Understanding Graphs through Spectral Densities

30 Jun 2018

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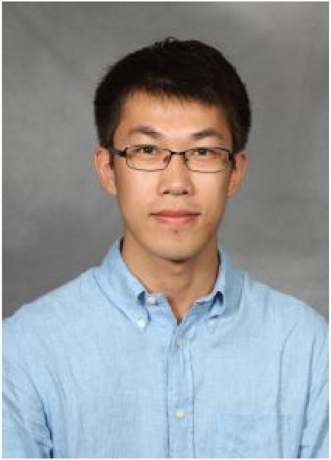
Acknowledgements



Thanks **Kun Dong** (Cornell CAM), along with Anna Yesypenko, Moteleolu Onabajo, Jianqiu Wang.

Also: NSF DMS-1620038.

Can One Hear the Shape of a Drum?

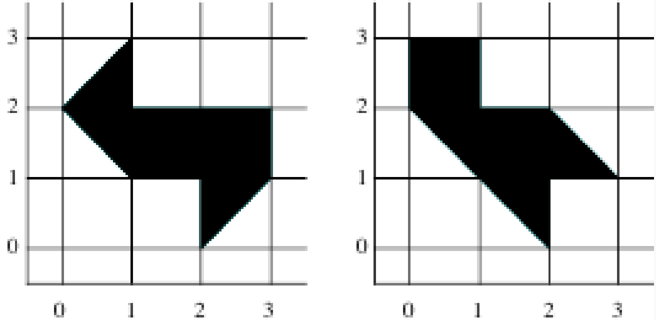
$$-\nabla^2 u = \lambda u \text{ on } \Omega, \qquad\qquad u = 0 \text{ on } \partial\Omega$$

Assume that for each n the eigenvalue λ_n for Ω_1 is equal to the eigenvalue μ_n for Ω_2. Question: Are the regions Ω_1 and Ω_2 congruent in the sense of Euclidean geometry?

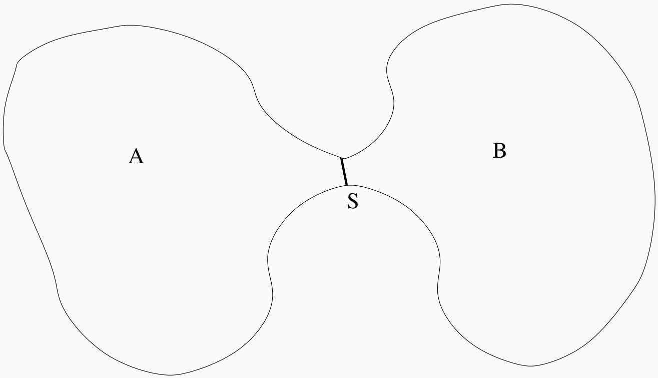
I first heard the problem posed this way some ten years ago from Professor Bochner. Much more recently, when I mentioned it to Professor Bers, he said, almost at once: "You mean, if you had perfect pitch could you find the shape of a drum."

Mark Kac, American Math Monthly, *1966*

Can One Hear the Shape of a Drum?



No in general (Gordon, Webb, Wolpert in 1992)
Yes with constraints (Zelditch in 2009)



Size of bottlenecks (Cheeger inequality)

$$h \leq 2\sqrt{\lambda_2}$$

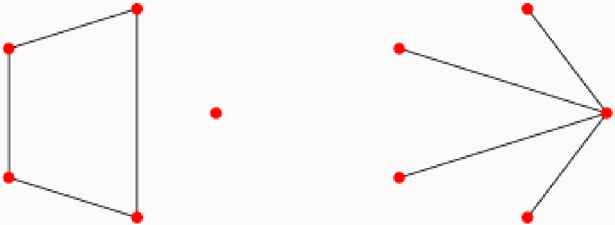
What Do You Hear?

Volume (Weyl law)

$$\lim_{x\to\infty} \frac{N(x)}{x^{d/2}} = (2\pi)^{-d}\omega_d \operatorname{vol}(\Omega), \quad N(x) = \{\#\text{ eigenvalues } \leq x\}$$

Also: lengths of geodesics for a closed Riemannian manifold.

Can One Hear the Shape of a Graph?



From eigenvalues of adjacency, Laplacian, normalized Laplacian?

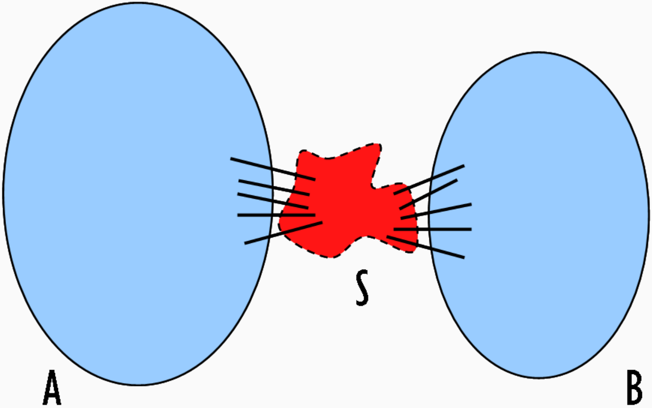
A Bestiary of Matrices

- Adjacency matrix: A
- Laplacian matrix: $L = D - A$
- Unsigned Laplacian: $L = D + A$
- **Random walk matrix**: $P = D^{-1}A$
- **Normalized adjacency**: $\bar{A} = D^{-1/2}AD^{-1/2}$
- **Normalized Laplacian**: $\bar{L} = I - \bar{A} = D^{-1/2}LD^{-1/2}$
- Modularity matrix: $B = A - \frac{dd^T}{2n}$
- Motif adjacency: $W = A^2 \odot A$

All have examples of co-spectral graphs

… through spectrum uniquely identifies *quantum graphs*

What Do You Hear?



Size of separators (Cheeger inequality) – L

What Do You Hear?

What information hides in the eigenvalue distribution?

1. Discretizations of Laplacian: something like Weyl's law
2. Sparse E-R random graphs: Wigner semicircular law
3. Some other random graphs: Wigner semicircle + a bit (Farkas *et al*, Phys Rev E (64), 2001)
4. "Real" networks: less well understood

But computing all eigenvalues seems *expensive*!

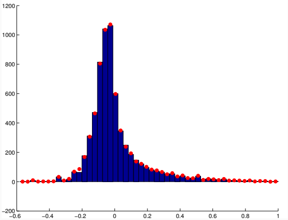
Reminder: Spectral Mapping

Consider a matrix H, and let f be analytic on the spectrum.
Then if $H = V\Lambda V^{-1}$,

$$f(H) = Vf(\Lambda)V^{-1}.$$

(generalizes to non-diagonalizable case)

Another Perspective: Density of States



Spectra define a *generalized function* (a *density*):

$$\mathrm{tr}(f(H)) = \int f(\lambda)\mu(\lambda)\,dx = \sum_{j=k}^{N} f(\lambda_k)$$

where f is an analytic test function. Smooth to get a picture: a *spectral histogram* or *kernel density estimate*.

Example: Estrada Index

Consider

$$\mathrm{tr}(\exp(\alpha A)) = \sum_{k=1}^{\infty} \frac{\alpha^k}{k!} \cdot (\#\text{ closed random walks of length } k) .$$

- Global measure of connectivity in a graph.
- Can clearly be computed via DoS.
- Generalizes to other weights.

Heat Kernels

DoS information equivalent to looking at the *heat kernel trace*:

$$h(s) = \mathrm{tr}(\exp(-sH)) = \mathcal{L}[\mu](s)$$

where H is a positive semi-definite operator.

$H = L$ (continuous time random walk generator) $\implies$
$h(s)/N = P$(self-return after time s from uniform start).

Power Moments

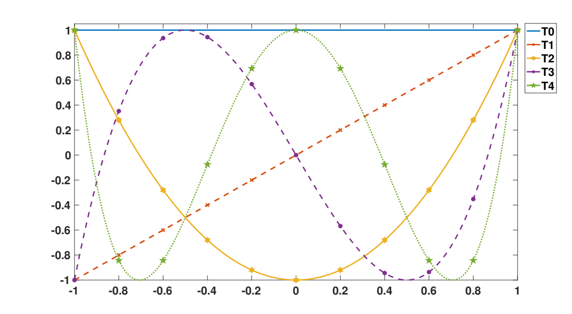
DoS information equivalent to looking at the *power moments*:

$$\mathrm{tr}(H^j).$$

Natural interpretation for matrices associated with graphs:

- A: number of length k cycles.
- $\bar{A}$ or P: return probability for k-step random walk (times N).
- L: ??

Chebyshev Moments



For numerics, prefer Chebyshev moments to power moments:

$$d_j = T_j(A)$$

where $T_j(z) = \cos(j \cos^{-1}(z))$ is the jth Chebyshev polynomial:

$$T_0(z) = 1, \quad T_1(z) = z, \quad T_{k+1}z = 2zT_k(z) - T_{k-1}(z).$$

Exploring Spectral Densities

Kernel polynomial method (see Weisse, Rev. Modern Phys.)

- Spectral distribution on $[-1, 1]$ is a generalized function:

$$\int_{-1}^{1} \mu(x) f(x)\, dx = \frac{1}{N} \sum_{k=1}^{N} f(\lambda_k)$$

- Write $f(x) = \sum_{j=1}^{\infty} c_j T_j(x)$ and $\mu(x) = \sum_{j=1}^{\infty} d_j \phi_j(x)$, where $\int_{-1}^{1} \phi_j(x) T_k(x)\, dx = \delta_{jk}$
- Estimate $d_j = \mathrm{tr}(T_j(H))$ by stochastic methods
- Truncate series for $\mu(x)$ and filter (avoid Gibbs)

Much cheaper than computing all eigenvalues!

Related methods

Golub and Meurant: Gauss quadrature for $\mu(x)$ via Lanczos

- Good: Approximately twice the convergence rate
- Bad: Gives quadrature rule vs a picture

Roder and Silver: Max entropy estimation

- Good: Better resolution from Chebyshev moments
- Bad: More complicated / expensive computation

Under investigation: Hybrid approaches.

Stochastic Trace and Diagonal Estimation

$Z \in \mathbb{R}^n$ with independent entries, mean 0 and variance 1.

$$E[(Z \odot HZ)_i] = \sum_j h_{ij} E[Z_i Z_j] = h_{ii}$$
$$\mathrm{Var}[(Z \odot HZ)_i] = \sum_j h_{ij}^2.$$

Serves as the basis for stochastic estimation of

- Trace (Hutchinson, others; review by Toledo and Avron)
- Diagonal (Bekas, Kokiopoulou, and Saad)

Independent probes $\implies 1/\sqrt{N}$ convergence (usual MC).

Beyond Independent Probes

For probes $Z = [Z_1, \cdots, Z_s]$, have *exact* diagonal

$$d = \left[(A \odot ZZ^T)e\right] \oslash [(Z \odot Z)e]$$

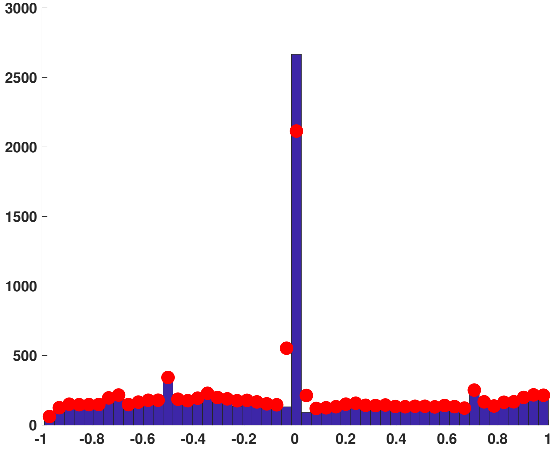
if $Z_{i,:}Zj, :^T = 0$ whenever $A_{ij} \neq 0$.

Idea:

- Pick rows $\{Z_{i,:}\}$ such that $Z_{i,:} \perp Z_{j,:}$ whenever $A_{ij} \neq 0$
- A an adjacency matrix $\implies$ graph coloring.

Combined with randomization, still gives unbiased estimates.

Example: PGP Network



Spike (non-smoothness) at eigenvalues of 0 leads to inaccurate approximation.

Suppose $PH = HP$. Then

$$\mathcal{V} \text{ a max invariant subspace for } P \implies \mathcal{V} \text{ a max invariant subspace for } H$$

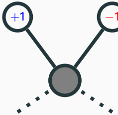
So *local symmetry* $\implies$ *localized eigenvectors*

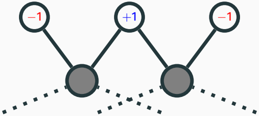
Suppose invariance under some symmetry group $\mathcal{G}$:

$$\forall P \in \mathcal{G}, \quad PH = HP$$

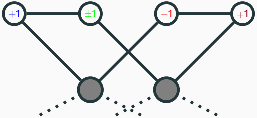
If $\mathcal{G}$ non-Abelian ($P_1P_2 \neq P_2P_1$), must have multiple eigenvalues.

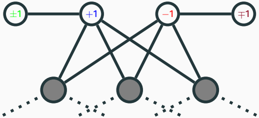
- $\lambda = 0$



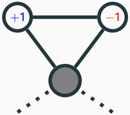


- $\lambda = \pm 1/2$

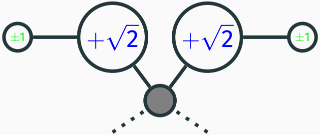




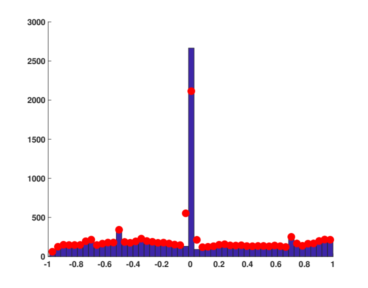
- $\lambda = -1/2$

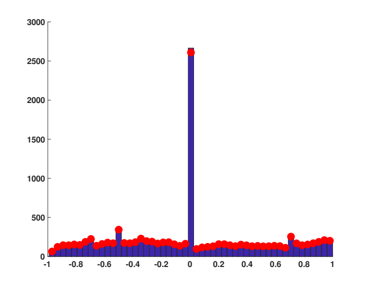


$\lambda = \pm 1/\sqrt{2}$



Motif Filtering





Motif "spikes" slow convergence – deflate motif eigenvectors!

If $P \in \mathbb{R}^{n \times m}$ an orthonormal basis for the quotient space,

- Apply estimator to $P^T \overline{A} P$ to reduce size for $m \ll n$.
- or use $Proj_P(Z)$ to probe the desired subspace.

Diagonal Estimation and LDoS

Diagonal estimation also useful for *local* DoS $\nu_k(x)$;
in the symmetric case with $H = Q\Lambda Q^T$, have

$$\int f(x)\nu_k(x)\,dx = f(H)_{kk} = e_k^T Q f(\Lambda) Q^T e_k$$

$$\nu_k(x) = \sum_{j=1}^{n} q_{kj}^2\,\delta(x - \lambda_j)$$

DoS is sum of local densities of states:

$$\mu(x) = \sum_{k=1}^{n} \nu_k(x)$$

KPM for LDoS

- Write $f(x) = \sum_{j=1}^{\infty} c_j T_j(x)$ and $\nu_k(x) = \sum_{j=1}^{\infty} d_j \phi_j(x)$, where $\int_{-1}^{1} \phi_j(x) T_k(x) \, dx = \delta_{jk}$
- Estimate $d_j = [T_j(H)]_{kk}$ by diag estimation
- Truncate series for $\mu(x)$ and filter (avoid Gibbs)

Diagonal estimator gives moments *for all k simultaneously*!

Other methods

Golub and Meurant: Gauss quadrature for $\nu_k(x)$ via Lanczos

- Good: No stochastic estimation error (vs KPM)
- Bad: Separate Lanczos *per node*

Roder and Silver: Max entropy estimation

- Good: Better resolution from Chebyshev moments
- Bad: More expensive computation per node

Under investigation: Hybrid approach.

LDoS Information

Can compute common *centrality measures* with LDoS

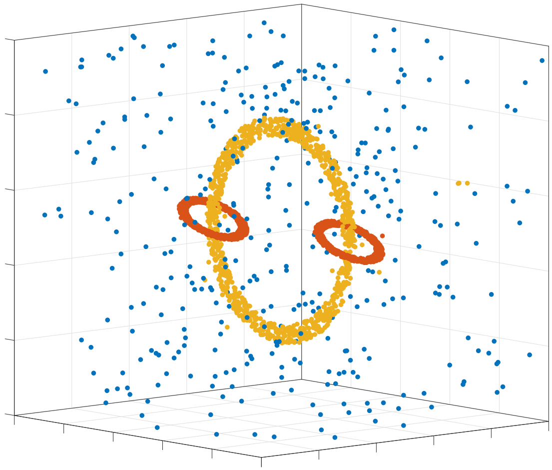
- Estrada centrality: $\exp(\gamma A)_{kk}$
- Resolvent centrality: $\left[(I - \gamma \bar{A})^{-1}\right]_{kk}$

Some motifs associated with localized eigenvectors:

- Chief example: Null vectors of $\bar{A}$ supported on leaves.
- Use LDoS + topology to find motifs?

What else?

LDoS and Clustering



Phase Retrieval in Graph Reconstruction

Reconstruct graph from *fully resolved* LDoS at all nodes?

- Assume $H = Q\Lambda Q^T$
- No multiple eigenvalues $\implies$ know $|Q|$ and Λ
- Can we recover signs in Q?

Feels a little like phase retrieval...

Of course, we usually have noisy LDoS estimates!

Exploring Spectral Densities (with David Gleich)

- Compute spectrum of normalized Laplacian / RW matrix
- Compare KPM to full eigencomputation

Things we know

- Eigenvalues in $[-1, 1]$; nonsymmetric in general
- Stability: change d edges, have

$$\lambda_{j-d} \leq \hat{\lambda}_j \leq \lambda_{j+d}$$

- kth moment = P(return after k-step random walk)
- Eigenvalue cluster near 1 $\sim$ well-separated clusters
- Eigenvalue cluster near 0 $\sim$ leaf clusters

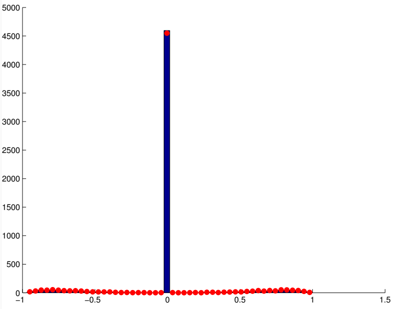
What else can we “hear”?

Experimental setup

- Global DoS
  - 1000 Chebyshev moments
  - 10 probe vectors (componentwise standard normal)
  - Histogram with 50 bins
- Local DoS
  - 100 Chebyshev moments
  - 10 probe vectors (componentwise standard normal)
  - Plot smoothed density on $[-1, 1]$
  - Spectrally order nodes by density plot

Suggestions for better pics are welcome!

Erdos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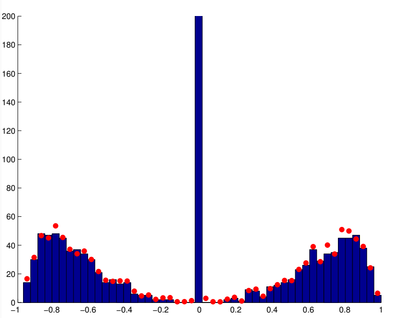
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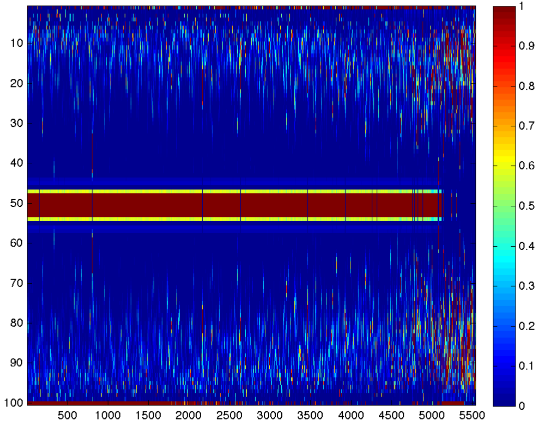
Erdos (local)



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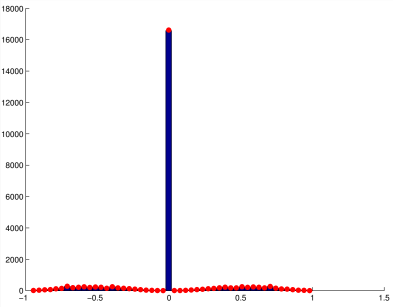
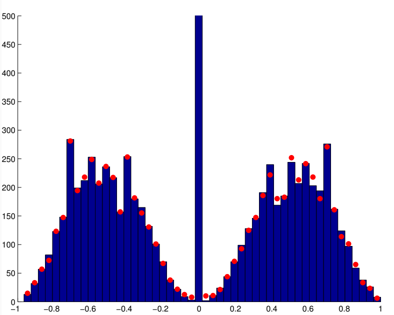
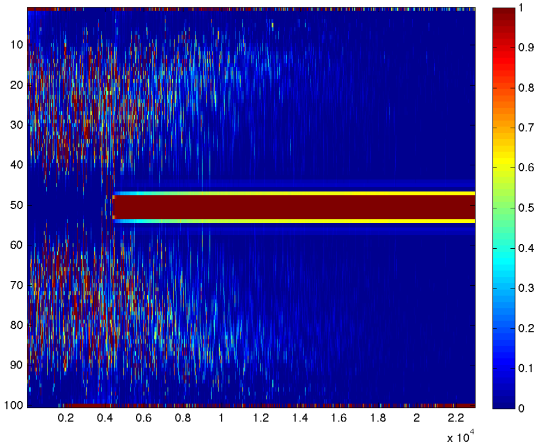
Internet topology

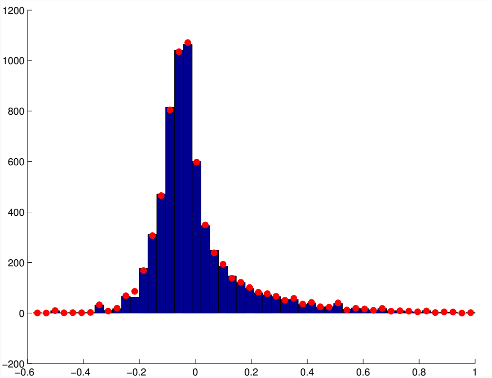




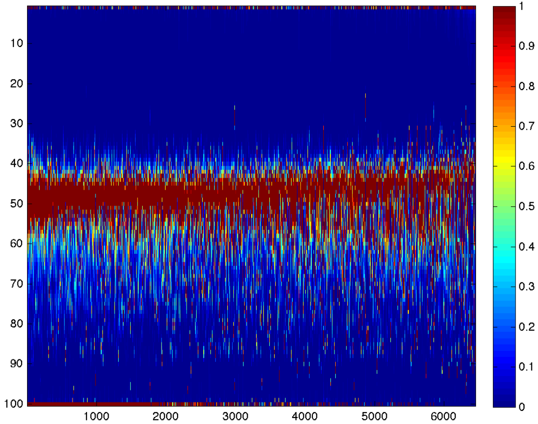
Internet topology (local)



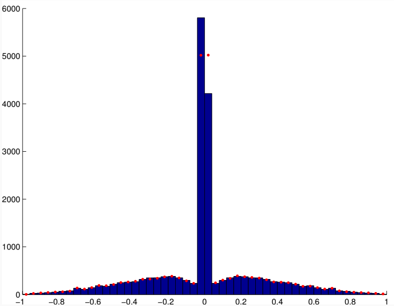
Marvel characters

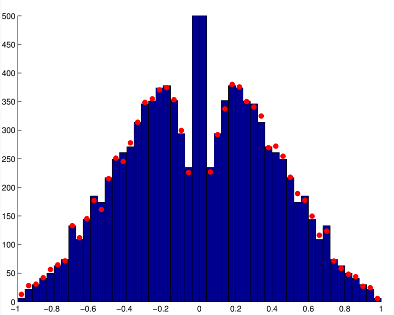


Marvel characters (local)

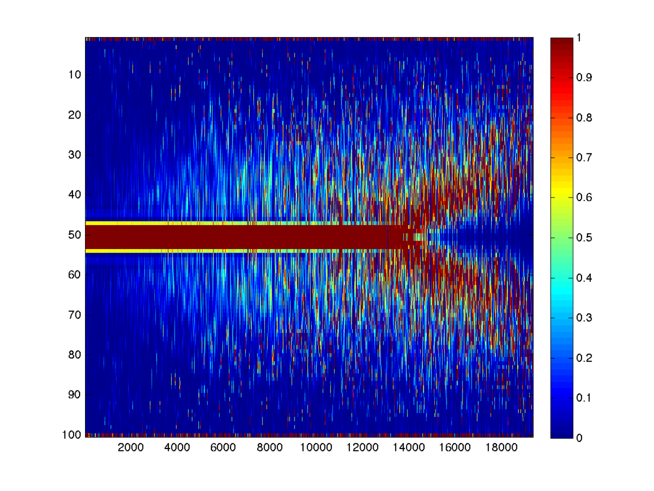


Marvel comics

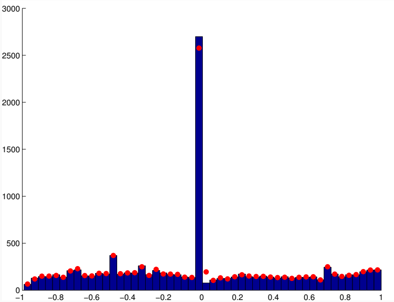




Marvel comics (local)



PGP



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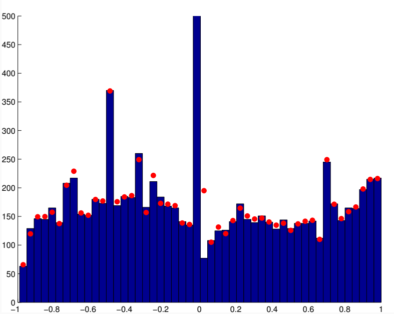

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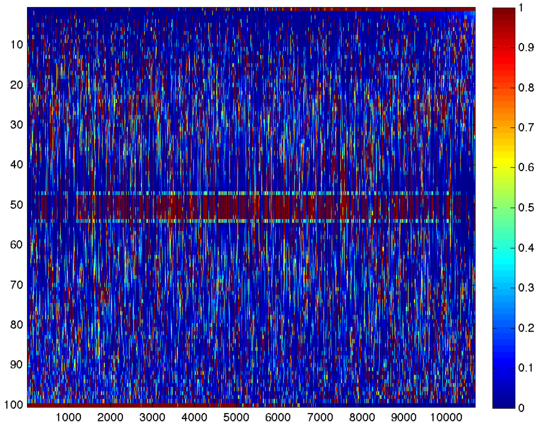
PGP (local)



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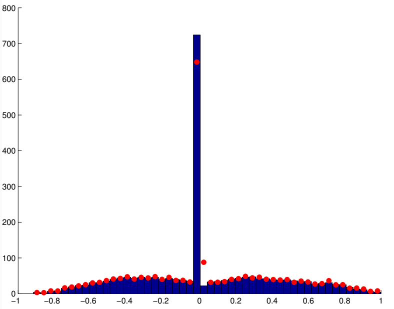
Yeast



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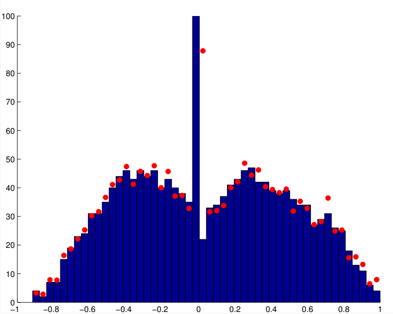

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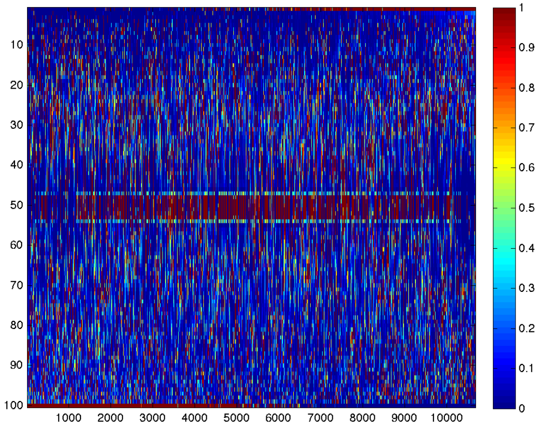
Yeast (local)



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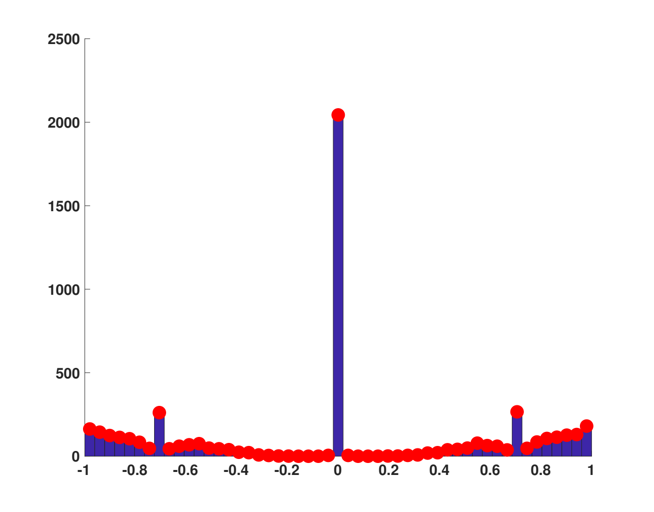
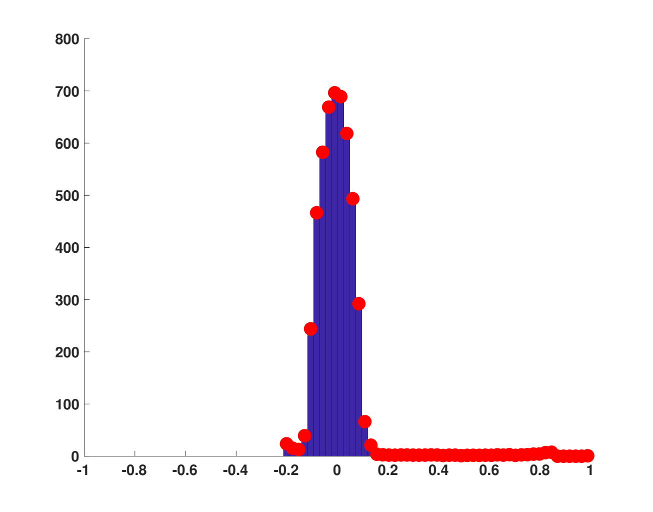
What about random graph models?

Barabási–Albert model



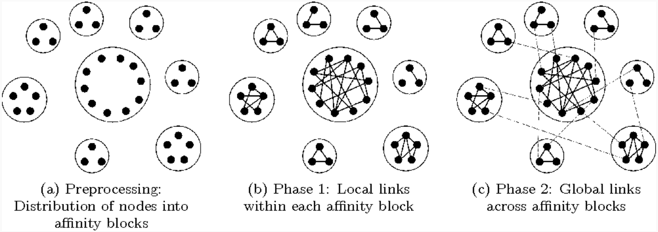
Scale-free network (5000 nodes, 4999 edges)

Watts–Strogatz



Small world network (5000 nodes, 260000 edges)

Model Verification: BTRE



Kolda et al, SISC (36), 2014

Block Two-Level Erdős-Rényi model (BTER)

- First Phase: Erdős-Rényi Blocks
- Second Phase: Using Chung-Lu Model to connect blocks with $p_{ij} = p(d_i, d_j)$

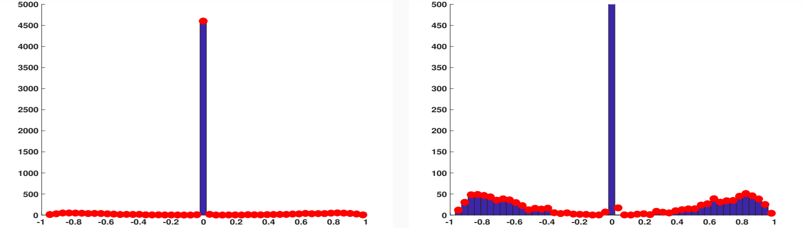


Figure 1: Erdos collaboration network.

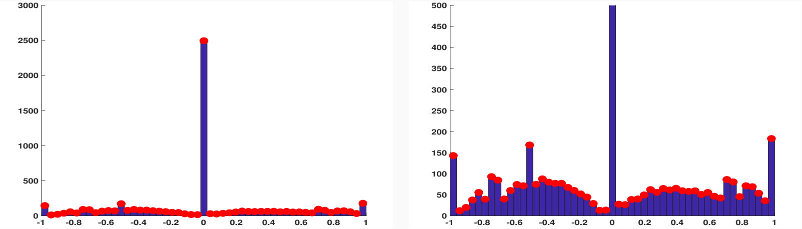
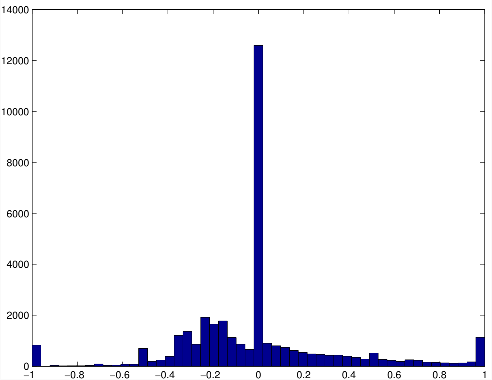


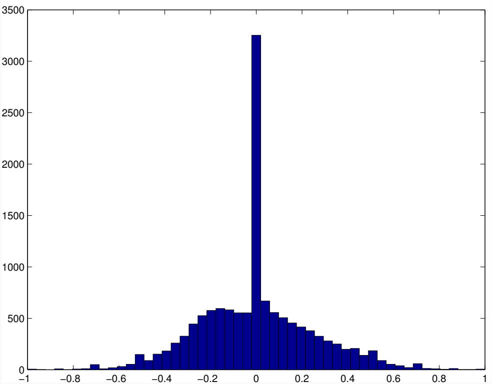
Figure 2: BTER model for Erdos collaboration network.

And a few more...

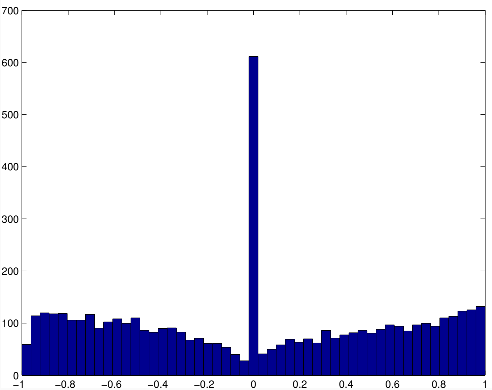
Enron emails (SNAP)



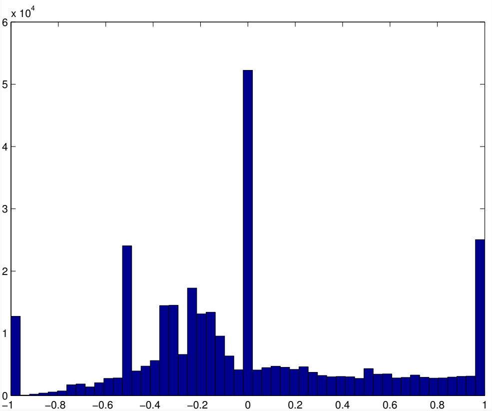
Reuters911 (Pajek)



US power grid (Pajek)

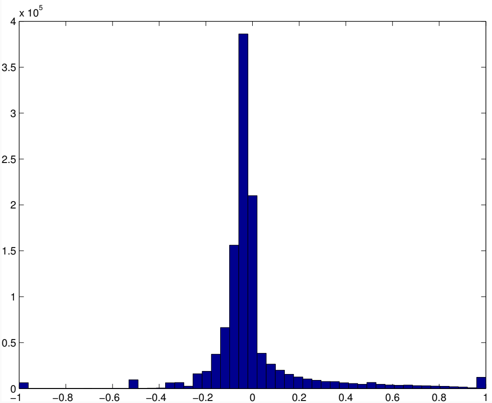


DBLP 2010 (LAW)



$N = 326186$, $nnz = 1615400$, 80 s (1000 moments, 10 probes)

Hollywood 2009 (LAW)



$N = 1139905$, $nnz = 113891327$, 2093 s (1000 moments, 10 probes)

Questions for You?

- Any isospectral graphs for multiple matrices?
- Can we recover topology from (exact) LDoS?
- Variance reduction in diagonal estimators?
- Random graphs with spectra that look “real”?
- Compression of moment information for diag estimators?
- More applications?

What Do You Hear?