Spectra of Large Random Stochastic Matrices & Relaxation in Complex Systems

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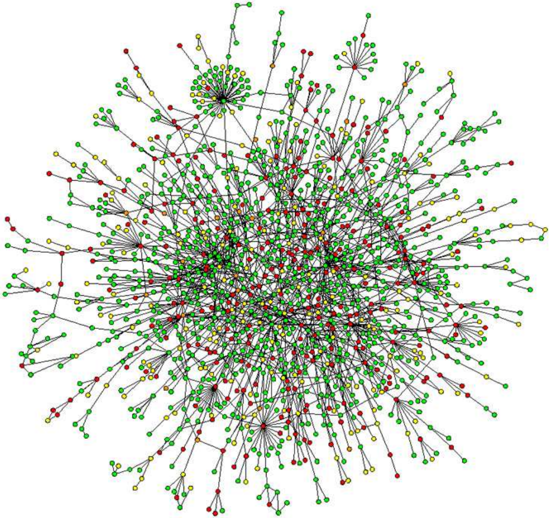
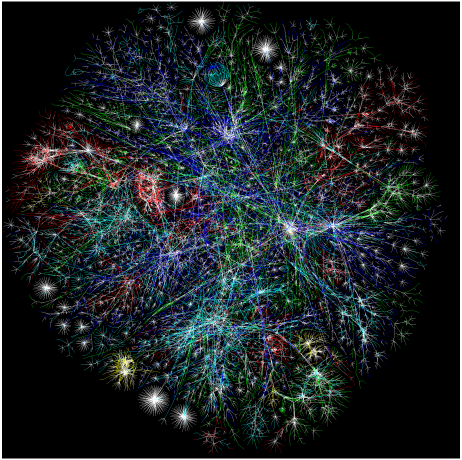


[Jeong et al (2001)]



[www.opte.org: Internet 2007]

Outline

1. Introduction
   - Discrete Markov Chains
   - Spectral Properties – Relaxation Time Spectra
2. Relaxation in Complex Systems
   - Markov Matrices Defined in Terms of Random Graphs
   - Applications: Random Walks, Relaxation in Complex Energy Landscapes
3. Spectral Density
   - Approach
   - Analytically Tractable Limiting Cases
4. Numerical Tests
5. Summary

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Discrete Markov Chains

- Discrete homogeneous Markov chain in an N-dimensional state space,

$$\mathbf{p}(t+1) = W\mathbf{p}(t) \qquad \Leftrightarrow \qquad p_i(t+1) = \sum_j W_{ij} p_j(t) \ .$$

- Normalization of probabilities requires that W is a stochastic matrix,

$$W_{ij} \geq 0 \quad \text{for all } i,j \qquad \text{and} \qquad \sum_i W_{ij} = 1 \quad \text{for all } j \ .$$

- Implies that generally

$$\sigma(W) \subseteq \{z; |z| \leq 1\} \ .$$

- If W satisfies a detailed balance condition, then

$$\sigma(W) \subseteq [-1,1] \ .$$

Spectral Properties – Relaxation Time Spectra

- Perron-Frobenius Theorems: exactly one eigenvalue $\lambda_1^\mu = +1$ for every irreducible component μ of state space.
- Assuming absence of cycles, all other eigenvalues satisfy

$$|\lambda_\alpha^\mu| < 1\ , \quad \alpha \neq 1\ .$$

- If system is overall irreducible: equilibrium is unique and convergence to equilibrium is exponential in time, as long as N remains finite:

$$\mathbf{p}(t) = W^t\,\mathbf{p}(0) = \mathbf{p}_{\mathrm{eq}} + \sum_{\alpha(\neq 1)} \lambda_\alpha^t\,\mathbf{v}_\alpha\,\big(\mathbf{w}_\alpha, \mathbf{p}(0)\big)$$

- Identify relaxation times

$$\tau_\alpha = -\frac{1}{\ln|\lambda_\alpha|}$$

$\Longleftrightarrow$ **spectrum of W relates to spectrum of relaxation times.**

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Markov matrices defined in terms of random graphs

- Interested in behaviour of Markov chains for large N, and transition matrices describing complex systems.
- Define in terms of weighted random graphs.
  - Start from a rate matrix $\Gamma = (\Gamma_{ij}) = (c_{ij} K_{ij})$
  - on a random graph specified by

$$\text{a connectivity matrix } C = (c_{ij})\ , \quad \text{and edge weights } K_{ij} > 0\ .$$

- Set Markov transition matrix elements to

$$W_{ij} = \begin{cases} \frac{\Gamma_{ij}}{\Gamma_j} & , \ i \neq j\ , \\ 1 & , \ i = j\ , \ \text{and} \ \ \Gamma_j = 0\ , \\ 0 & , \ \text{otherwise} \ \ , \end{cases}$$

where $\Gamma_j = \sum_i \Gamma_{ij}$.

Symmetrization

- Markov transition matrix can be symmetrized by a similarity transformation, if it satisfies a detailed balance condition w.r.t. an equilibrium distribution $p_i = p_i^{\mathrm{eq}}$

$$W_{ij} p_j = W_{ji} p_i$$

- Symmetrized by $\mathcal{W} = P^{-1/2} W P^{1/2}$ with $P = \mathrm{diag}(p_i)$

$$\mathcal{W}_{ij} = \frac{1}{\sqrt{p_i}} W_{ij} \sqrt{p_j} = \mathcal{W}_{ji}$$

- Symmetric structure is inherited by transformed master-equation operator $\mathcal{M} = P^{-1/2} M P^{1/2}$, with $M_{ij} = W_{ij} - \delta_{ij}$.
- **Computation of spectra below so far restricted to this case.**

Applications I – Unbiased Random Walk

- Unbiased random walks on complex networks: $K_{ij} = 1$; transitions to neighbouring vertices with equal probability:

$$W_{ij} = \frac{c_{ij}}{k_j} \ , \quad i \neq j \ ,$$

and $W_{ii} = 1$ on isolated sites ($k_i = 0$).

- Symmetrized version is

$$\mathcal{W}_{ij} = \frac{c_{ij}}{\sqrt{k_i k_j}} \ , \quad i \neq j \ ,$$

and $\mathcal{W}_{ii} = 1$ on isolated sites.

- Symmetrized master-equation operator known as normalized graph Laplacian

$$\mathcal{L}_{ij} = \begin{cases} \frac{c_{ij}}{\sqrt{k_i k_j}} & , \ i \neq j \\ -1 & , \ i = j \ \text{, and } k_i \neq 0 \\ 0 & , \ \text{otherwise} \ . \end{cases}$$

Applicatons II – Non-uniform Edge Weights

- Internet traffic (hopping of data packages between routers)
- Relaxation in complex energy landscapes; Kramers transition rates for transitions between long-lived states; e.g.:

$$\Gamma_{ij} = c_{ij} \exp\left\{ -\beta(V_{ij} - E_j) \right\}$$

with energies E_i and barriers V_{ij} from some random distribution.
$\Leftrightarrow$ generalized trap models.

- Markov transition matrices of generalized trap models satisfy a detailed balance condition with

$$p_i = \frac{\Gamma_i}{\mathcal{Z}} \mathrm{e}^{-\beta E_i}$$

$\Rightarrow$ can be symmetrized.

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Spectral Density and Resolvent

- Spectral density from resolvent

$$\rho_A(\lambda) = \frac{1}{\pi N} \mathrm{Im}\, \mathrm{Tr} \left[\lambda_\varepsilon \mathbb{1} - A\right]^{-1} , \qquad \lambda_\varepsilon = \lambda - \mathrm{i}\varepsilon$$

- Express as [S F Edwards & R C Jones (1976)]

$$\begin{aligned} \rho_A(\lambda) &= \frac{1}{\pi N} \mathrm{Im} \frac{\partial}{\partial \lambda} \mathrm{Tr} \ln \left[\lambda_\varepsilon \mathbb{1} - A\right] \\ &= -\frac{2}{\pi N} \mathrm{Im} \frac{\partial}{\partial \lambda} \ln Z_N , \end{aligned}$$

where Z_N is a Gaussian integral:

$$Z_N = \int \prod_k \frac{\mathrm{d}u_k}{\sqrt{2\pi/\mathrm{i}}} \exp\left\{ -\frac{\mathrm{i}}{2} \sum_{k,\ell} u_k (\lambda_\varepsilon \delta_{k\ell} - A_{k\ell}) u_\ell \right\} .$$

- Spectral density expressed in terms of single site-variances

$$\rho_A(\lambda) = \frac{1}{\pi N} \mathrm{Re} \sum_i \langle u_i^2 \rangle ,$$

Large Single Instances

- I. Investigate single large instances
  - Use cavity method to evaluates single-site marginals

$$P(u_i) \propto \exp\left\{-\frac{\mathrm{i}}{2}\lambda_\varepsilon u_i^2\right\} \int \prod_{j\in\partial i} \mathrm{d}u_j \exp\left\{\mathrm{i}\sum_{j\in\partial i} A_{ij}u_iu_j\right\} P_j^{(i)}(u_j)\ ,$$

  - On a (locally) tree-like graph get recursion for the cavity distributions,

$$P_j^{(i)}(u_j) \propto \exp\left\{-\frac{\mathrm{i}}{2}\lambda_\varepsilon u_j^2\right\} \prod_{\ell\in\partial j\setminus i} \int \mathrm{d}u_\ell \exp\left\{\mathrm{i}A_{j\ell}u_ju_\ell\right\} P_\ell^{(j)}(u_\ell)\ .$$

  - Cavity recrsions self-consistently solved by (complex) Gaussians.

$$P_j^{(i)}(u_j) = \sqrt{\omega_j^{(i)}/2\pi}\, \exp\left\{-\frac{1}{2}\omega_j^{(i)}u_j^2\right\}\ ,$$

  - generate recursion for inverse cavity variances

$$\omega_j^{(i)} = \mathrm{i}\lambda_\varepsilon + \sum_{\ell\in\partial j\setminus i} \frac{A_{j\ell}^2}{\omega_\ell^{(j)}}\ .$$

  - Solve iteratively on single instances for $N = \mathcal{O}(10^5)$

Thermodynamic Limit

Sparse Symmetric Random Matrices

- Recursions for inverse cavity variances can be interpreted as stochastic recursions, generating a self-consistency equation for their pdf $\pi(\omega)$.
  - Structure for (up to symmetry) i.i.d matrix elements $A_{ij} = c_{ij} K_{ij}$

    [RK (2008)]

    $$\pi(\omega) = \sum_{k\geq 1} p(k) \frac{k}{c} \int \prod_{\nu=1}^{k-1} \mathrm{d}\pi(\omega_\nu)\, \langle \delta(\omega - \Omega_{k-1}) \rangle_{\{K_\nu\}}$$

    with

    $$\Omega_{k-1} = \Omega_{k-1}(\{\omega_\nu, K_\nu\}) = \mathrm{i}\lambda_\varepsilon + \sum_{\nu=1}^{k-1} \frac{K_\nu^2}{\omega_\nu} \ .$$

  - Solve using population dynamics algorithm. [Mézard, Parisi (2001)]
    & get spectral density:

    $$\rho(\lambda) = \frac{1}{\pi} \mathrm{Re} \sum_k p(k) \int \prod_{\nu=1}^{k} \mathrm{d}\pi(\omega_\ell) \left\langle \frac{1}{\Omega_k(\{\omega_\nu, K_\nu\})} \right\rangle_{\{K_\nu\}}$$

  - Can identify continuous and pure point contributions to DOS.

Thermodynamic Limit

General Markov Matrices

- Same structure superficially;
  – first: transformation $u_i \leftarrow u_i/\sqrt{\Gamma_i}$ on non-isolated sites
  – second: differences due to column constraints
  ($\Rightarrow$ dependencies between matrix elements beyond degree)

$$\pi(\omega) = \sum_{k\geq 1} p(k)\frac{k}{c}\int \prod_{\nu=1}^{k-1} \mathrm{d}\pi(\omega_\nu)\ \left\langle \delta\big(\omega - \Omega_{k-1}\big)\right\rangle_{\{K_\nu\}}$$

with

$$\Omega_{k-1} = \sum_{\nu=1}^{k-1}\left[\mathrm{i}\lambda_\varepsilon K_\nu + \frac{K_\nu^2}{\omega_\nu + \mathrm{i}\lambda_\varepsilon K_\nu}\right] .$$

- In terms of these

$$\rho(\lambda) = p(0)\,\delta(\lambda-1) + \frac{1}{\pi}\mathrm{Re}\sum_{k\geq 1} p(k)\int \prod_{\nu=1}^{k} \mathrm{d}\pi(\omega_\ell)\ \left\langle \frac{\sum_{\nu=1}^{k} K_\nu}{\Omega_k(\{\omega_\nu, K_\nu\})}\right\rangle_{\{K_\nu\}}$$

Analytically Tractable Limiting Cases

Unbiased Random Walk on Random Regular & Large-c Erdös-Renyi Graph

- Recall FPE

$$\pi(\omega) = \sum_{k\geq 1} p(k)\frac{k}{c}\int \prod_{\nu=1}^{k-1} d\pi(\omega_\nu)\ \delta(\omega - \Omega_{k-1})$$

with

$$\Omega_{k-1} = i\lambda_\varepsilon k + \sum_{\nu=1}^{k-1} \frac{1}{\omega_\nu}\ .$$

- Regular Random Graphs $p(k) = \delta_{k,c}$. All sites equivalent.
- $\Rightarrow$ Expect

$$\pi(\omega) = \delta(\omega - \bar{\omega})\ , \qquad \Leftrightarrow \qquad \bar{\omega} = i\lambda_\varepsilon c + \frac{c-1}{\bar{\omega}}$$

- Gives

$$\rho(\lambda) = \frac{c}{2\pi}\,\frac{\sqrt{4\frac{c-1}{c^2} - \lambda^2}}{1-\lambda^2}$$

- $\Leftrightarrow$ Kesten-McKay distribution adapted to Markov matrices
- Same result for large c Erdös-Renyi graphs $\Rightarrow$ Wigner semi-circle

Analytically Tractable Limiting Cases

General Markov Matricies for large-c Erdös-Renyi Graph

- Recall FPE
$$\pi(\omega) = \sum_{k\geq 1} p(k)\frac{k}{c}\int \prod_{\ell=1}^{k-1} d\pi(\omega_\ell)\ \langle \delta(\omega - \Omega_{k-1})\rangle_{\{K_\nu\}}$$
with
$$\Omega_{k-1} = \sum_{\nu=1}^{k-1}\left[i\lambda_\varepsilon K_\nu + \frac{K_\nu^2}{\omega_\nu + i\lambda_\varepsilon K_\nu}\right].$$
- Large c: contributions only for large k. Approximate Ω_{k-1} by sum of averages (LLN). $\Rightarrow$ Expect
$$\pi(\omega) \simeq \delta(\omega - \bar{\omega})\ , \qquad \Leftrightarrow \qquad \bar{\omega} \simeq c\left[i\lambda_\varepsilon\langle K\rangle + \left\langle \frac{K^2}{\bar{\omega} + i\lambda_\varepsilon K}\right\rangle\right].$$
- Gives
$$\rho(\lambda) = \frac{1}{\pi}\mathrm{Re}\left[\frac{c\langle K\rangle}{\bar{\omega}}\right]$$
- Is remarkably precise already for $c \simeq 20$. For large c, get semicircular law
$$\rho(\lambda) = \frac{c}{2\pi}\frac{\langle K\rangle^2}{\langle K^2\rangle}\sqrt{\frac{4\langle K^2\rangle}{c\langle K\rangle^2} - \lambda^2}$$

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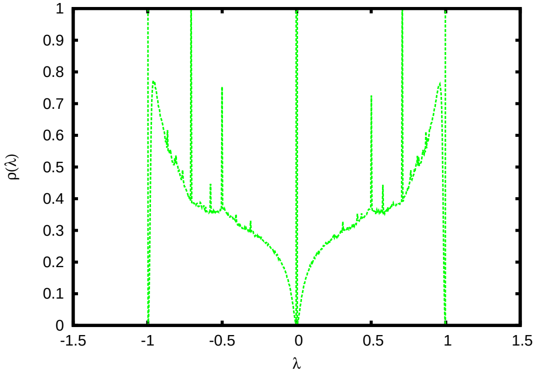
Unbiased Random Walk

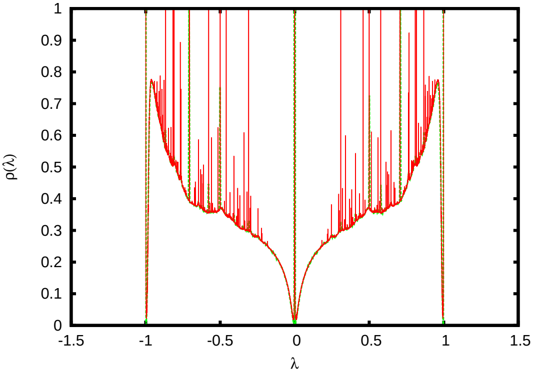
- Spectral density: $k_i \sim$ Poisson(2), $\mathcal{W}$ unbiased RW



Simulation results, averaged over 5000 1000×1000 matrices (green)

Unbiased Random Walk

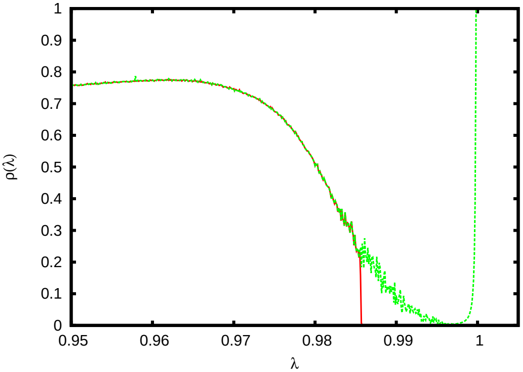
- Spectral density: $k_i \sim$ Poisson(2), $\mathcal{W}$ unbiased RW



Simulation results, averaged over 5000 1000×1000 matrices (green) ; population-dynamics results (red) added.

Unbiased Random Walk

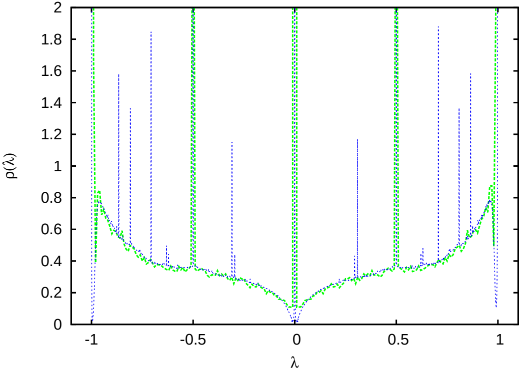
- Spectral density: $k_i \sim$ Poisson(2), $\mathcal{W}$ unbiased RW



zoom into the edge of the spectrum: extended states (red), total DOS (green).

Unbiased Random Walk

- population dynamics – cavity on single instance $k_i \sim$ Poisson(2)

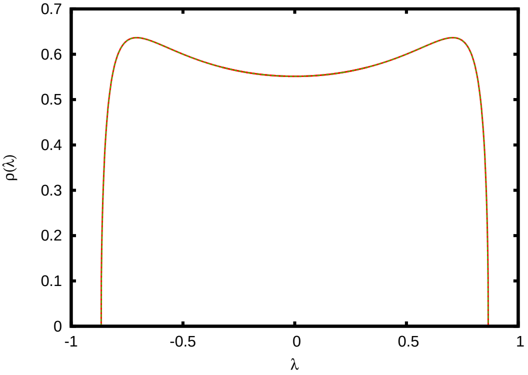


Population dynamics results (blue) compared to results from cavity approach

on a single instance of $N = 10^4$ sites (green), both for total DOS

Unbiased Random Walk–Regular Random Graph

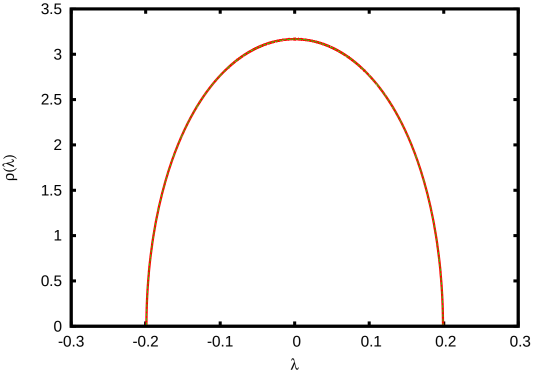
- comparison population dynamics – analytic result



Population dynamics results (red) compared to analytic result (green) for RW on regular random graph at $c = 4$.

Unbiased Random Walk–Large=c Erdös-Renyi

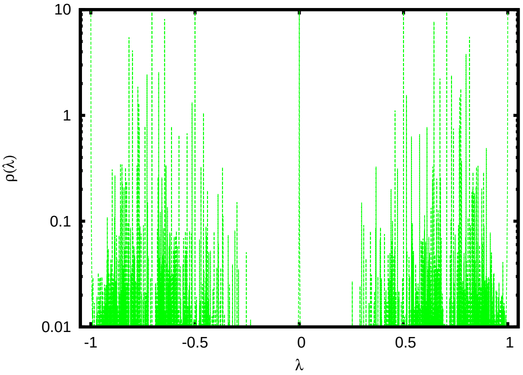
- comparison population dynamics – analytic result



Population dynamics results (red) compared to analytic result (green) for RW on Erdös-Renyi random graph at $c = 100$.

Unbiased Random Walk–Scale Free Graphs

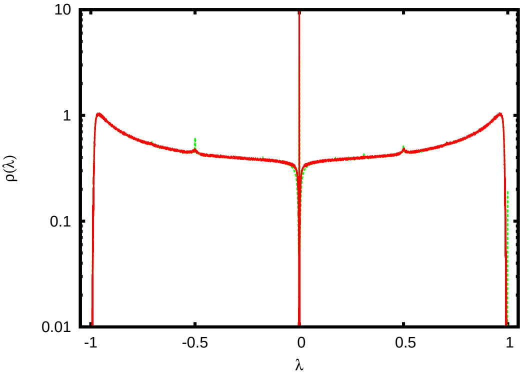
- Random graphs with $p(k) \propto k^{-\gamma}, k \geq k_{\min}$



Population dynamics results for RW on scale-free graph $\gamma = 4\ , k_{\min} = 1$.

Unbiased Random Walk–Scale Free Graphs

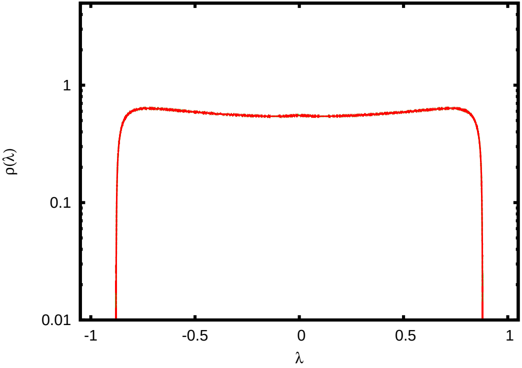
- Random graphs with $p(k) \propto k^{-\gamma}, k \geq k_{\min}$



Simulation results (green) compared with population dynamics results (red) for a RW on scale-free graph $\gamma = 4, k_{\min} = 2$.

Unbiased Random Walk–Scale Free Graphs

- Random graphs with $p(k) \propto k^{-\gamma}, k \geq k_{\min}$

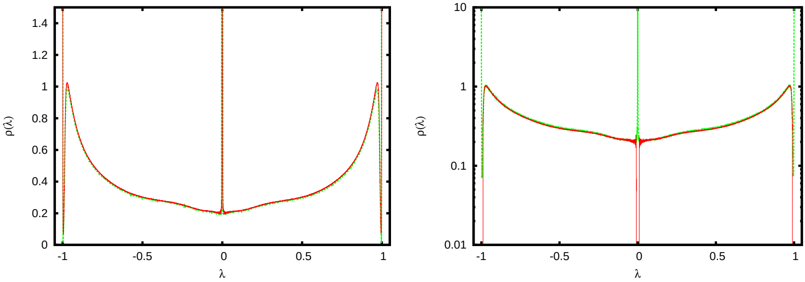


Population dynamics results (extende DOS red, total DOS green) for a RW on scale-free graph $\gamma = 4, k_{\min} = 3$.

Stochastic Matrices

- Spectral density: $k_i \sim \text{Poisson}(2)$, $p(K_{ij}) \propto K_{ij}^{-1}; K_{ij} \in [e^{-\beta}, 1]$

$$\Leftrightarrow K_{ij} = exp\{-\beta V_{ij}\} \text{ with } V_{ij} \sim U[0,1] \Leftrightarrow \text{ Kramers rates.}$$

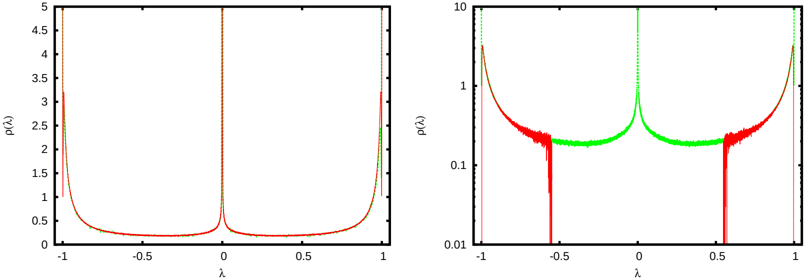


Spectral density for stochastic matrices defined on Poisson random graphs with $c = 2$, and $\beta = 2$. Left: Simulation results (green) compared with population dynamics results (red). Right: Population dynamics results, extended states (red), total DOS (green).

Stochastic Matrices

- Spectral density: $k_i \sim$ Poisson(2), $p(K_{ij}) \propto K_{ij}^{-1}; K_{ij} \in [\mathrm{e}^{-\beta}, 1]$

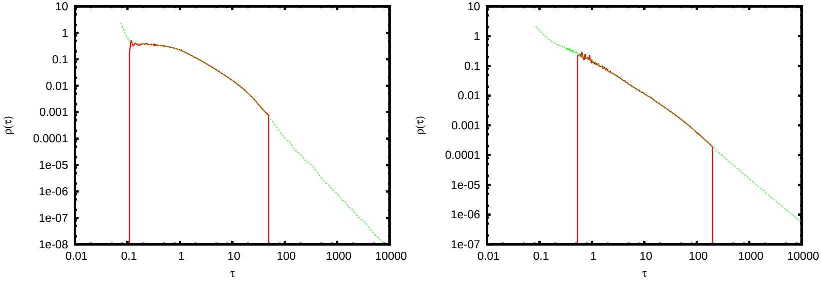
$$\Leftrightarrow K_{ij} = exp\{-\beta V_{ij}\} \ \text{ with } \ V_{ij} \sim U[0,1] \Leftrightarrow \ \text{Kramers rates.}$$



Spectral density for stochastic matrices defined on Poisson random graphs with $c = 2$, and $\beta = 5$. Left: Simulation results (green) compared with population dynamics results (red); Right: Population dynamics results, extended states (red), total DOS (green).

Stochastic Matrices – Relaxation time spectra

- Kramers rates: relaxation time spectra



Relaxation time spectra; scale-free graph $p_k \sim k^{-3}$ for $k \geq 2$. Kramers rates at $\beta = 2$ (left) and $\beta = 5$ (right). DOS of extended modes (red full line) and total DOS (green dashed line).

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Summary

- Computed DOS of Stochastic matrices defined on random graphs.
- Analysis equivalent to alternative replica approach.
- Restrictions: detailed balance & finite mean connectivity
- Closed form solution for unbiased random walk on regular random graphs
- Algebraic approximations for general Markov matrices on large c random regular and Erdös Renyi graphs.
- Get semicircular laws asymptotically at large c.
- Localized states at edges of specrum implies finite maximal relaxation time for extended states (transport processes) even in thermodynamic limit.
- For $p(K_{ij}) \propto K_{ij}^{-1}; K_{ij} \in [\mathrm{e}^{-\beta}, 1]$ see localization effects at large β and concetration of DOS at edges of the spectrum ($\leftrightarrow$ relaxation time spectrum dominated by slow modes $\Rightarrow$ Glassy Dynamics?

Open Problems

- Analytic determination of mobility edges.

  Generalize approach of Abou-Chacra, Anderson, Thouless (1973)

- Computation of IPRs, statistics of eigenvector components

  eigenvector corresponding to largest EV: via Ritz variational principle, Kabashima et al (2010)

- Asymptotics for $\lambda \ll 1$ (fast modes) and $|1 - |\lambda|| \ll 1$ (slow modes).
- Disentangling results pertaining to giant component and finite clusters

  combine cavity approaches for RMT spectra and percolation theory on graphs

- Generalization to systems without detailed balance (directed links).