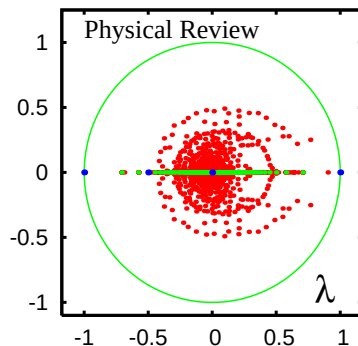
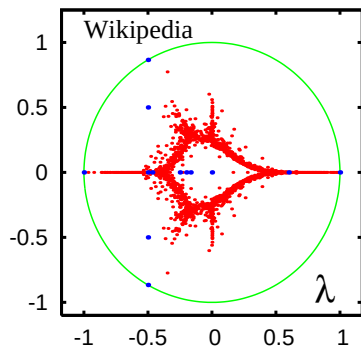




Spectral properties of Google matrix

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Quantum chaos: fundamentals and applications

Luchon, March 14 - 21, 2015

Contents

Perron-Frobenius operators	3
PF Operators for directed networks	4
PageRank	6
Numerical diagonalization	7
University Networks	9
Wikipedia	12
Twitter network	14
Random Perron-Frobenius matrices	16
Poisson statistics of PageRank	18
Physical Review network	20
Perron-Frobenius matrix for chaotic maps	26
References	35

Perron-Frobenius operators

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

$$p_i(t+1) = \sum_j G_{ij} p_j(t) \quad \text{with} \quad \sum_i G_{ij} = 1 \quad , \quad G_{ij} \geq 0 .$$

The transition probabilities G_{ij} provide a **Perron-Frobenius** matrix. Conservation of probability: $\sum_i p_i(t+1) = \sum_i p_i(t) = 1$.

In general $G^T \neq G$ and eigenvalues λ may be complex and obey $|\lambda| \leq 1$. The vector $e^T = (1, \dots, 1)$ is left eigenvector with $\lambda_1 = 1$
 $\Rightarrow$ existence of (at least) one right eigenvector P for $\lambda_1 = 1$ also called **PageRank** in the context of Google matrices: $G P = 1 P$

For non-degenerate λ_1 and finite gap $|\lambda_2| < 1$: $\lim_{t \rightarrow \infty} p(t) = P$

$\Rightarrow$ **Power method** to compute P with rate of convergence $\sim |\lambda_2|^t$.

PF Operators for directed networks

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

Adjacency matrix:

$A_{jk} = 1$ if there is a link $k \rightarrow j$ and $A_{jk} = 0$ otherwise.

Sum-normalization of each non-zero column of $A \Rightarrow S_0$.

Replacing each zero column (**dangling nodes**) with $e/N \Rightarrow S$.

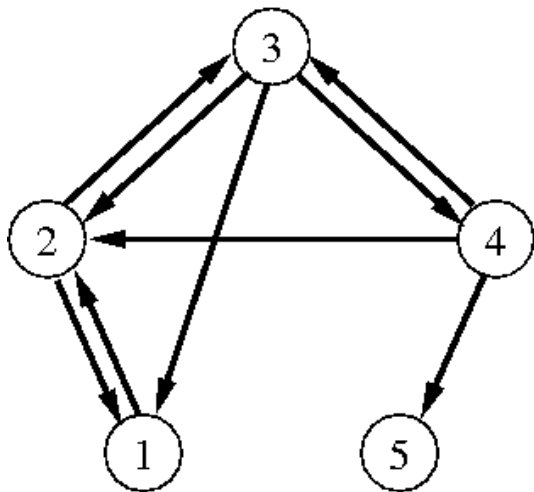
Eventually apply the **damping factor** $\alpha < 1$ (typically $\alpha = 0.85$):

Google matrix:
$$G(\alpha) = \alpha S + (1 - \alpha) \frac{1}{N} ee^T .$$

$\Rightarrow \lambda_1$ is non-degenerate and $|\lambda_2| \leq \alpha$.

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

Example:



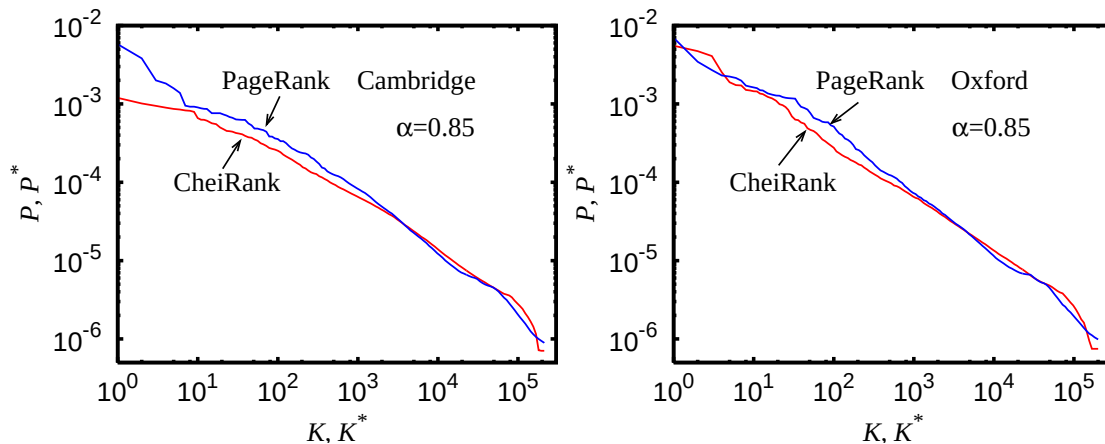
$$A = \begin{pmatrix} 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

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

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

PageRank

Example for university networks of Cambridge 2006 and Oxford 2006 ($N \approx 2 \times 10^5$ and $N_\ell \approx 2 \times 10^6$).



$$P(i) = \sum_j G_{ij} P(j)$$

$P(i)$ represents the “importance” of “node/page i ” obtained as sum of all other pages j pointing to i with weight $P(j)$. Sorting of $P(i) \Rightarrow$ index $K(i)$ for order of appearance of search results in search engines such as Google.

Numerical diagonalization

- **Power method** to obtain P : rate of convergence for $G(\alpha) \sim \alpha^t$.
- Full “exact” diagonalization ($N \lesssim 10^4$).
- **Arnoldi method** to determine largest $n_A \sim 10^2 - 10^4$ eigenvalues. Idea: write

$$G \xi_k = \sum_{j=0}^{k+1} H_{jk} \xi_j \quad \text{for } k = 0, \dots, n_A - 1$$

where ξ_{k+1} is obtained from **Gram-Schmidt** orthogonalization of $G\xi_k$ to $\xi_0, \dots, \xi_k$ with ξ_0 being some suitable normalized initial vector. $\xi_0, \dots, \xi_{n_A-1}$ span a **Krylov space** of dimension n_A and the eigenvalues of the “small” representation matrix H_{jk} are (very) good approximations to the largest eigenvalues of G .

Example for Twitter network of 2009: $N \approx 4 \times 10^7$ and $N_\ell \approx 1.5 \times 10^9$ with $n_A = 640$ (lower N in other examples allows for higher n_A).

- Practical problems due to ***invariant subspaces*** of nodes in realistic WWW networks creating large degeneracies of λ_1 (or λ_2 if $\alpha < 1$). Decomposition in subspaces and a core space

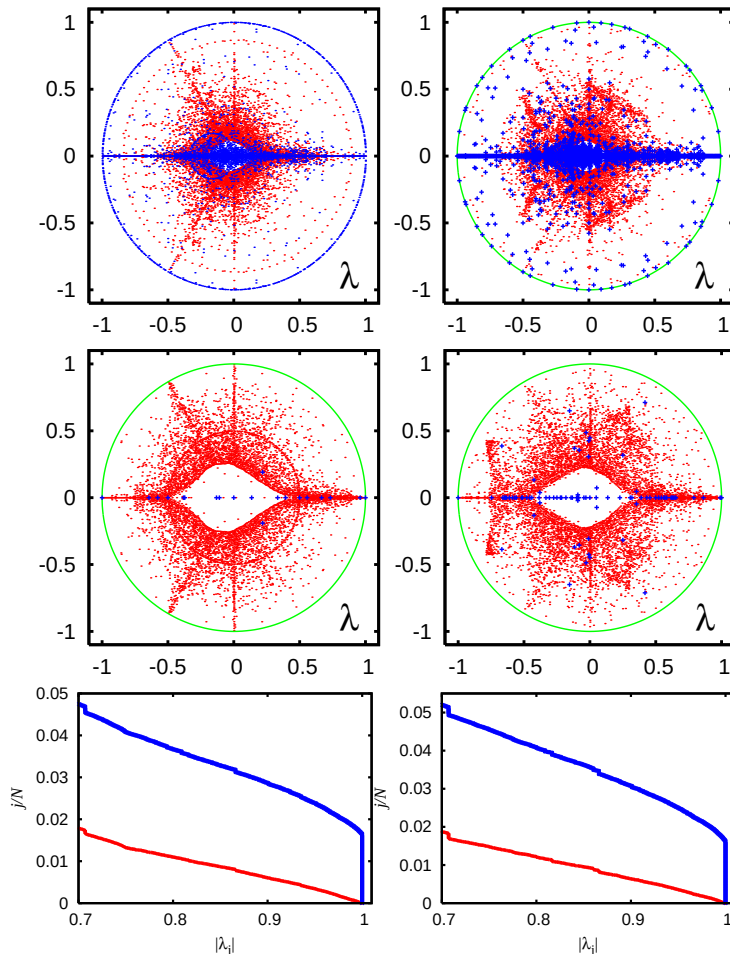
$$\Rightarrow S = \begin{pmatrix} S_{ss} & S_{sc} \\ 0 & S_{cc} \end{pmatrix}$$

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 and the Arnoldi method to S_{cc} to determine the largest core space eigenvalues λ_j (note: $|\lambda_j| < 1$).

- Strange numerical problems to determine accurately “small” eigenvalues, in particular for (nearly) ***triangular network structure*** due to large Jordan-blocks (e.g. citation network of Physical Review).

University Networks



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

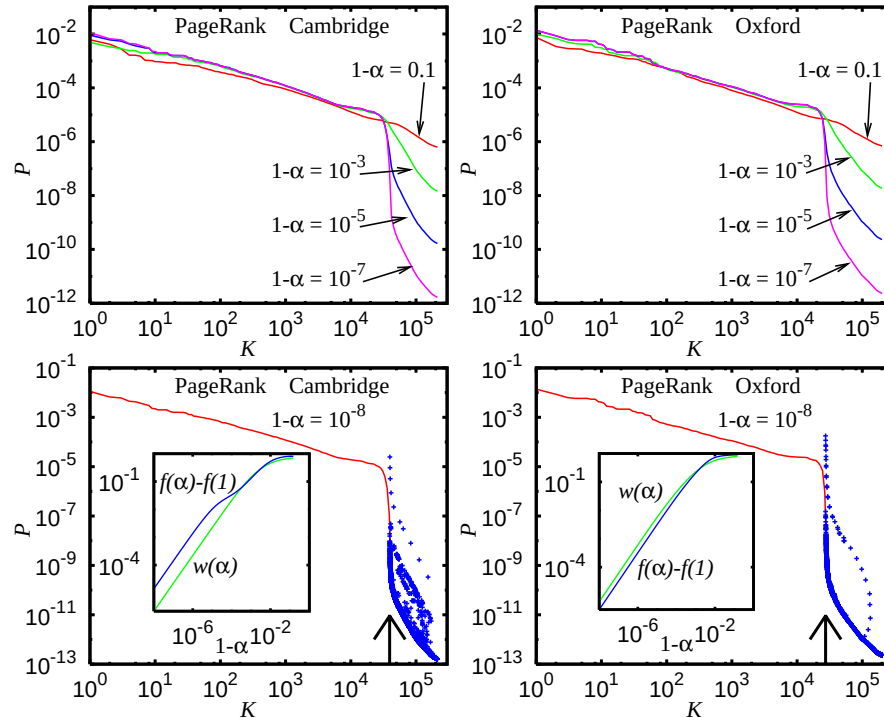
Oxford 2006 (right),
 $N = 200823$, $N_s = 30579$

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

Blue: subspace eigenvalues

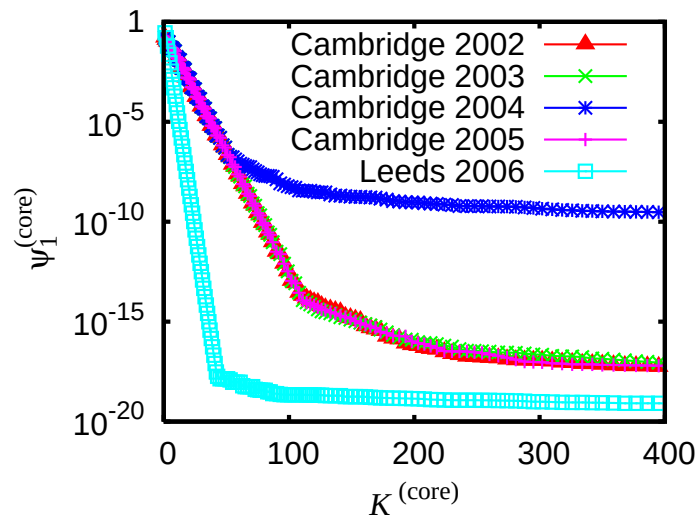
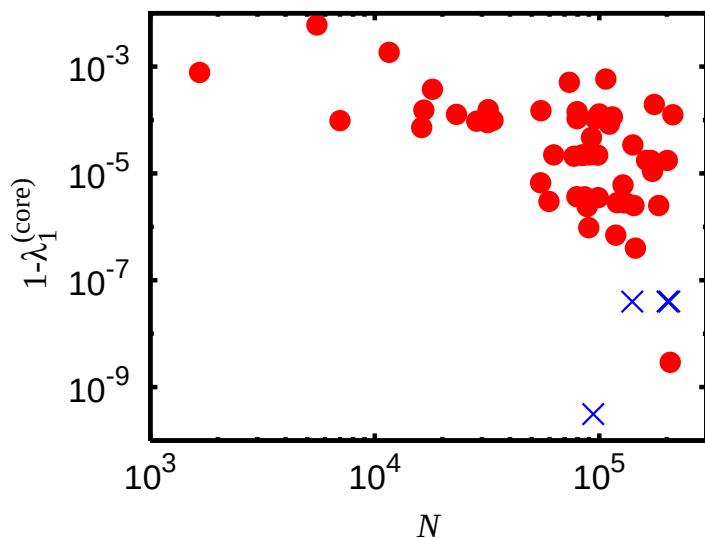
Red: core space eigenvalues (with
 Arnoldi dimension $n_A = 20000$)

PageRank for $\alpha \rightarrow 1$:



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

Core space gap and quasi-subspaces



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

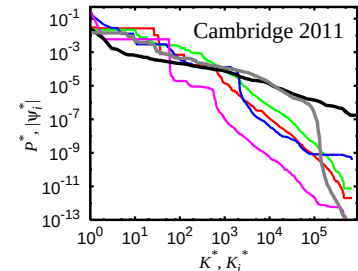
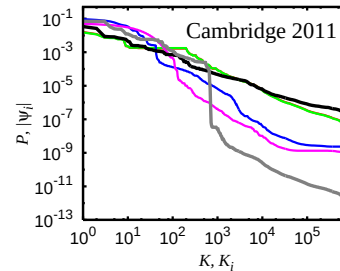
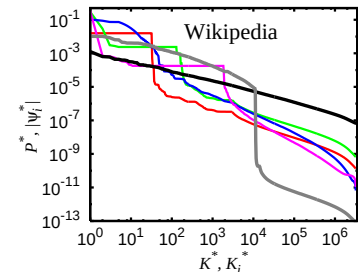
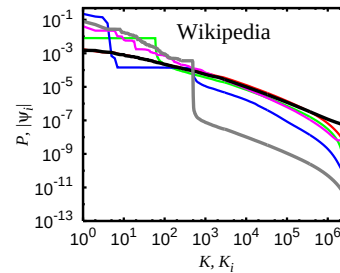
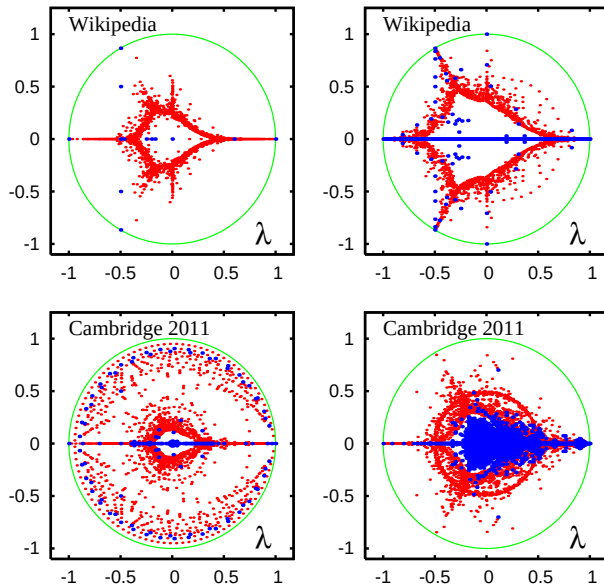
Red dots for gap $> 10^{-9}$; blue crosses (moved up by 10^9) for gap $< 10^{-16}$.

Right: first core space eigenvector 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.

Wikipedia

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



left (right): PageRank (CheiRank)

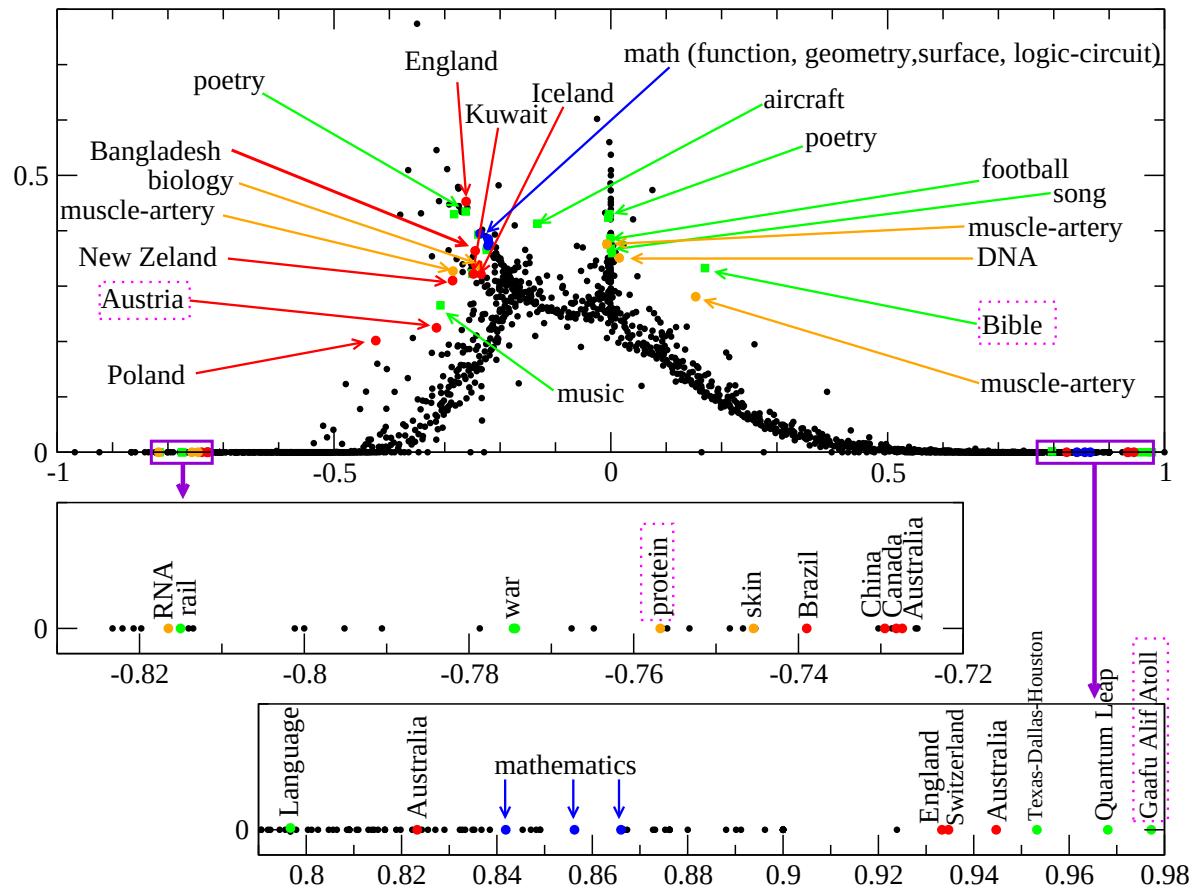
black: PageRank (CheiRank) at $\alpha = 0.85$

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

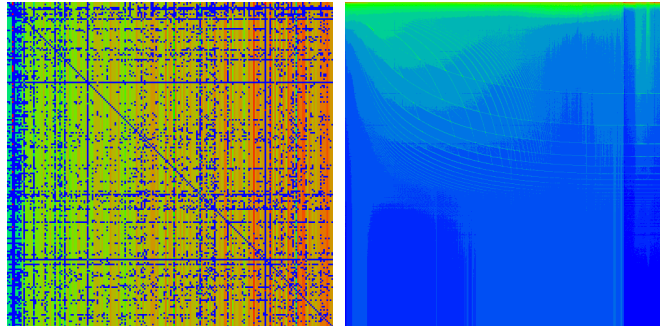
“Themes” of certain Wikipedia eigenvectors:



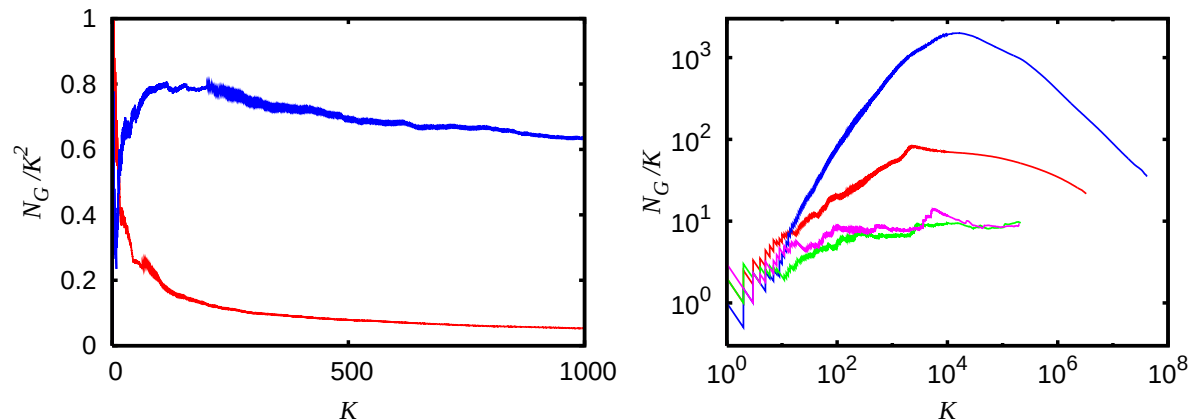
Twitter network

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

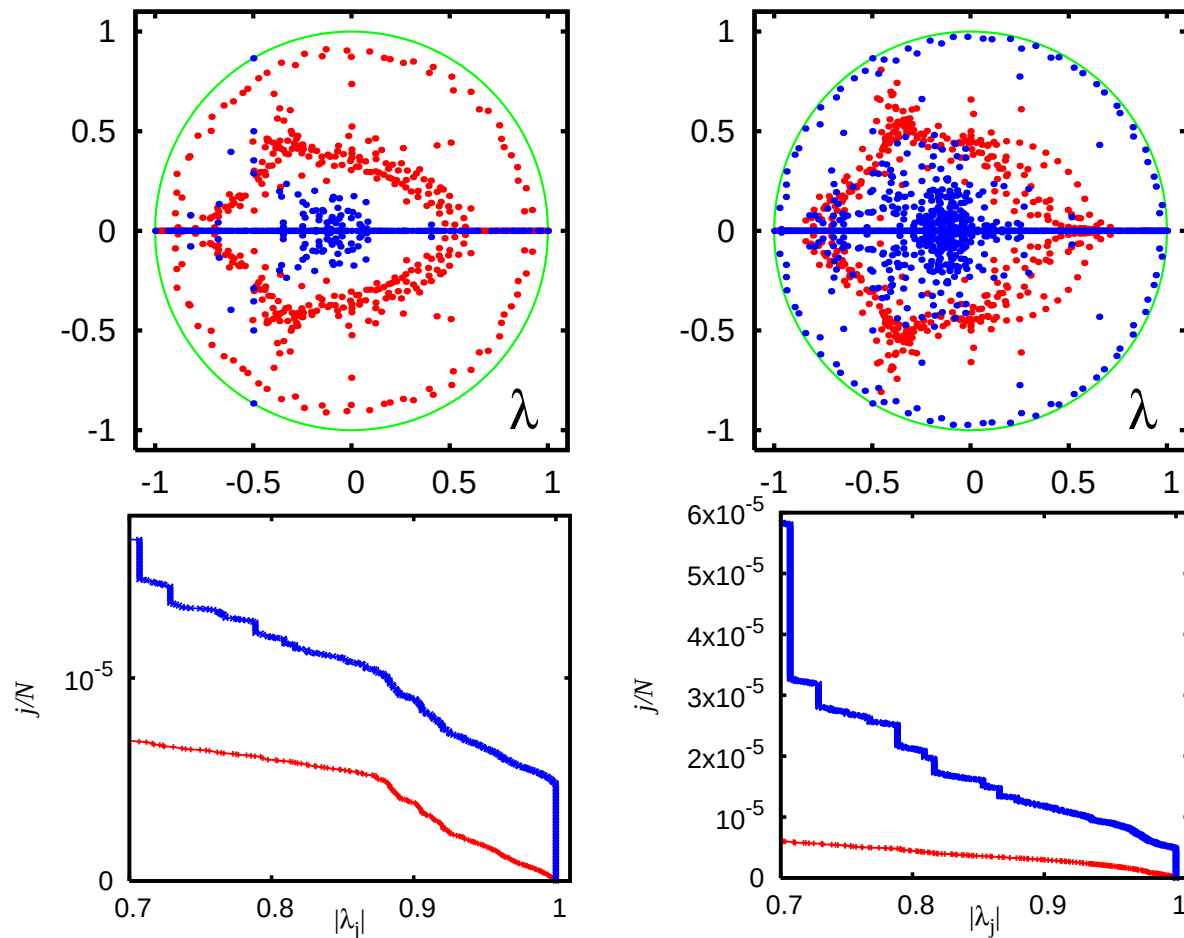
Matrix structure in K-rank order:



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



Spectrum for the Twitter network



$n_A = 640 \Rightarrow$ requires ~ 200 GB of RAM memory.

Random Perron-Frobenius matrices

Construct random matrix ensembles G_{ij} such that:

$G_{ij} \geq 0$, G_{ij} are (approximately) non-correlated and distributed with the same distribution $P(G_{ij})$ (of finite variance σ^2),

$$\sum_j G_{ij} = 1 \quad \Rightarrow \quad \langle G_{ij} \rangle = 1/N$$

$\Rightarrow$ 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:

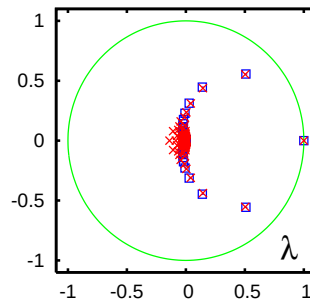
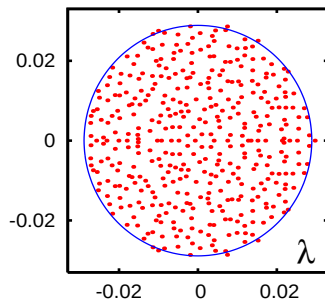
full $\Rightarrow R = 1/\sqrt{3N}$

sparse with Q non-zero elements per column $\Rightarrow R \sim 1/\sqrt{Q}$

power law with $P(G) \sim G^{-b}$ for $2 < b < 3$ $\Rightarrow R \sim N^{1-b/2}$

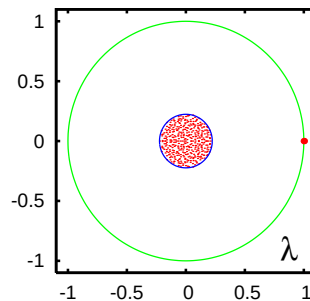
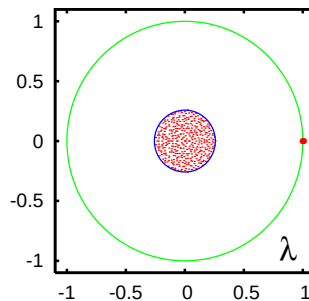
Numerical verification:

uniform full:
 $N = 400$



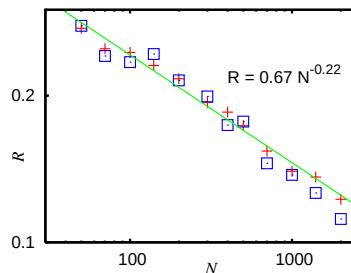
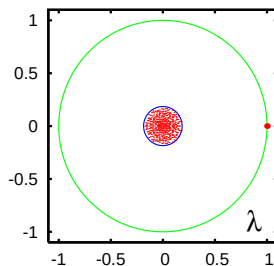
triangular
random and
average

uniform sparse:
 $N = 400$,
 $Q = 20$



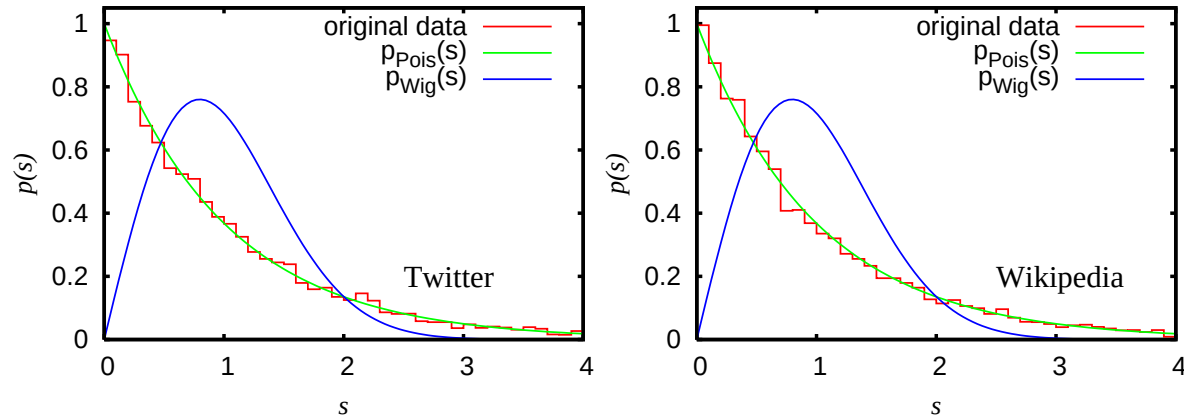
constant sparse:
 $N = 400$,
 $Q = 20$

power law:
 $b = 2.5$



power law case:
 $R_{\text{th}} \sim N^{-0.25}$

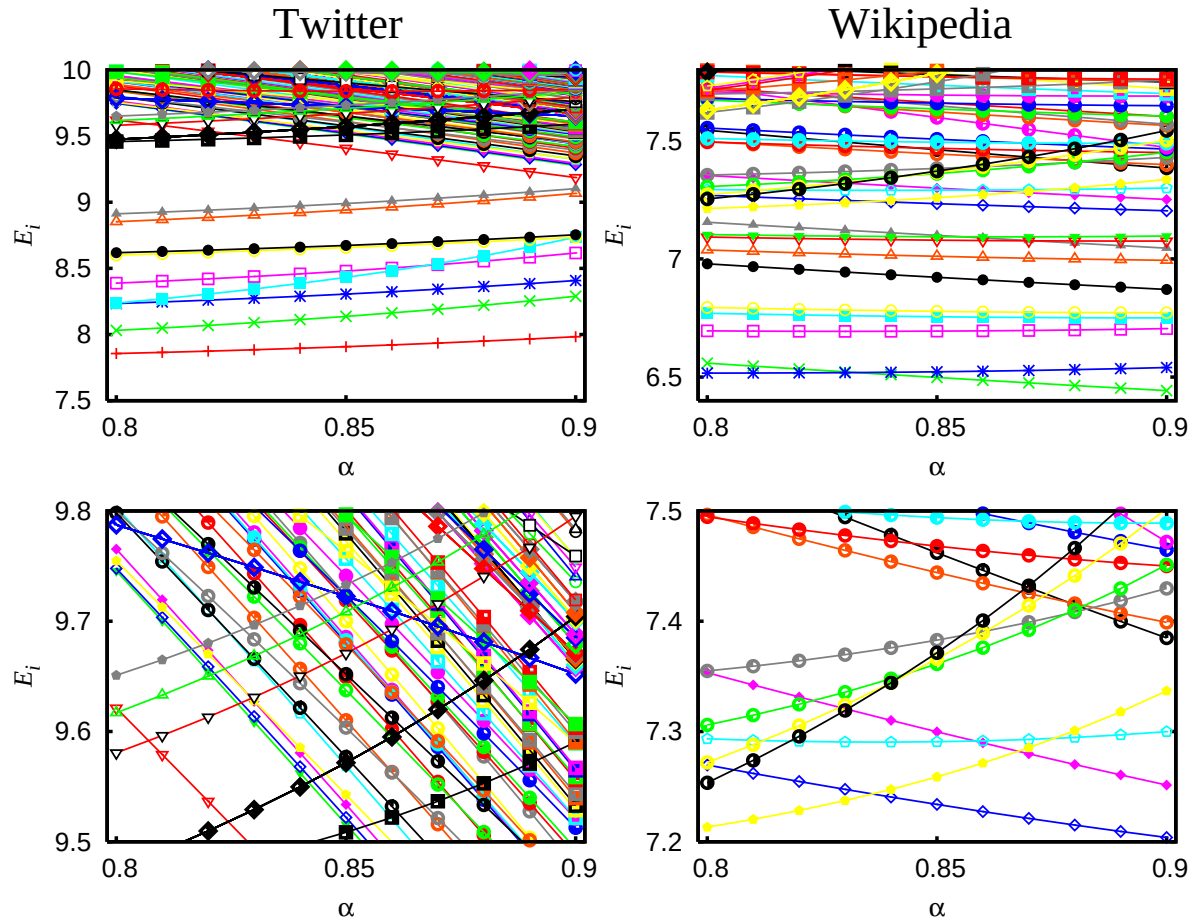
Poisson statistics of PageRank



Identify PageRank values to “energy-levels”:

$$P(i) = \exp(-E_i/T)/Z$$

with $Z = \sum_i \exp(-E_i/T)$ and an effective temperature T (can be chosen: $T = 1$).

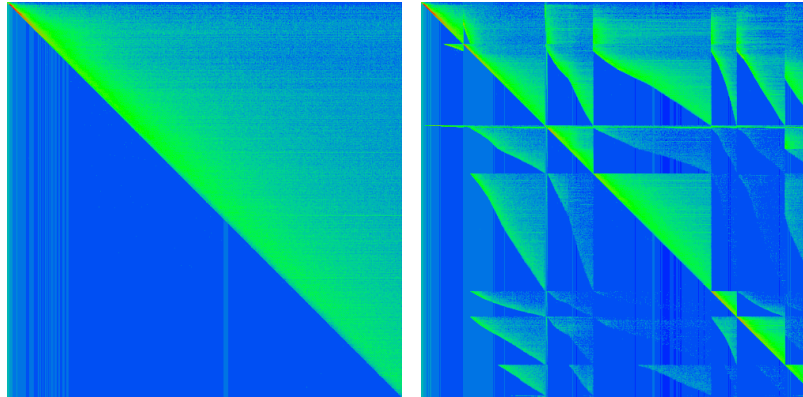


Parameter dependance of $E_i = -\ln(P(i))$ on the damping factor α .

Physical Review network

$N = 463347$ nodes and $N_\ell = 4691015$ links.

Coarse-grained matrix structure (500×500 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 adjacency matrix: most citations links $t \rightarrow t'$ are for $t > t'$ (“past citations”) but there is a small number ($12126 = 2.6 \times 10^{-3} N_\ell$) of links $t \rightarrow t'$ with $t \leq t'$ corresponding to **future citations**.

Strong numerical problems due to large Jordan subspaces!

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***:

$$S_0^l = 0 \quad \text{with } l = 352.$$

Let ψ be an eigenvector of S with eigenvalue λ 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.

If $C \neq 0 \Rightarrow \lambda \neq 0$ since the equation $S_0\psi = -C e/N$ does not have a solution $\Rightarrow \lambda\mathbf{1} - S_0$ invertible.

$$\Rightarrow \psi = C (\lambda\mathbf{1} - S_0)^{-1} e/N = \frac{C}{\lambda} \sum_{j=0}^{l-1} \left(\frac{S_0}{\lambda}\right)^j e/N .$$

$$\text{From } \lambda^l = (d^T \psi / C) \lambda^l \Rightarrow \boxed{\mathcal{P}_r(\lambda) = 0}$$

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

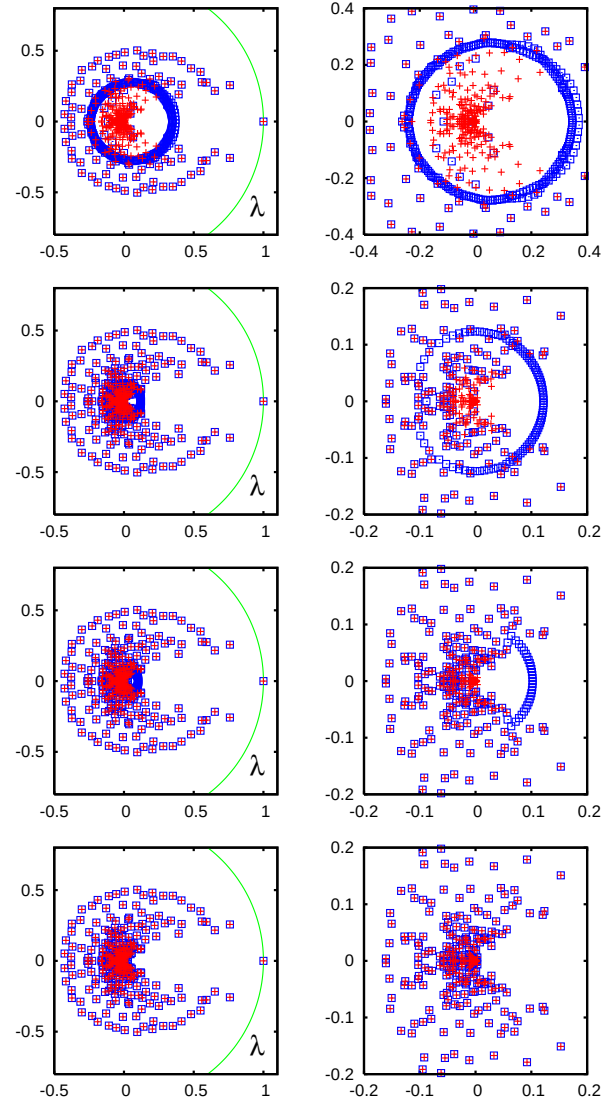
Solution:

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.

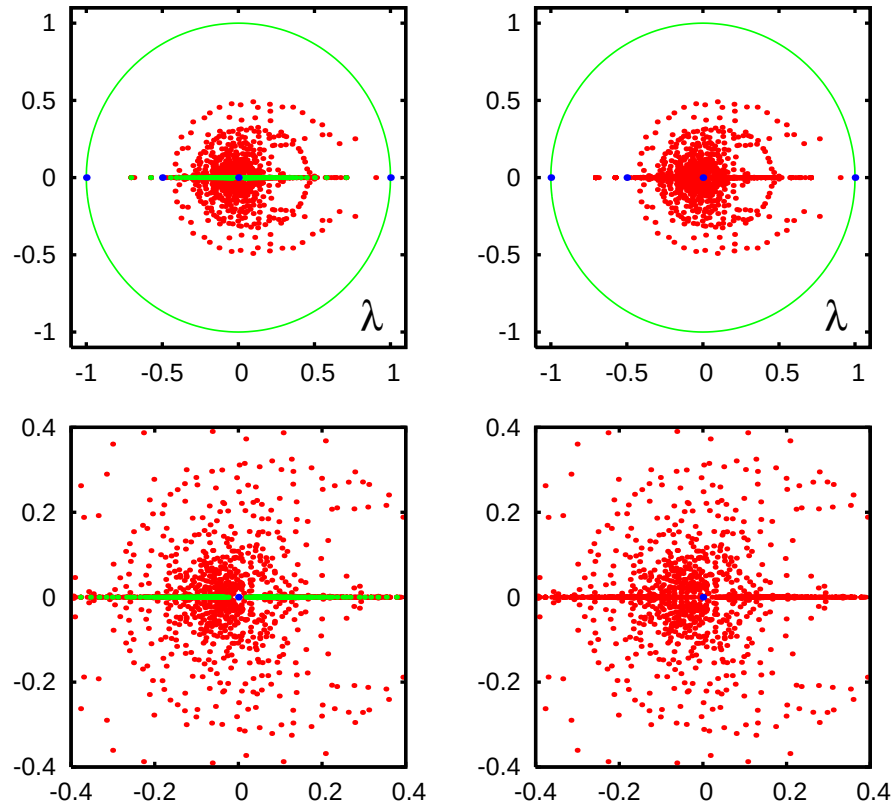
red crosses: zeros of $\mathcal{P}_r(\lambda)$ from 256 binary digits calculation

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.

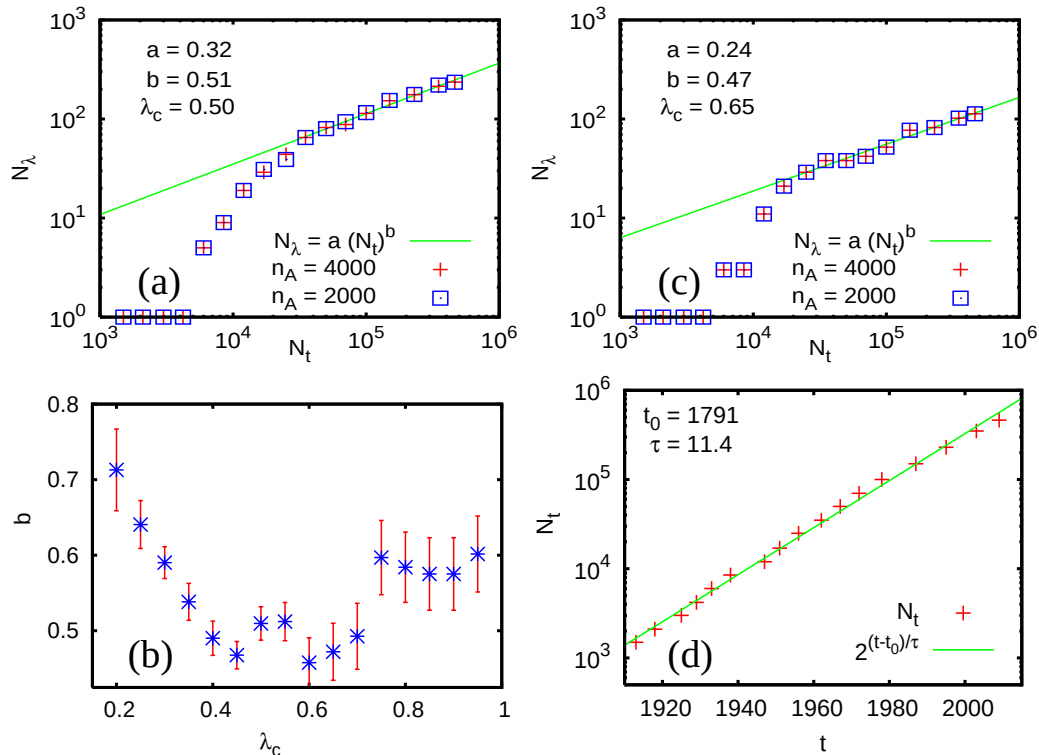


Full Physical Review network

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



Fractal Weyl law



N_λ = number of complex eigenvalues with $\lambda_c \leq |\lambda| \leq 1$.

N_t = reduced network size of Physical Review at time t .

$$N_\lambda = a N_t^b$$

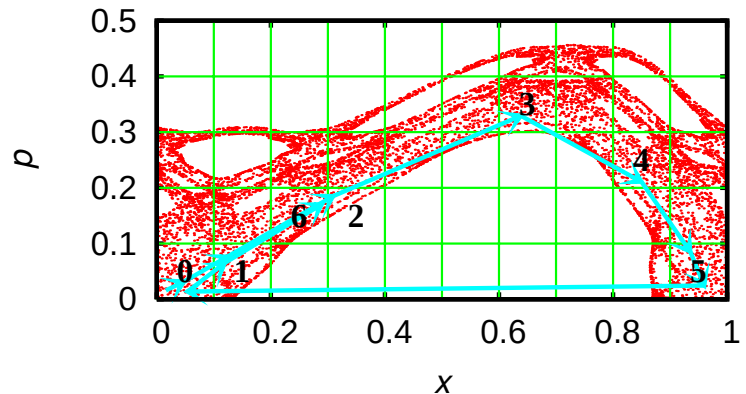
Perron-Frobenius matrix for chaotic maps

A new variant of the **Ulam Method** to construct the **Perron-Frobenius matrix** for the case of a mixed phase space:

Subdivide phase space in square cells of size M^{-1} and iterate a classical trajectory ($t \sim 10^{11} - 10^{12}$) and attribute a new number to each new cell which is entered. At the same time count the number of transitions from cell i to cell j ($\Rightarrow n_{ji}$) $\Rightarrow$ $N \times N$ -PF-Matrix (N =number of non-empty cells) by:

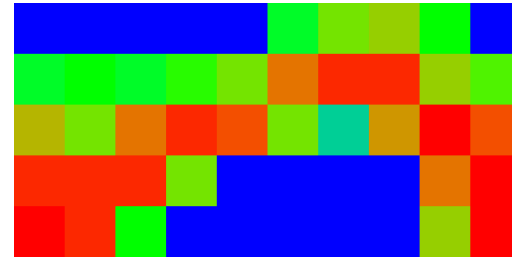
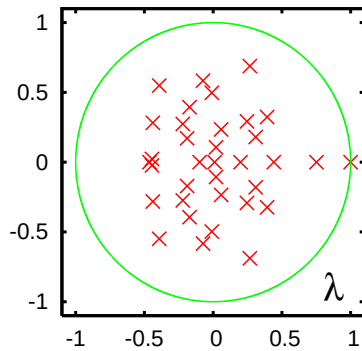
$$G_{ji} = \frac{n_{ji}}{\sum_l n_{li}}$$

Example: Chirikov map at
 $k = k_c = 0.971635406$
with $M = 10$.



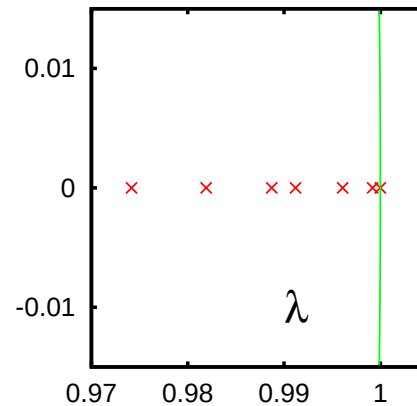
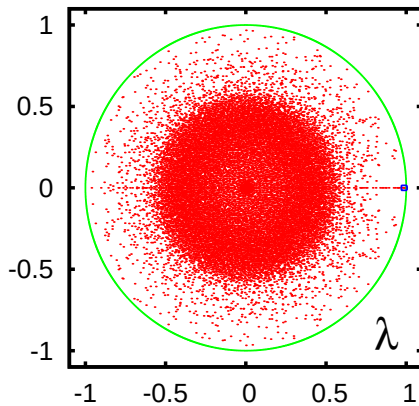
Eigenvalues

for $M = 10, t = 10^6$ and $N = 35$



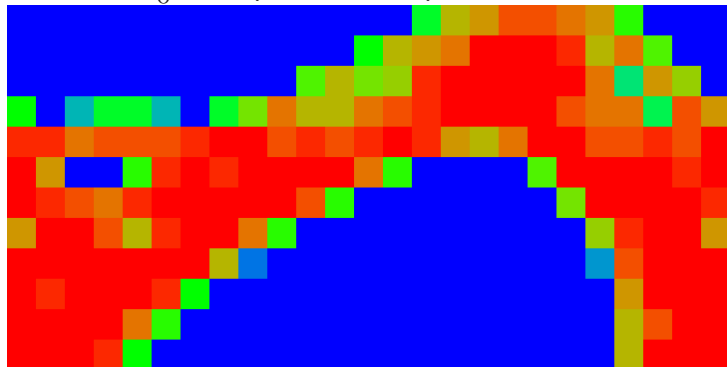
Phase space representation of the eigenvector for $\lambda_0 = 1$.

for $M = 280, t = 10^{12}$ and $N = 16609$

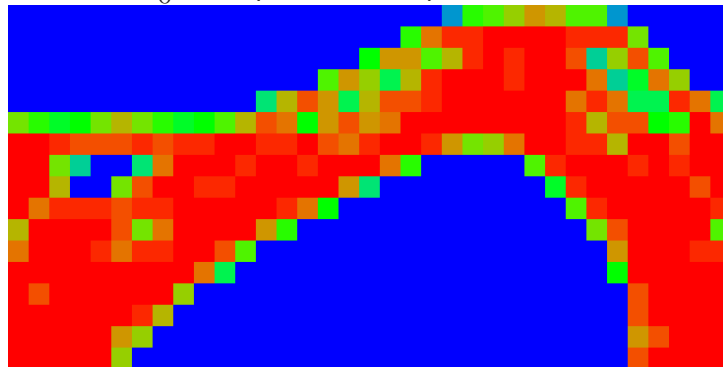


Eigenvectors

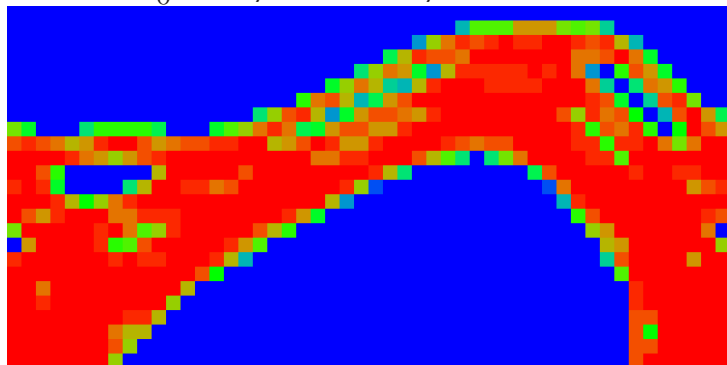
$$\lambda_0 = 1, M = 25, N = 177$$



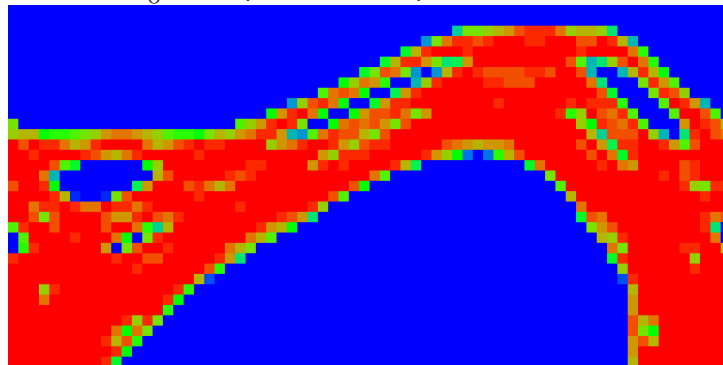
$$\lambda_0 = 1, M = 35, N = 332$$

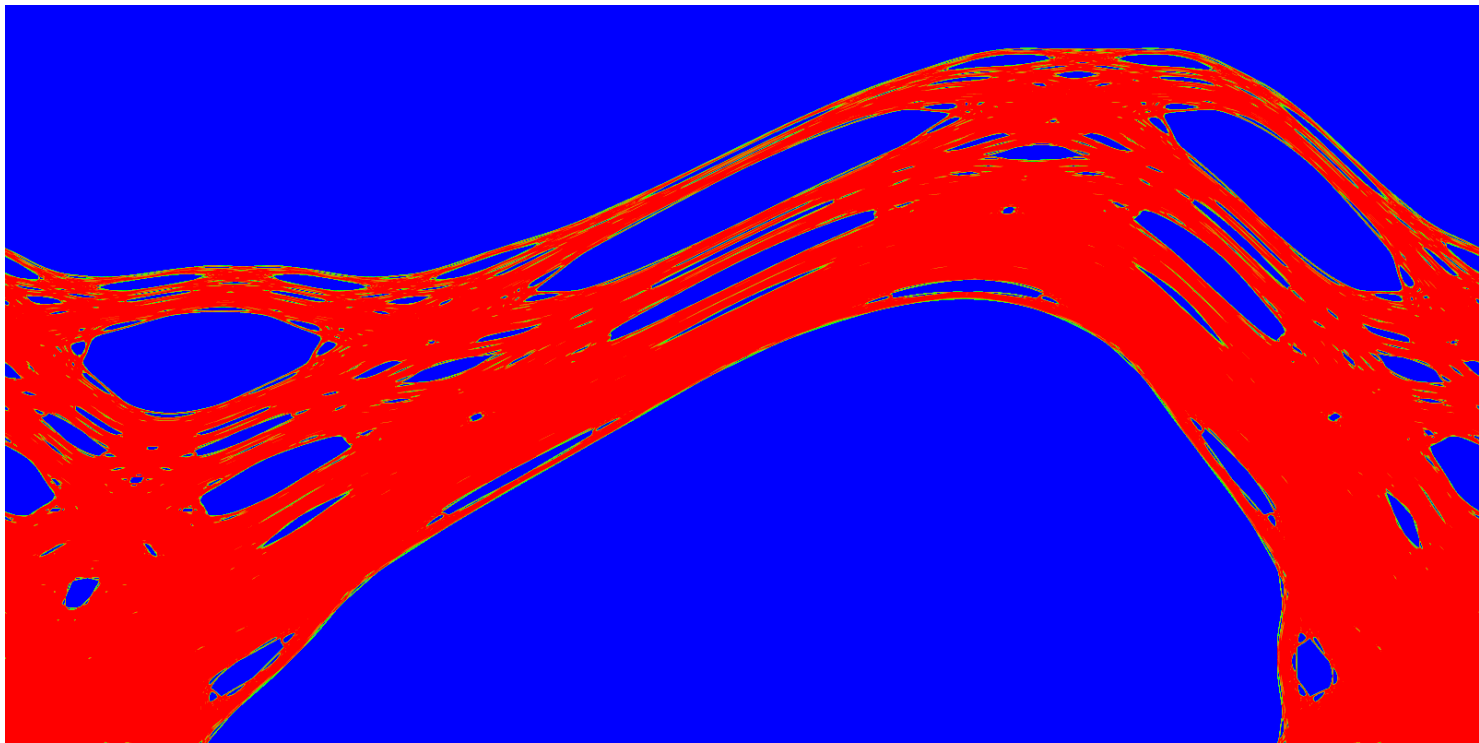


$$\lambda_0 = 1, M = 50, N = 641$$

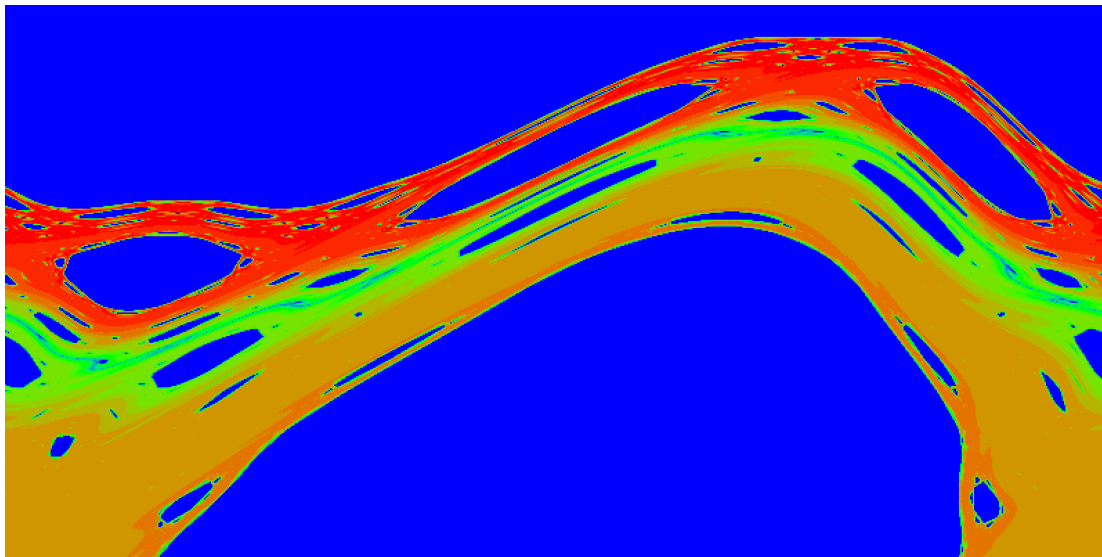


$$\lambda_0 = 1, M = 70, N = 1189$$





$$\lambda_0 = 1, M = 1600, N = 494964, n_A = 3000$$

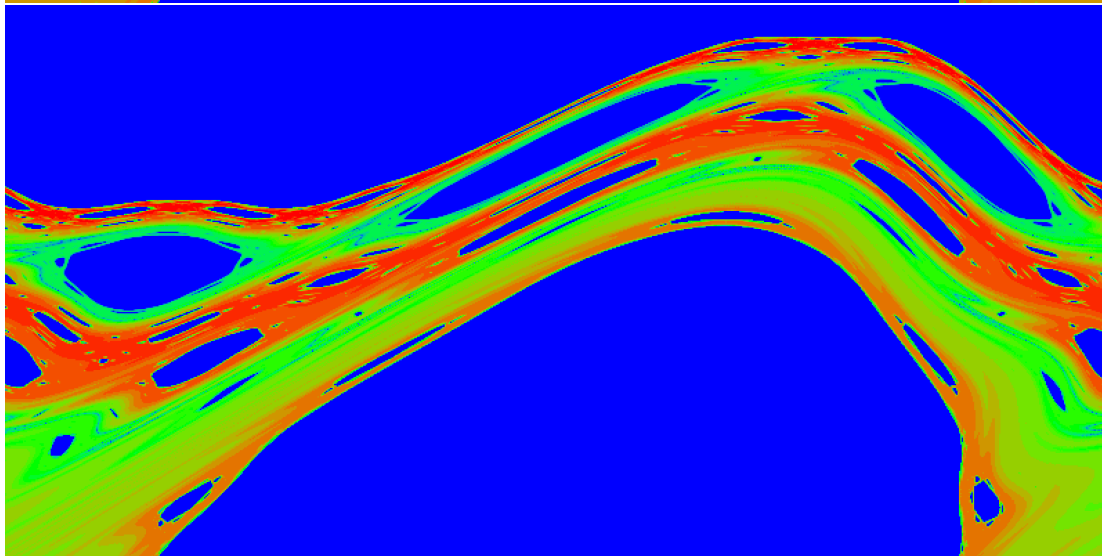


$$\lambda_1 = 0.99980431$$

$$M = 800$$

$$N = 127282$$

$$n_A = 2000$$

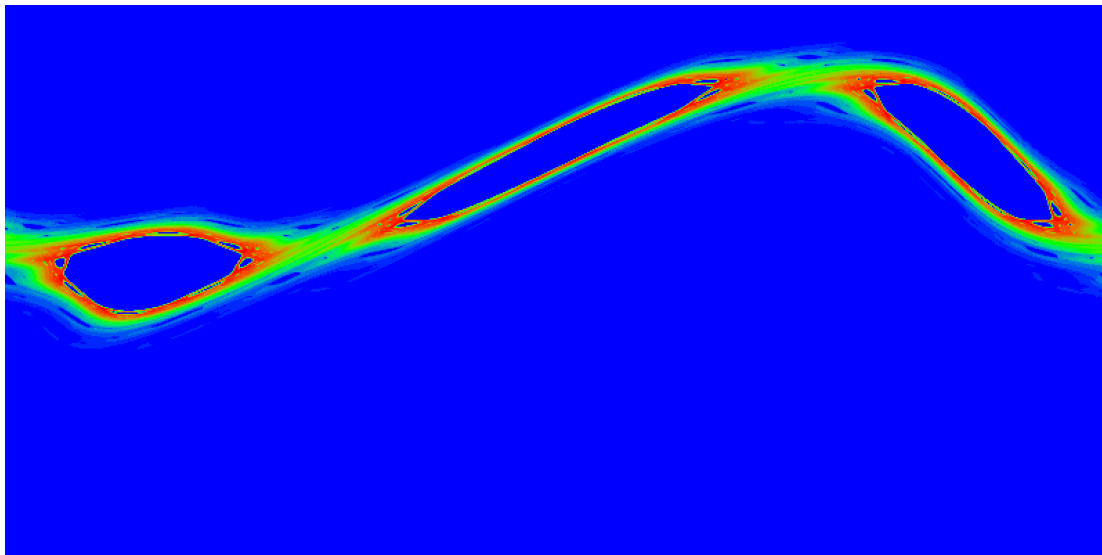


$$\lambda_2 = 0.99878108$$

$$M = 800$$

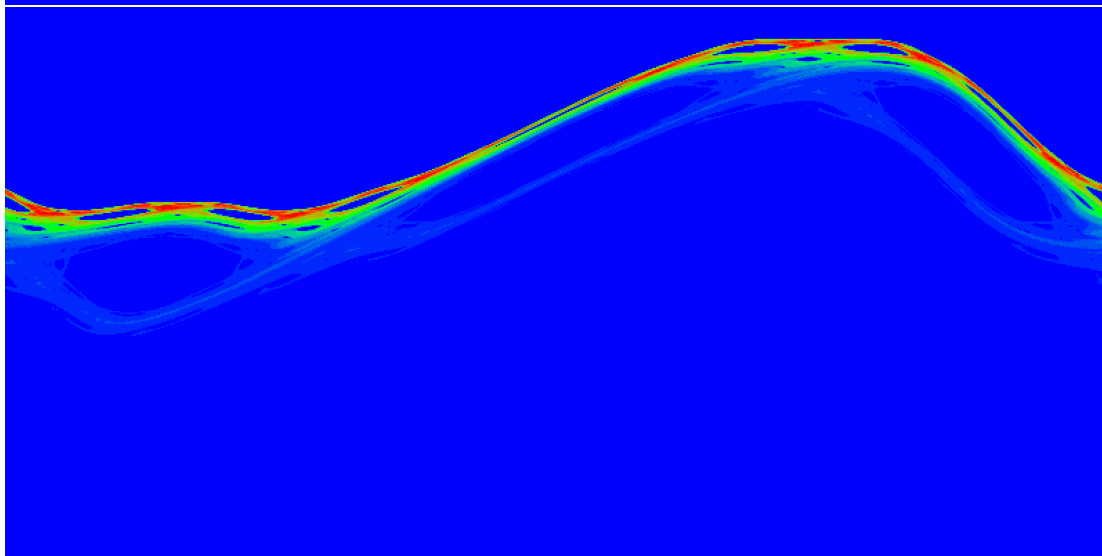
$$N = 127282$$

$$n_A = 2000$$



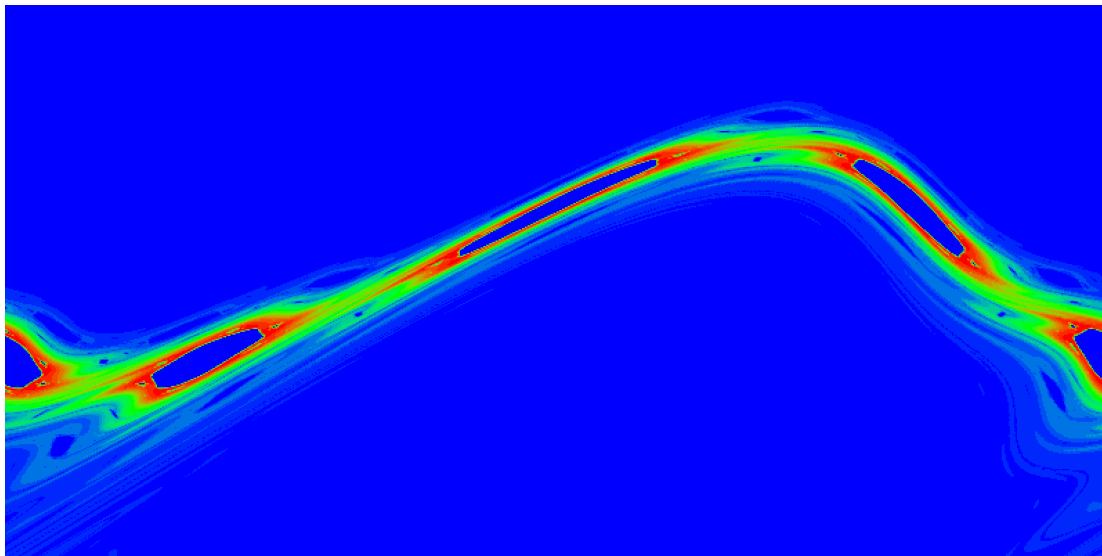
$$\begin{aligned}\lambda_6 &= \\ &-0.49699831 \\ &+i\,0.86089756 \\ &\approx |\lambda_6| e^{i2\pi/3}\end{aligned}$$

$$\begin{aligned}M &= 800 \\ N &= 127282 \\ n_A &= 2000\end{aligned}$$



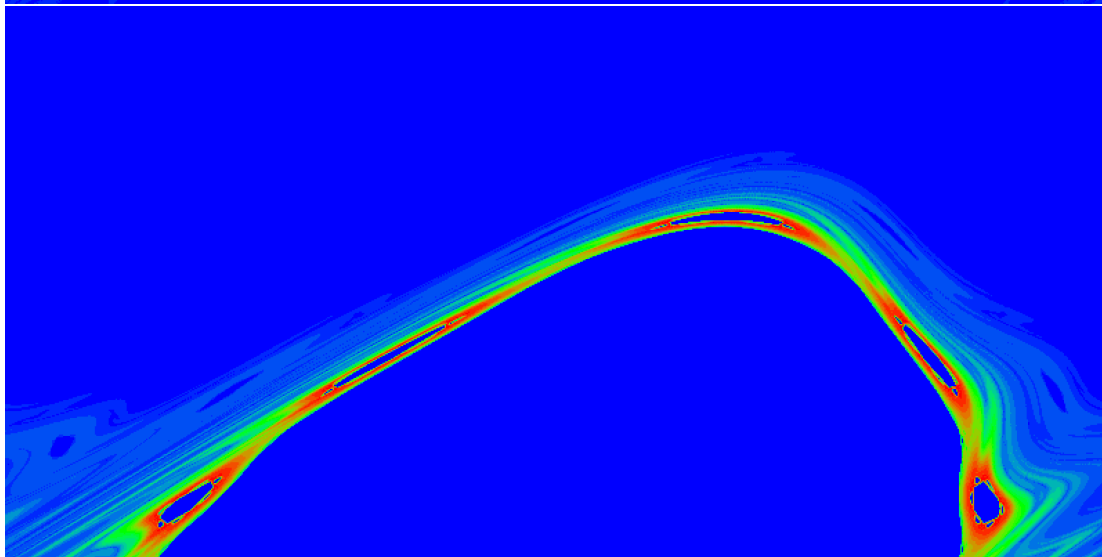
$$\begin{aligned}\lambda_{19} &= \\ &-0.71213331 \\ &+i\,0.67961609 \\ &\approx |\lambda_{19}| e^{i2\pi(3/8)}\end{aligned}$$

$$\begin{aligned}M &= 800 \\ N &= 127282 \\ n_A &= 2000\end{aligned}$$



$$\begin{aligned}\lambda_8 &= \\ 0.00024596 \\ +i 0.99239222 \\ &\approx |\lambda_8| e^{i 2\pi/4}\end{aligned}$$

$$\begin{aligned}M &= 800 \\ N &= 127282 \\ n_A &= 2000\end{aligned}$$



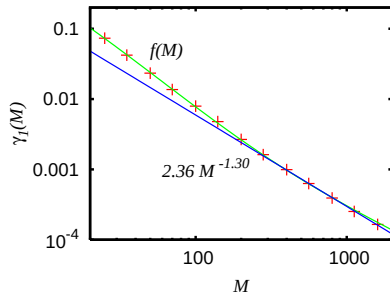
$$\begin{aligned}\lambda_{13} &= \\ 0.30580631 \\ +i 0.94120900 \\ &\approx |\lambda_{13}| e^{i 2\pi/5}\end{aligned}$$

$$\begin{aligned}M &= 800 \\ N &= 127282 \\ n_A &= 2000\end{aligned}$$

Extrapolation of eigenvalues

$$(\gamma_j = -2 \ln(|\lambda_j|))$$

$\gamma_1(M)$ in the limit $M \rightarrow \infty$:



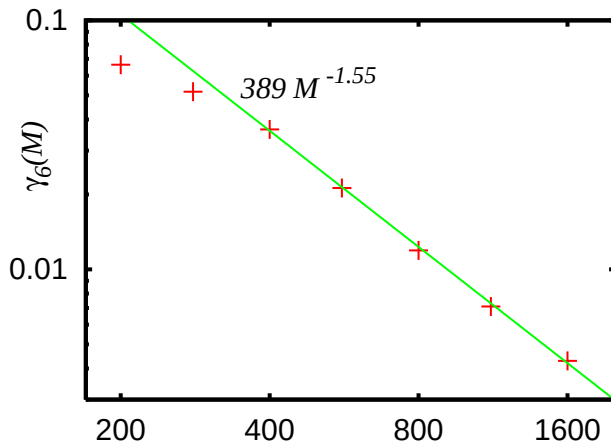
$$f(M) = \frac{D}{M} \frac{1 + \frac{C}{M}}{1 + \frac{B}{M}}$$

$$D = 0.245$$

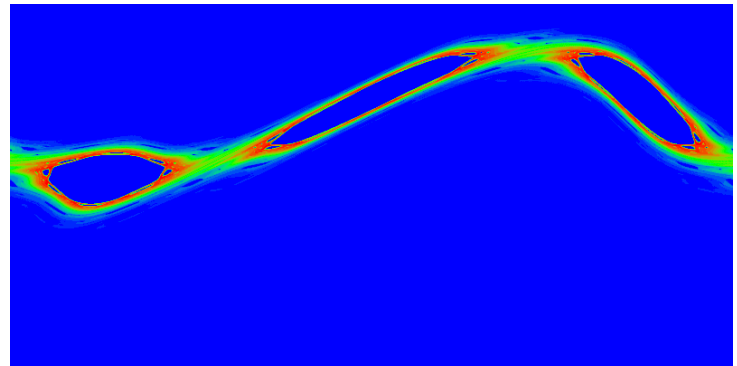
$$B = 13.1$$

$$C = 258$$

$\gamma_6(M)$ in the limit $M \rightarrow \infty$:

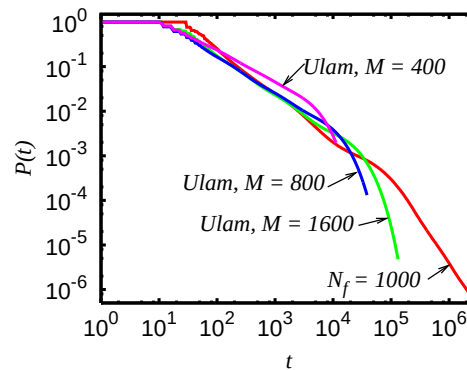
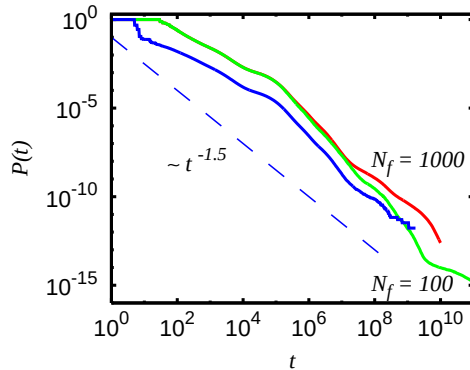


$$\gamma_6(M) \approx 389 M^{-1.55} \text{ for } M \geq 400.$$

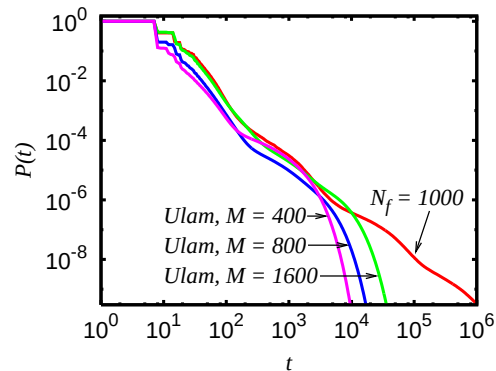
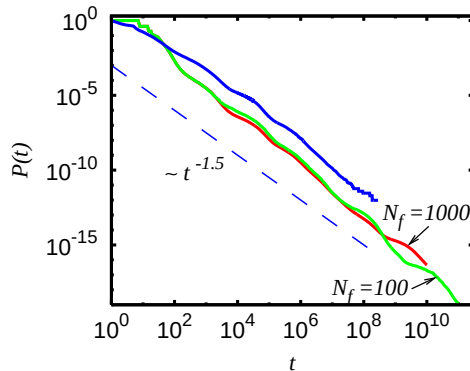


Absorption for $p < 0.05$

Chirikov map



Separatrix map



Red, green (left): Survival Monte-Carlo Method

Blue (left): Data of Weiss et al. PRL **89**, 239401 (2002) and Chirikov et al. PRL **89**, 239402 (2002).

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