Spectra of Random Stochastic Matrices and Relaxation in Complex Systems

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We compute spectra of large stochastic matrices $W$, defined on sparse random graphs, where edges $(i,j)$ of the graph are given positive random weights $W_{ij} > 0$ in such a fashion that column sums are normalized to one. We compute spectra of such matrices both in the thermodynamic limit, and for single large instances. The structure of the graphs and the distribution of the non-zero edge weights $W_{ij}$ are largely arbitrary, as long as the mean vertex degree remains finite in the thermodynamic limit and the $W_{ij}$ satisfy a detailed balance condition. Knowing the spectra of stochastic matrices is tantamount to knowing the complete spectrum of relaxation times of stochastic processes described by them, so our results should have many interesting applications for the description of relaxation in complex systems. Our approach allows to disentangle contributions to the spectral density related to extended and localized states, respectively, allowing to differentiate between time-scales associated with transport processes and those associated with the dynamics of local rearrangements.

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There are numerous processes, both natural and artificial, which can be understood in terms of random walks on complex networks [1–3], including the spread of diseases in social networks [4, 5], the transmission of information in communication networks (e.g. [6]), search algorithms [7, 8], the out-of-equilibrium dynamics of glassy systems at low temperatures as described in terms of hopping between long-lived states in state space [9–11], the dynamics of major conformational changes in macromolecules [12], or cell-signalling through protein-protein interaction networks [13], to name but a few. For reviews that cover conformational changes in macromolecules [12], or cell-signalling through protein-protein interaction networks [13], to name but a few. For reviews that cover the evolution of initial probability vector $p(0)$ over $t$ time steps, i.e. by considering $p(t) = W^t p(0)$. Using a spectral decomposition of $W$, and assuming the system to be irreducible and free of cycles, one obtains

$$p(t) = p^{\text{eq}} + \sum_{\alpha \neq 1} \lambda_\alpha \omega_\alpha \left(\omega_\alpha, p(0)\right)$$

where we have used that $1 = \lambda_1 > |\lambda_\alpha|$ for $\alpha \neq 1$, given the assumptions [17], and where $\omega_\alpha$ and $\omega_\alpha$ denote the right and left eigenvectors of $W$, respectively, with $\omega_1 \equiv p^{\text{eq}}$, and $\omega_1 = (1, \ldots, 1)$. Eq. (2) allows to relate relaxation times of the system to eigenvalues of $W$ via $\tau_\alpha = -1/\ln |\lambda_\alpha|$ for $\alpha \neq 1$.

We construct random stochastic matrices in terms of unnormalized transition matrices $\Gamma = (\Gamma_{ij}) = (c_{ij}K_{ij})$, with connectivity matrix elements $c_{ij} \in \{0,1\}$ (and $c_{ii} = 0$) specifying the network structure of possible transitions, and positive edge weights $K_{ij} > 0$, and setting $W_{ij} = \Gamma_{ij}/\Gamma_j$ if $\Gamma_j \equiv \sum_i \Gamma_{ij} \neq 0$, and $W_{ii} = 1$ for isolated sites for which $\Gamma_i = 0$. The present investigation will be restricted to the case where $W$ satisfies a detailed balance condition, and can thus be symmetrized by a similarity transformation, as discussed above. The spectrum of fully connected matrices of this type was shown to converge to a semi-circular law [18] in the large system limit, and to a circular law, if the detailed balance condition is dropped [19]. Asymptotic results related to the circular law were obtained for Erdös-Renyi graphs with
mean connectivity diverging in the thermodynamic limit [20]. For some recent related results concerning spectra of graph Laplacians, we refer to [21–23].

We follow [24] and express the spectral density $\rho_W(\lambda)$ of the stochastic matrix $W$ in terms of a derivative

$$
\rho_W(\lambda) = -\lim_{\varepsilon \to 0} \frac{2}{\pi N} \Im \frac{\partial}{\partial \lambda} \log Z_W(\lambda) ,
$$

of the logarithm of a Gaussian integral

$$
Z_W(\lambda) = \int \prod_{i=1}^{N} \frac{du_i}{\sqrt{2\pi i}} \exp \left\{ -iH_W(\lambda, u) \right\}
$$

defined in terms of the quadratic form

$$
H_W(\lambda, u) = \frac{1}{2} \sum_{i,j} (\lambda_\varepsilon \delta_{ij} - W_{ij}) u_i u_j ,
$$

with $\lambda_\varepsilon = \lambda - i\varepsilon$. Here, $W$ is the symmetrized version of $W$, obtained via a similarity transform that involves the equilibrium distribution $p^\text{eq}$ as discussed above. The representation (3) allows to interpret the spectral density as a sum over single site variances

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

of the complex Gaussian measure

$$
P_W(u) = \frac{1}{Z_W} e^{-iH_W(\lambda, u)} .
$$

Here and in what follows we shall omit explicitly writing the limit $\varepsilon \to 0$, and take it to be understood.

In the thermodynamic limit, the spectral density is expected to be non-random and is obtained by averaging Eq. (3) over the matrix ensemble in question, using the replica method to perform averages as proposed in [24], and taking the limit $N \to \infty$. Methods developed in [25] can be used to efficiently deal with the sparsity of the ensemble of matrices considered in the present letter. Alternatively, one can analyse single large instances using a cavity approach proposed in [26] to obtain the single instance spectral density in terms of variances of single-site marginals. In the thermodynamic limit, recursion relations for the cavity-variances obtained within that approach can be interpreted as stochastic recursions, allowing to formulate self-consistency relations for their distributions, which turn out to be equivalent to those obtained using replica. This is the approach we shall briefly outline in what follows.

In order not to overburden the present exposition with technicalities, we shall restrict our attention here to cases where the unnormalized transition matrix $\Gamma$ is symmetric, in which case the symmetrized normalized Markov matrix is of the form

$$
W_{ij} = \frac{\Gamma_{ij}}{\sqrt{\Gamma_{ii} \Gamma_{jj}}} ,
$$

for $\Gamma_{ij} > 0$, hence $\Gamma_i > 0$ and $\Gamma_j > 0$, and $W_{ii} = 1$ for isolated sites.

To obtain the single-site marginals of (7) required to evaluate $\rho_W(\lambda)$ according to (6), we distinguish between single-site marginals on isolated sites, which are of the form $p_W(u_i) \propto e^{-\frac{1}{2}(\lambda_\varepsilon-1) u_i^2}$, and those for sites that are not isolated. On the latter, we perform a transformation of variables, $\frac{\pi N}{\lambda} \to u_i$. In terms of the transformed variables, we have

$$
\rho_W(\lambda) = p_N(0) \delta(\lambda - 1) + \Re \frac{1}{\pi N} \sum_i \Gamma_i (u_i^2) ,
$$

with $p_N(0) = \frac{N_\text{is}}{N}$ denoting the fraction of isolated sites, and only non-isolated sites with $\Gamma_i > 0$ contributing to the second sum.

On a locally tree-like graph a marginal $P_i(u_i)$ of a (transformed) variable on a non-isolated site can be expressed in terms of cavity marginals $P_j^{(i)}(u_j)$ on sites in the neighbourhood $\partial i$ of $i$ as

$$
P_i(u_i) \propto e^{-\frac{1}{2} \Gamma_{ij} \lambda_\varepsilon u_i^2} \prod_{j \in \partial i} \int du_j e^{iK_{ij} u_i u_j} P_j^{(i)}(u_j) .
$$

The cavity marginals satisfy a set of self consistency equations

$$
P_j^{(i)}(u_j) \propto e^{-\frac{1}{2} \Gamma_{ij} \lambda_\varepsilon u_j^2} \prod_{\ell \in \partial j \setminus i} \int du_\ell e^{iK_{ij} u_j u_\ell} P_\ell^{(j)}(u_\ell) .
$$

These relations are exact on trees; for finitely connected random graphs they become asymptotically exact in the thermodynamic limit. They are solved [26] by complex Gaussians of the form

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

with $\Re \omega_j^{(i)} \geq 0$, entailing that the inverse cavity variances satisfy the self-consistency equations

$$
\omega_j^{(i)} = i\lambda_\varepsilon \Gamma_j + \sum_{\ell \in \partial j \setminus i} K_{ij}^\ell / \omega_\ell^{(j)} .
$$

These can be solved iteratively on large single instances. Single-site marginals, too, will be Gaussian with inverse variances expressed in terms of solutions of (10) as $\omega_i = i\lambda_\varepsilon \Gamma_i + \sum_{j \in \partial i} K_{ij}^i / \omega_j^{(i)}$. In terms of these inverse variances of single-site marginals then, we have

$$
\rho_W(\lambda) = p_N(0) \delta(\lambda - 1) + \Re \frac{1}{\pi N} \sum_i \frac{\Gamma_i}{\omega_i} .
$$
cavity variances of the form

Cavities

of which the problem was originally formulated, and this issue we return to the Gaussian integral in terms that extends beyond degree. In order to deal with numerical diagonalization of an ensemble of 1000 × 1000 matrices (green dashed curve) and analytic results obtained by solving (12) via population dynamics (red full curve).

Specializing to the case of unbiased random walk, we have \( \Gamma_{ij} = c_{ij} \), hence \( \Gamma_j = k_j \) and \( W_{ij} = c_{ij} / \sqrt{k_i k_j} \) for non-isolated sites, where \( k_i \) and \( k_j \) are degrees of vertices \( i \) and \( j \). In this case, Eqs. (10)-(11) readily lend themselves for averaging over a graph-ensemble in the thermodynamic limit, giving rise to an integral equation for a probability density function \( \pi(\omega) \) for inverse cavity variances of the form

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

in which \( p(k) \) is the degree distribution (thus \( p(k)k/c \) the probability of an edge to be connected to a site with degree \( k \), and \( \Omega_{k-1} = \Omega(\omega_1^{k-1}) = i\lambda k + \sum_{\nu=1}^{k-1} \omega_{\nu} \). In terms of the solution of (12), one obtains the spectral density of \( W \) for a random graph with degree distribution \( p(k) \) as

\[
\rho(\lambda) = p(0)\delta(\lambda - 1) + \frac{1}{\pi} \text{Re} \sum_{k \geq 1} p(k) \int \prod_{\nu=1}^{k-1} d\pi(\omega_{\nu}) \frac{k}{\Omega_k}.
\]

Contributions related to extended and localized states can be identified as explained in [25]. The same results have been obtained within a replica approach [27].

For Markov processes other than the unbiased random walk, straightforward averaging of cavity recursions over the ensemble of Markov matrices is prevented by the fact that the \( K_{ij} \) in (10) are not independent due to column sum constraints, in a way that extends beyond degree. In order to deal with this issue we return to the Gaussian integral in terms of which the problem was originally formulated, and rewrite the quadratic form (using transformed variables on non-isolated sites) as

\[
H_W = \frac{1}{2} \sum_{ij}(\lambda c - 1)u_i^2 + \frac{1}{2} \sum_{ij}c_{ij} \left[ \frac{1}{2} \lambda c K_{ij} (u_i^2 + u_j^2) - K_{ij} u_i u_j \right].
\]

Using this setup, one easily obtains the following reformulated recursion for inverse variances of cavity marginals

\[
\omega^{(i)}_j = \sum_{\ell \in \partial j \setminus i} \left( \frac{i\lambda c K_{j\ell} + K^2_{j\ell}}{\omega^{(i)}_{j\ell} + i\lambda c K_{j\ell}} \right),
\]

This version allows ensemble averaging, giving rise to the self-consistency equation

\[
\pi(\omega) = \sum_{k \geq 1} p(k) \frac{k}{c} \prod_{\nu=1}^{k-1} d\pi(\omega_{\nu}) \left\{ \delta(\omega - \Omega_{k-1}) \right\}_{\{\nu\}}
\]

with now

\[
\Omega_{k-1} = \sum_{\nu=1}^{k-1} \left( i\lambda c K_{\nu} + \frac{K^2_{\nu}}{\omega_{\nu} + i\lambda c K_{\nu}} \right),
\]

which is efficiently solved using a population dynamics algorithm. In terms of its solution, the spectral density in the thermodynamic limit is given by

\[
\rho(\lambda) = p(0)\delta(\lambda - 1) + \frac{1}{\pi} \text{Re} \sum_{k \geq 1} p(k) \int \prod_{\nu=1}^{k-1} d\pi(\omega_{\nu}) \left\{ \frac{\sum_{\nu=1}^{k} K_{\nu}}{\Omega_k} \right\}_{\{\nu\}}.
\]

Fig. 1 shows the spectrum of the transition matrix for an unbiased random walk on an Erdős-Rényi graph of mean connectivity \( c = 2 \), comparing results of numerical diagonalization of 1000 × 1000 matrices, showing excellent agreement except that our population dynamics algorithm picks of 1000 matrices, showing excellent agreement except that our population dynamics algorithm picks systems of this type were studied within a heterogeneous mean-field approximation to dynamics in [11], generalizing earlier work [9, 10] to include barrier height distributions and incompletely connected networks of traps. Two aspects are particularly notable: (i) as \( \beta \) is increased the spectral density gives more weight to regions near \( \lambda = \pm 1 \),
expression for the spectral density when inserted into (13), allows to obtain a closed-form quadratic self-consistency equation for \(\bar{\omega}\) weights. This expression is invariant under rescaling of the edge weights \(K_{ij}\), as it should, because \(K\) scales are immaterial in normalized Markov transition matrices.

For the unbiased random walk problem on a regular random graph with \(\rho(k) = \delta_{k,c}\), Eqs (12) are solved by a \(\delta\)-function, \(\pi(\omega) = \delta(\omega - \bar{\omega})\), giving rise to a quadratic self-consistency equation for \(\bar{\omega}\); its solution, when inserted into (13), allows to obtain a closed-form expression for the spectral density

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

which is readily recognised as a variant of the Kesten-McKay distribution [28], adapted to capture the spectral problem of the Markov transition matrix for an unbiased random walk on random regular graphs. The same result is found to provide an accurate approximate description for \(\rho(\lambda)\) at large mean degree \(c\), which becomes asymptotically exact as \(c \to \infty\), where (18) approaches a semicircular law. An analogous line of reasoning allows to obtain the spectral density for more general Markov matrices on Erdős-Rényi and random regular random graphs in the large \(c\) limit, viz. the semi-circular law

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

This expression is invariant under rescaling of the edge weights \(K_{ij}\), as it should, because \(K\) scales are immaterial in normalized Markov transition matrices.

In summary, we computed spectra of random stochastic matrices defined in terms of random graphs, assuming that they satisfy a detailed balance condition. Of particular relevance is the possible appearance of localized states in such systems. Referring to Eq. (2), one can indeed argue that most modes corresponding to localized states will not contribute to the relaxation dynamics, if initial conditions are themselves localized, an issue we have not seen systematically investigated in the literature. Further details on several of the issues which could be just touched upon in the present letter will be provided in a forthcoming paper [27]. We expect our methods and results to be of interest for the study of a broad range of relaxation phenomena in complex systems.