Spectra of Large Random Stochastic Matrices & Relaxation in Complex Systems

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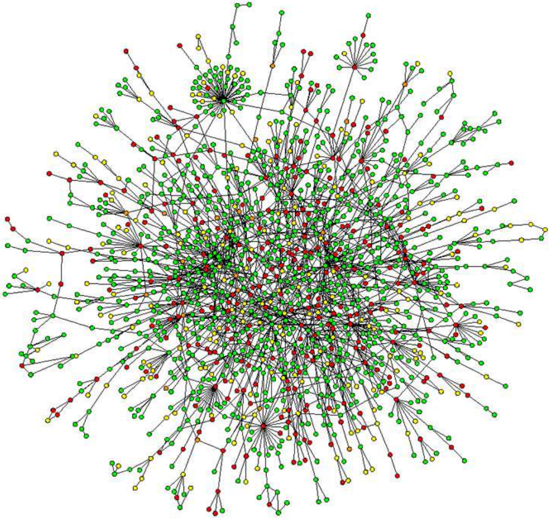
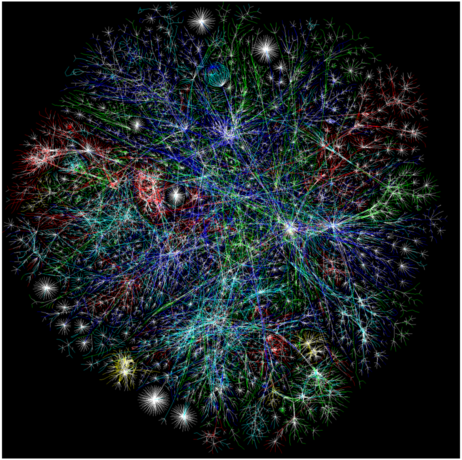


[Jeong et al (2001)]



[www.opte.org: Internet 2007]

Outline

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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

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:

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

- Identify relaxation times

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

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

Outline

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

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

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

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

  - 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

- 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.

Self-Consistency Equations & Spectral Density

Unbiased Random Walk

- Self-consistency equations for pdf of inverse cavity variances;
  – first: transformation $u_i \leftarrow u_i/\sqrt{k_i}$ on non-isolated sites

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

  with

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

- Solve using stochastic (population dynamics) algorithm.
- In terms of these

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

Self-Consistency Equations & Spectral Density

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

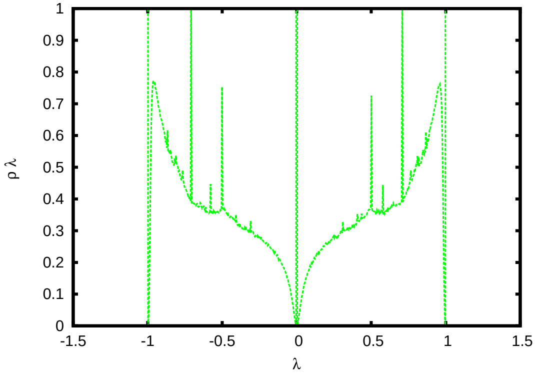
General Markov Matricies for large-c Erdös-Renyi Graph

- 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
$$\rho(\lambda) = \frac{c}{2\pi}\frac{\langle K\rangle^2}{\langle K^2\rangle}\sqrt{\frac{4\langle K^2\rangle}{c\langle K\rangle^2} - \lambda^2}$$

Outline

Unbiased Random Walk

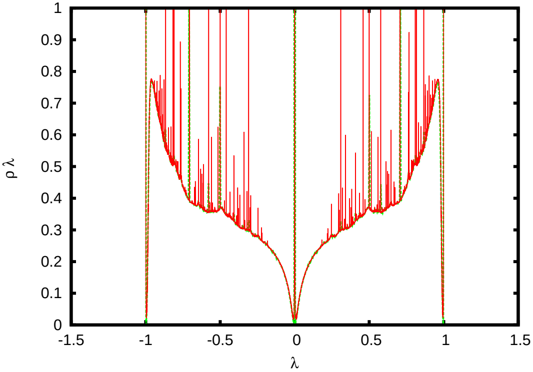
- Spectral density: $k_i \sim$ Poisson(2), $\mathcal{W}$ unbiased RW



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

Unbiased Random Walk

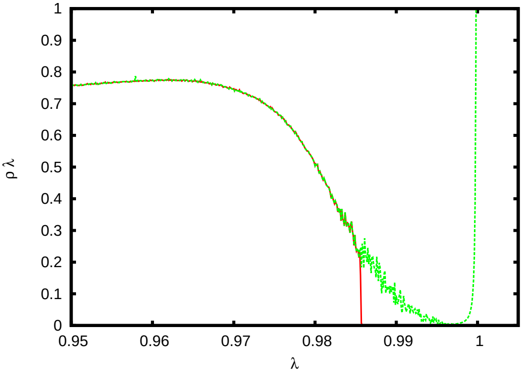
- Spectral density: $k_i \sim$ Poisson(2), $\mathcal{W}$ unbiased RW



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

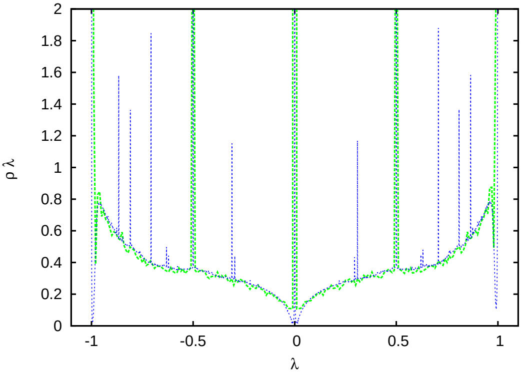


Simulation results, averaged over 5000 1000×1000 matrices (green); population-dynamics results (red) added;

population dynamics results: zoom into $\lambda \simeq 1$ region. (total DOS green, extended states (red).

Unbiased Random Walk

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

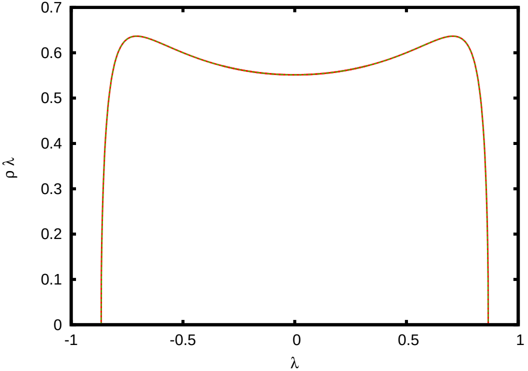


Population dynamics results (blue) compared to results from cavity approach

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

Unbiased Random Walk–Regular Random Graph

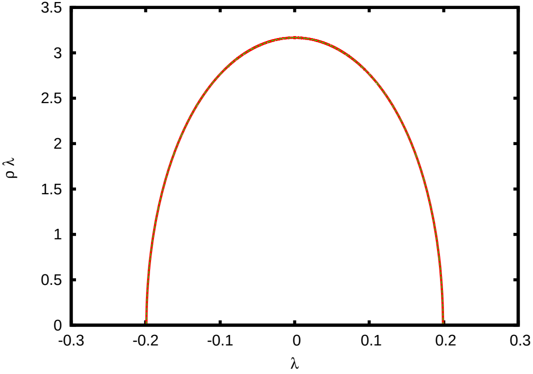
- comparison population dynamics – analytic result



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

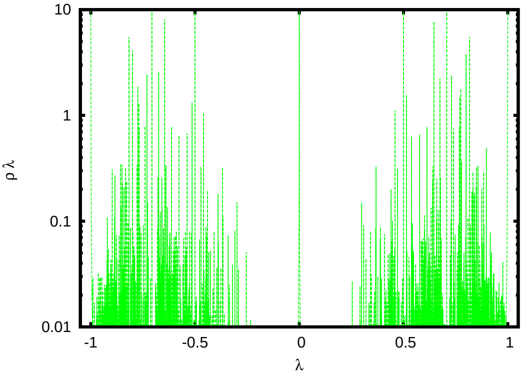
- comparison population dynamics – analytic result



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

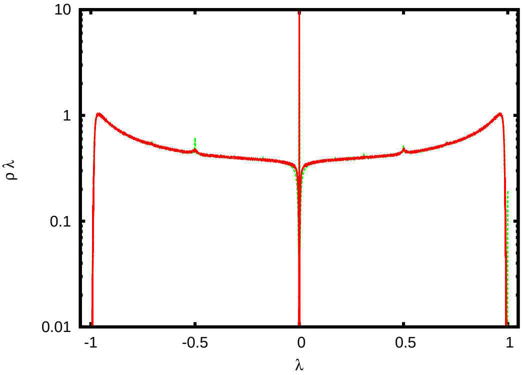
- Random graphs with $p(k) \propto k^{-\gamma}$, $k \geq k_{\text{min}}$



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

Unbiased Random Walk–Scale Free Graphs

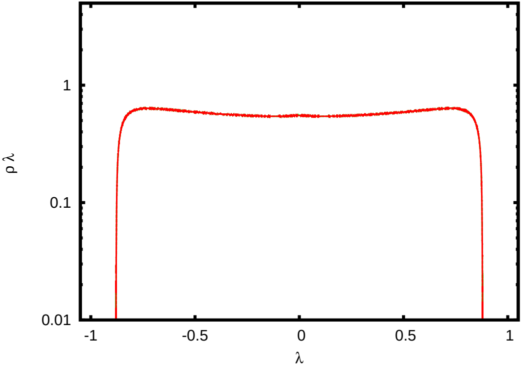
- Random graphs with $p(k) \propto k^{-\gamma}$, $k \geq k_{\rm min}$



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

Unbiased Random Walk–Scale Free Graphs

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

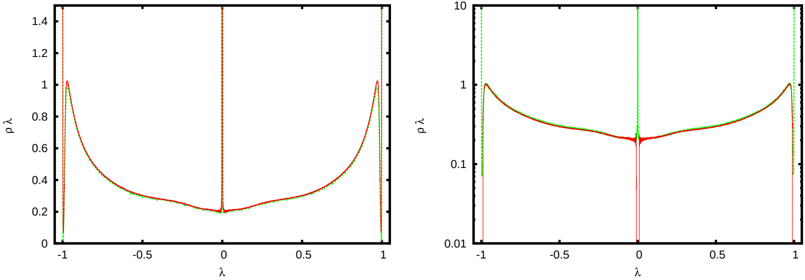


Population dynamics results (extende DOS red, total DOS green) for a RW on scale-free graph $\gamma = 4$, $k_{\text{min}} = 3$.

Stochastic Matrices

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

  $\Leftrightarrow K_{ij} = exp\{-\beta V_{ij}\}$ with $V_{ij} \sim U[0,1] \Leftrightarrow$ 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: $k_i \sim \text{Poisson}(2)$, $p(K_{ij}) \propto K_{ij}^{-1}$; $K_{ij} \in [\mathrm{e}^{-\beta}, 1]$

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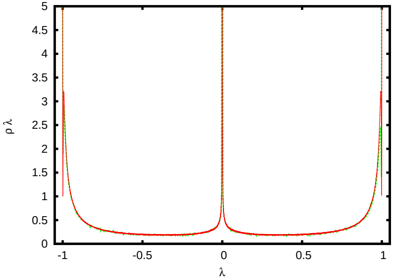
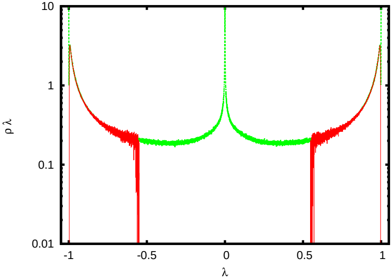




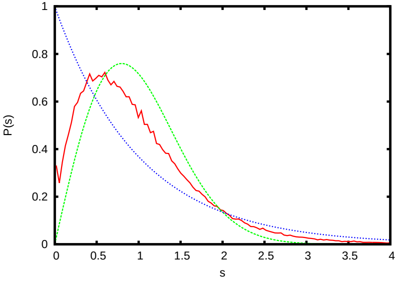
Spectral density for stochastic matrices defined on Poisson random graphs with $c = 2$, and $\beta = 5$. Left: Simulation results (green) compared with population dynamics results (red); Right: Population dynamics results, extended states (red), total DOS (green).

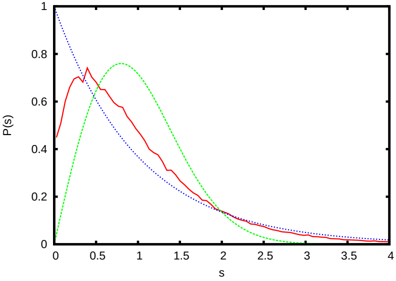
Stochastic Matrices

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

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

- Level spacings

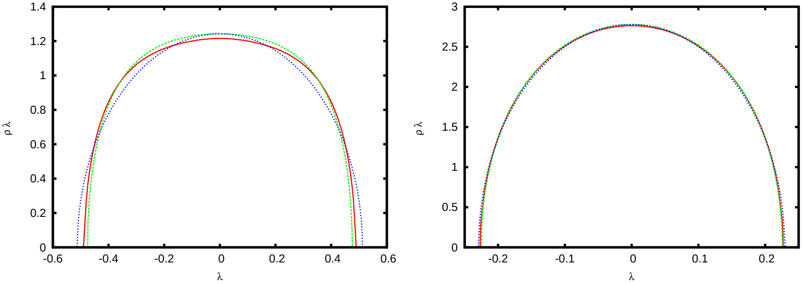




Level-spacing distribution for stochastic matrices defined on Poisson random graphs with $c = 2$, and $\beta = 2$ (left), $\beta = 5$ (right). Also shown are the predicions for GOE matrices (green) and the spacing distribution for Poisson points (blue).

Stochastic Matrices – Large *c* Erdös Renyi

- Kramers rates: comparison population dynamics – analytic result



Population dynamics results (green) compared to analytic approximation (red) and asymptotic semicircular law (blue) for a Poisson random graph at $c = 20$ (left) and $c = 100$ (right), with Kramers rates at $\beta = 2$.

Outline

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 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?