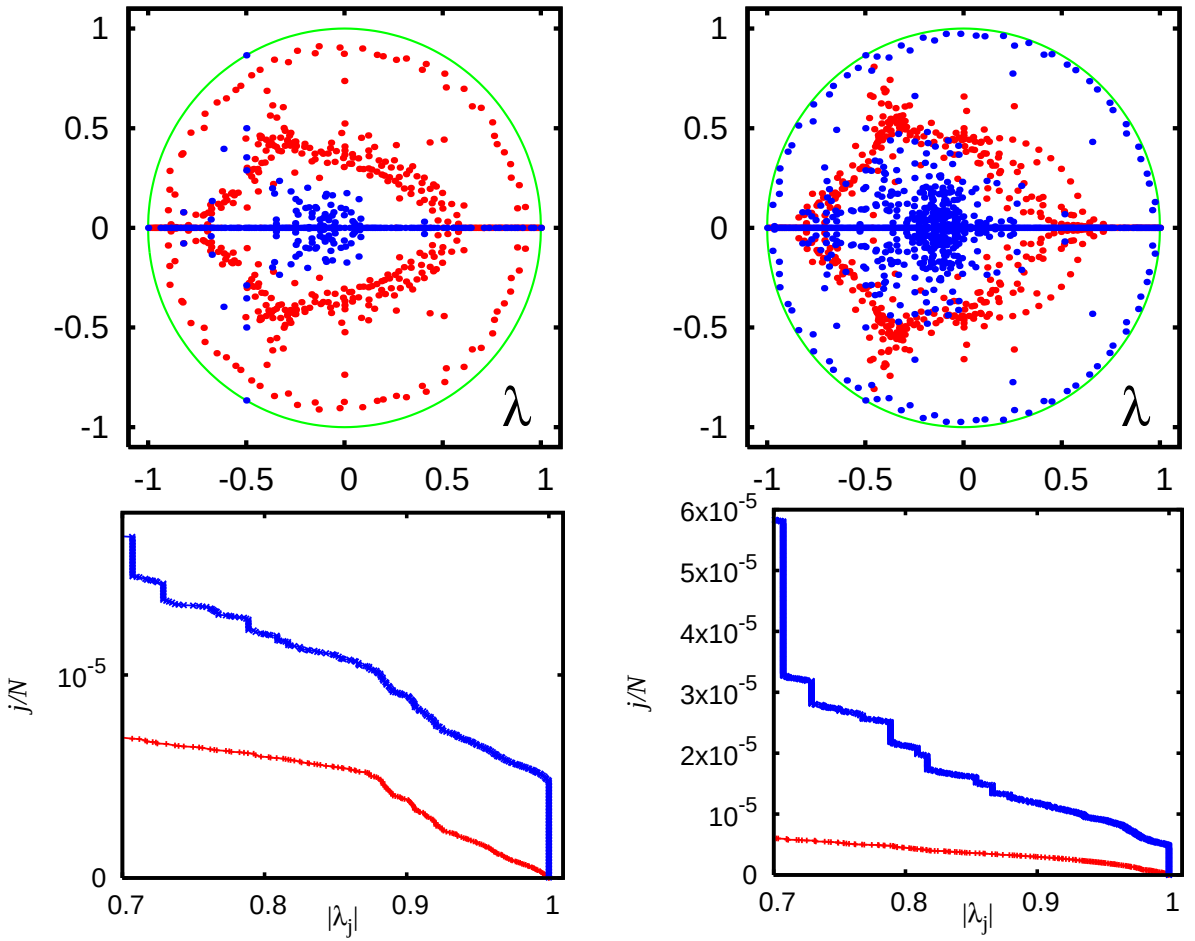
Matrix structure in K-rank order:



Number N_G of non-empty matrix elements in $K \times K$-square:

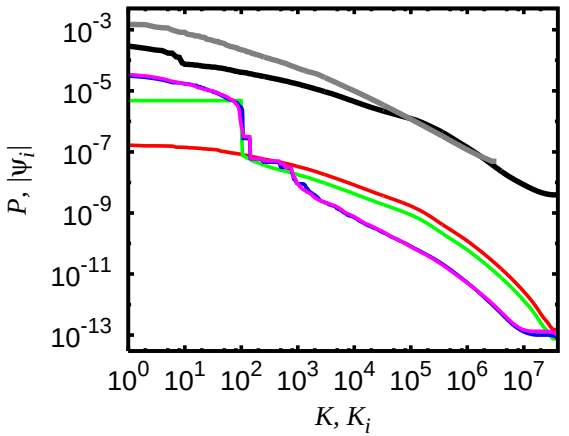


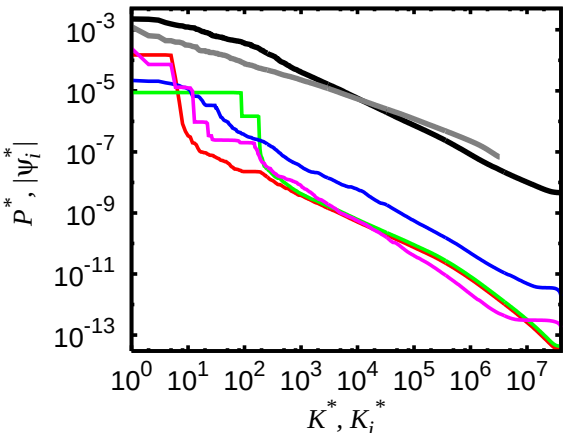
Spectrum



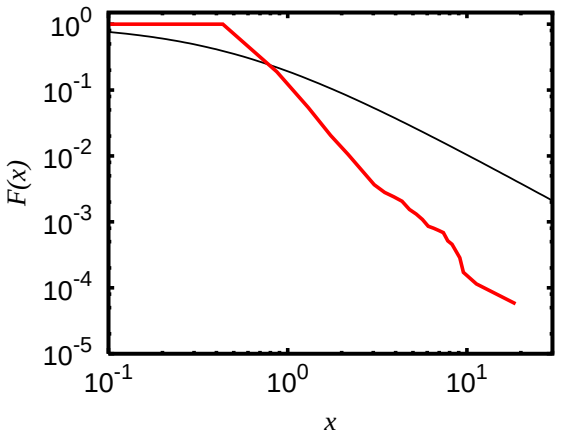
$n_A = 640 \quad \Rightarrow \quad 250$ GB of RAM memory.

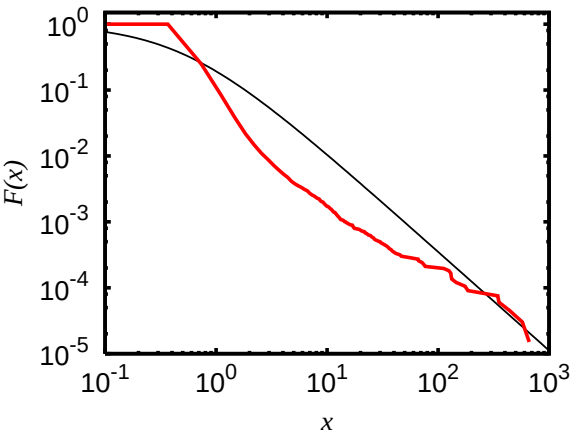
PageRank, CheiRank, eigenvectors





Subspace distribution





Black line: $F(x) = 1/(1+2x)^{3/2}$.

References

1. K. M. Frahm and D. L. Shepelyansky, ***Ulam method for the Chirikov standard map***, Eur. Phys. J. B **76**, 57 (2010).

2. K. M. Frahm, B. Georgeot and D. L. Shepelyansky, ***Universal emergence of PageRank***, J. Phys. A: Math. Theor. **44**, 465101 (2011).

3. K. M. Frahm and D. L. Shepelyansky, ***Google matrix of Twitter***, Eur. Phys. J. B **85**, 355 (2012).

4. L. Ermann, K. M. Frahm and D. L. Shepelyansky, **Spectral properties of Google matrix of Wikipedia and other networks**, Eur. Phys. J. B **86**, 193 (2013).