Top eigenpair statistics for sparse symmetric random matrices

Vito Antonio Rocco Susca, Pierpaolo Vivo and Reimer Kühn
King's College London, Department of Mathematics
EPSRC CANES CDT in Cross-Disciplinary Approaches to Non-Equilibrium Systems

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Abstract

We develop a formalism to compute the statistics of the largest eigenpair of weighted sparse graphs with Poissonian connectivity and a bounded maximal degree. By framing the problem in terms of optimization of a quadratic form on the sphere and introducing a fictitious temperature, we employ the cavity and replica methods to find the solution in terms of self-consistent equations for auxiliary probability density functions, which can be solved by population dynamics. This derivation allows us to identify and disentangle the individual contributions to the top eigenvector's components coming from nodes of different degree and is in perfect agreement with numerical diagonalization of large matrices.

Statistical Mechanics formulation

- We consider sparse random $N \times N$ symmetric matrices with real i.i.d entries $J_{ij} = c_{ij} K_{ij}$, where c_{ij} represents the connectivity matrix, i.e. an adjacency matrix of a graph, and K_{ij} encodes the bond weights. We consider Poissonian highly sparse connectivity, such that the probability of two nodes being connected is equal to $p = {}^{c}/_{N}$, with the mean degree c a finite constant. The maximum degree is s_{max}. The bond weights are i.i.d. drawn from a parent pdf $p(K)$. Such a matrix admits real eigenvalues, the largest being λ_1 with the corresponding eigenvector $\boldsymbol{v}_1$.
- The goal of this work is to set up a formalism based on the statistical mechanics of disordered systems to find the average or typical value of the largest eigenvalue $\overline{\lambda_1}$ and the density of the corresponding top eigenvector's components $\rho(u)$ in the limit $N \to \infty$.
- The search for the largest eigenpair can be formulated as a constrained optimization problem over a sphere of radius N as in [1]

$$\min_{||\boldsymbol{v}||=N} -\frac{1}{2}(\boldsymbol{v}, J\boldsymbol{v}) = \min_{||\boldsymbol{v}||=N} H(\boldsymbol{v}) = N\lambda_1 .$$

- For any fixed matrix J, this minimum can be computed by introducing a fictitious canonical ensemble of vectors $\boldsymbol{v} \in \mathbb{R}^N$, whose Gibbs-Boltzmann distribution at inverse temperature β is

$$P_\beta(\boldsymbol{v}) = \frac{1}{Z(\beta, J)} \exp\left[\frac{\beta}{2}(\boldsymbol{v}, J\boldsymbol{v})\right] \delta(|\boldsymbol{v}|^2 - N) .$$

- In the zero temperature limit $\beta \to \infty$, only the ground "state" of the systems is populated, corresponding to $\boldsymbol{v}_1$.
- To deal with this distribution, we employ both the **replica** and **cavity** method, showing that these two conceptually different techniques lead to the same solution. The partition function $Z(\beta, J)$ is the starting point of the replica treatment.
- Alternatively, one could start from a 'soft constraint' version of the same distribution, which will prove more convenient as a starting point for the analysis based on the cavity method.

Cavity Method

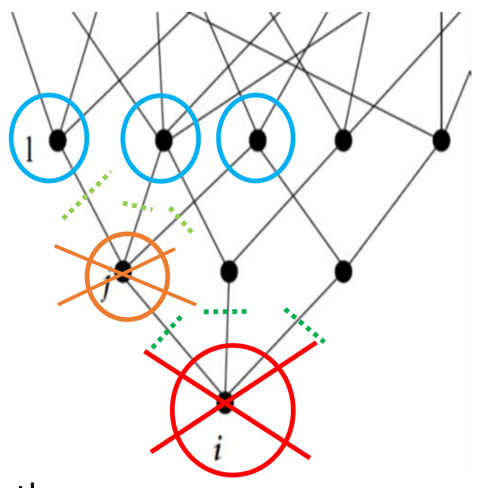
- Given a **single instance** of the matrix J and considering the grand canonical ensemble of the vectors $\boldsymbol{v} \in \mathbb{R}^N$ (equivalent to the canonical one for large N), the marginal distribution of the i-th component is

$$P_i(v_i) = \frac{1}{Z_i} \exp\left(-\frac{\beta}{2}\lambda v_i^2\right) \int \mathrm{d}\boldsymbol{v}_{\partial i} \exp\left(\beta \sum_{j\in\partial i} v_i J_{ij} v_j\right) P^{(i)}(\boldsymbol{v}_{\partial i}) ,$$

where $P^{(i)}(\boldsymbol{v}_{\partial i})$ is the *cavity probability distribution* and ∂i indicates the neighbourhood of i. Tree-like approximation holds for very sparse connectivity: removing the node i makes the branches departing from it independent

$$P_i(v_i) = \frac{1}{Z_i} \exp\left(-\frac{\beta}{2}\lambda v_i^2\right) \prod_{j\in\partial i} \int \mathrm{d}v_j \exp(\beta v_i J_{ij} v_j) P_j^{(i)}(v_j) .$$

- Marginalizing corresponds to "removing" the node i from the network. With the same reasoning applied to the network in which the node i has been already removed, a self-consistent equation can be derived for the *cavity marginal distribution* $P_j^{(i)}(v_j)$



$$P_j^{(i)}(v_j) = \frac{1}{Z_j^{(i)}} \exp\left(-\frac{\beta}{2}\lambda v_j^2\right) \prod_{\ell\in\partial j\setminus i} \int \mathrm{d}v_\ell \exp(\beta v_j J_{j\ell} v_\ell) P_\ell^{(j)}(v_\ell) .$$

- The above self-consistent equation is solved by a non-zero mean Gaussian ansatz

$$P_j^{(i)}(v_j) = \sqrt{\frac{\beta\omega_j^{(i)}}{2\pi}} \exp\left(-\frac{\beta {h_j^{(i)}}^2}{2\omega_j^{(i)}}\right) \exp\left\{-\frac{\beta}{2}\omega_j^{(i)} v_j^2 + \beta h_j^{(i)} v_j\right\} ,$$

where the coefficients $\omega_j^{(i)}$ and $h_j^{(i)}$ are called *cavity fields.* They are determined by the update rules:

$$\omega_j^{(i)} = \lambda - \sum_{\ell\in\partial j\setminus i} \frac{J_{j\ell}^2}{\omega_\ell^{(j)}} \qquad h_j^{(i)} = \sum_{\ell\in\partial j\setminus i} \frac{J_{j\ell} h_\ell^{(j)}}{\omega_\ell^{(j)}} .$$

In turn, the single-site marginal $P_i(v_i)$ can also be expressed as a non-zero mean Gaussian whose coefficients are given by

$$\Omega_i = \lambda - \sum_{j\in\partial i} \frac{J_{ij}^2}{\omega_j^{(i)}} \qquad H_i = \sum_{j\in\partial i} \frac{J_{ij} h_j^{(i)}}{\omega_j^{(i)}} .$$

- In the limit $\beta \to \infty$, the single site marginal $P_i(v_i)$ converges to the distribution of the component v_{1i} of the first eigenvector of the matrix J

$$\lim_{\beta\to\infty} P_i(v_i) = \delta\left(v_{1i} - \frac{H_i}{\Omega_i}\right) = P_i(v_{1i}) \cdot$$

- In the **thermodynamic limit** $N \to \infty$, we consider a collection of infinitely large single-instance matrices J. The cavity fields and marginal coefficients updates translate into *stochastic iterations* for the *joint pdf of cavity fields and joint pdf of marginal coefficients*

$$q(\omega, h) = \sum_{s=1}^{s_{max}} \frac{s}{c} p(s) \int \left[\prod_{\ell=1}^{s-1} \mathrm{d}q(\omega_\ell, h_\ell)\right] \left\langle \delta\left(\omega - \left(\lambda - \sum_{\ell=1}^{s-1} \frac{K_\ell^2}{\omega_\ell}\right)\right) \delta\left(h - \sum_{\ell=1}^{s-1} \frac{K_\ell h_\ell}{\omega_\ell}\right) \right\rangle_{\{K_\ell\}} ,$$

$$Q(\Omega, H) = \sum_{s=0}^{s_{max}} p(s) \int \left[\prod_{\ell=1}^{s} \mathrm{d}q(\omega_\ell, h_\ell)\right] \left\langle \delta\left(\Omega - \left(\lambda - \sum_{\ell=1}^{s} \frac{K_\ell^2}{\omega_\ell}\right)\right) \delta\left(H - \sum_{\ell=1}^{s} \frac{K_\ell h_\ell}{\omega_\ell}\right) \right\rangle_{\{K_\ell\}} ,$$

where $p(s)$ is the degree distribution with mean c and $\{K_\ell\}$ is a set of i.i.d random variables, each drawn from $p(K)$, i.e. the pdf of the weights K_{ij} of the matrix entries $J_{ij} = c_{ij} K_{ij}$. Convergence is attained when $\lambda = \lambda_1$.

- The distribution of the first eigenvector component is

$$\rho(u) = \int \mathrm{d}Q(\Omega, H)\, \delta\left(u - \frac{H}{\Omega}\right) \quad \text{with} \quad T = \int \mathrm{d}Q(\Omega, H) \frac{H^2}{\Omega^2} = 1 \cdot$$

Replica Method

- Starting from the partition function $Z(\beta, J)$ of the canonical ensemble of vectors $\boldsymbol{v} \in \mathbb{R}^N$, the **typical largest eigenvalue** is expressed as $\overline{\lambda_1} = \lim_{\beta\to\infty} \frac{2}{\beta N} \overline{\ln Z(\beta, J)}$, where the overline indicates the ensemble average.

Applying the replica trick $\overline{\ln Z(\beta, J)} = \lim_{n\to 0} \frac{1}{n} \ln \overline{Z^n(\beta, J)}$ and introducing the order parameter ϕ and its conjugate $\hat{\phi}$, the average replicated partition function can be written in a form suitable for a saddle-point approximation

$$\overline{Z^n(\beta, J)} = \int \mathcal{D}\phi\, \mathcal{D}\hat{\phi}\, \mathrm{d}\vec{\lambda} \exp\{N S_n(\phi, \hat{\phi}, \vec{\lambda})\} \qquad S_n(\phi, \hat{\phi}, \vec{\lambda}) = S_1(\phi, \hat{\phi}) + S_2(\phi) + S_3(\vec{\lambda}) + S_4(\hat{\phi}, \vec{\lambda})$$

$$S_1(\phi, \hat{\phi}) = -\mathrm{i} \int \mathrm{d}\vec{v}\, \phi(\vec{v}) \hat{\phi}(\vec{v}) \qquad S_2(\phi) = \frac{c}{2} \int \mathrm{d}\vec{v}\mathrm{d}\vec{v}'\, \phi(\vec{v})\phi(\vec{v}') \left[\left\langle \exp\left(\beta K \sum_a v_a v_a'\right)\right\rangle_K - 1\right]$$

$$S_3(\vec{\lambda}) = \mathrm{i}\frac{\beta}{2} \sum_a \lambda_a \qquad S_4(\hat{\phi}, \vec{\lambda}) = \mathrm{Log} \int \mathrm{d}\vec{v} \exp\left[-\mathrm{i}\frac{\beta}{2} \sum_a \lambda_a v_a^2 + \mathrm{i}\hat{\phi}(\vec{v})\right] ,$$

where $\vec{v} \in \mathbb{R}^n$ is a vector in the replica space.

- Replica-symmetric ansatz [2]: at the saddle point we assume that $\lambda_a = \lambda \quad \forall a = 1, \dots, n$ and that

$$\phi(\vec{v}) = \int \mathrm{d}\omega \mathrm{d}h \frac{\pi(\omega, h)}{Z(\omega, h)^n} \prod_{a=1}^{n} \exp\left(-\frac{\beta}{2}\omega v_a^2 + \beta h v_a\right) \quad \text{where} \quad Z(\omega, h) = \sqrt{\frac{2\pi}{\beta\omega}} \exp\left(\frac{\beta h^2}{2\omega}\right) ,$$

$$\mathrm{i}\hat{\phi}(\vec{v}) = \hat{c} \int \mathrm{d}\hat{\omega}\mathrm{d}\hat{h}\, \hat{\pi}(\hat{\omega}, \hat{h}) \prod_{a=1}^{n} \exp\left(\frac{\beta}{2}\hat{\omega} v_a^2 + \beta \hat{h} v_a\right) .$$

- The stationarity conditions w.r.t. ϕ, $\hat{\phi}$ and λ yield respectively

$$\hat{\pi}(\hat{\omega}, \hat{h}) = \int \mathrm{d}\pi(\omega', h') \left\langle \delta\left(\hat{\omega} - \frac{K^2}{\omega'}\right) \delta\left(\hat{h} - \frac{K h'}{\omega'}\right) \right\rangle_K$$

$$\pi(\omega, h) = \sum_{s=1}^{s_{max}} \frac{s}{c} p(s) \int \left[\prod_{\ell=1}^{s-1} \mathrm{d}\hat{\pi}(\hat{\omega}_\ell, \hat{h}_\ell)\right] \delta\left(\omega - \left(\mathrm{i}\lambda^* - \sum_{\ell=1}^{s-1} \hat{\omega}_\ell\right)\right) \delta\left(h - \sum_{\ell=1}^{s-1} \hat{h}_\ell\right)$$

$$1 = \sum_{s=0}^{s_{max}} p(s) \int \left[\prod_{\ell=1}^{s} \mathrm{d}\pi(\omega_\ell, h_\ell)\right] \left\langle \left(\frac{\sum_{\ell=1}^{s} \frac{K_\ell h_\ell}{\omega_\ell}}{\mathrm{i}\lambda^* - \sum_{\ell=1}^{s} \frac{K_\ell^2}{\omega_\ell}} \right)^2 \right\rangle_{\{K_\ell\}} ,$$

where the shortcut $\mathrm{d}\pi(\omega, h) = \mathrm{d}\omega \mathrm{d}h\, \pi(\omega, h)$ has been used. Inserting $\hat{\pi}(\hat{\omega}, \hat{h})$ into $\pi(\omega, h)$, one finds the exact same self-consistent equation found in cavity for $q(\omega, h)$! Moreover, evaluating the action S_n at the saddle point, one finds that $\overline{\lambda_1} = \mathrm{i}\lambda^* = \lambda \in \mathbb{R}$. Note: the degree distribution $p(s)$ can be replaced by any other with finite mean.

- The **density of the top eigenvector components** is defined as

$$\rho(u) = \lim_{\beta\to\infty} \rho_\beta(u) = \lim_{\beta\to\infty} \overline{\left\langle \frac{1}{N} \sum_{i=1}^{N} \delta(u - v_i) \right\rangle} ,$$

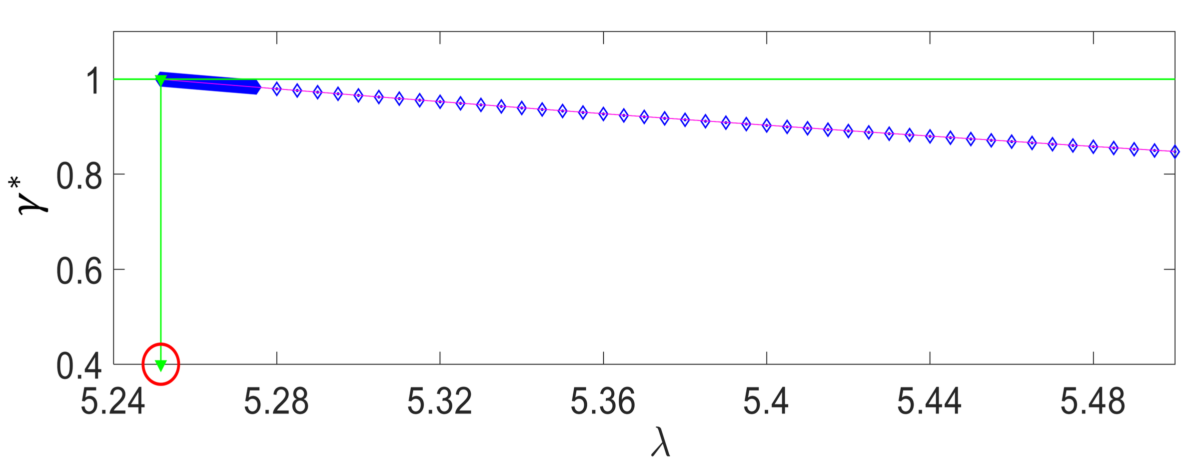
where the angular brackets indicate the thermal averaging and the overline indicate the ensemble averaging. The evaluation of $\rho_\beta(u)$ entails the same replica calculation which has been performed for $\overline{\lambda_1}$. Moreover, the explicit expression for $\rho_\beta(u)$ appears naturally in the eigenvalue calculation when looking at the single-site term of the action, S_4. Eventually, one finds

$$\rho(u) = \sum_{s=0}^{s_{max}} p(s) \int \left[\prod_{\ell=1}^{s} \mathrm{d}\pi(\omega_\ell, h_\ell)\right] \left\langle \delta\left(u - \frac{\sum_{\ell=1}^{s} \frac{K_\ell h_\ell}{\omega_\ell}}{\mathrm{i}\lambda^* - \sum_{\ell=1}^{s} \frac{K_\ell^2}{\omega_\ell}}\right) \right\rangle_{\{K_\ell\}} ,$$

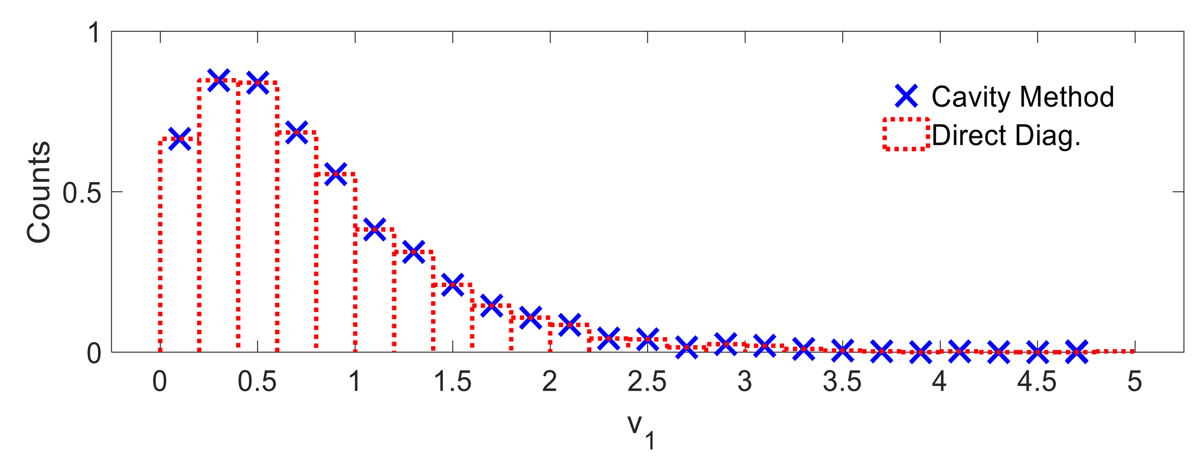
where the distribution $\pi(\omega, h)$ is exactly the same appearing in the eigenvalue computation, satisfying the above relation.

Results

Cavity single instance



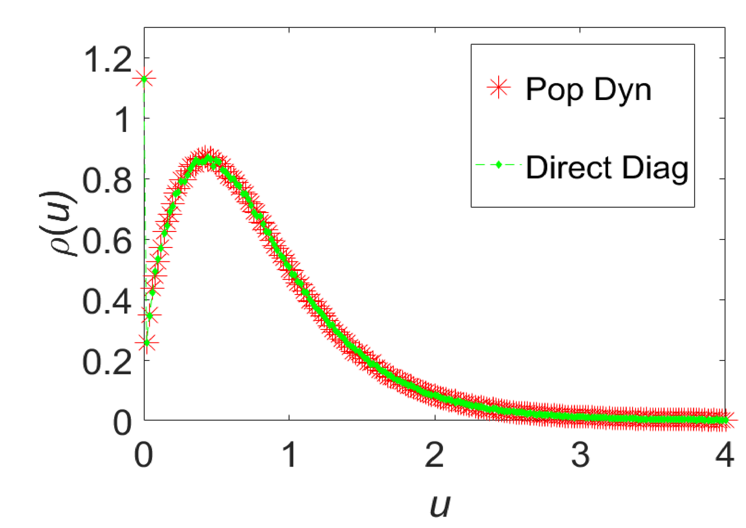
$\lambda_1 = 5.251599$
$\lambda_1^{diag} = 5.251575$
$\epsilon_{\lambda_1} = 0.001\%$

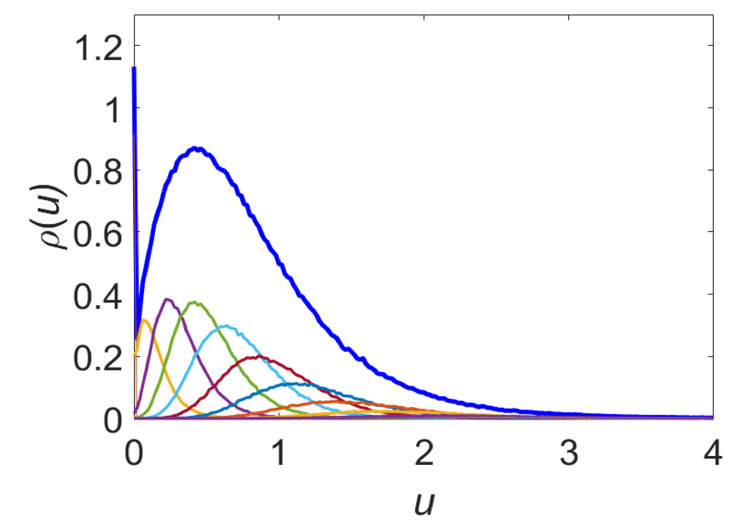


$$\frac{\left\|\boldsymbol{v}_1 - \boldsymbol{v}_1^{diag}\right\|}{\left\|\boldsymbol{v}_1^{diag}\right\|} = \mathcal{O}(10^{-15})$$

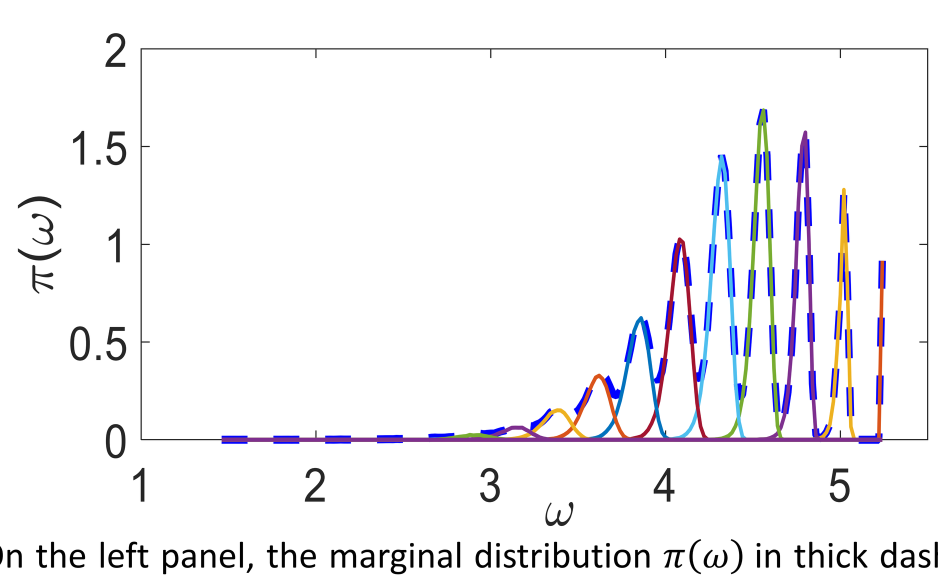
Erdős–Rényi Adjacency matrix, with $c = 4$. Top: $\lambda = \lambda_1$ when the largest eigenvalue γ^* of the *Non-Backtracking operator* B becomes 1. B is defined as $B_{(i,j),(k,\ell)} = \frac{J_{j\ell}}{\omega_j^{(\ell)}}$ if $j = k \wedge i \neq \ell$ and 0 otherwise; it appears in the $h_j^{(i)}$'s update. Bottom: normalized histogram of the components of the largest eigenvector $\boldsymbol{v}_1$ obtained via cavity method against the same eigenvector $\boldsymbol{v}_1^{diag}$ computed via direct diagonalization of the same matrix.

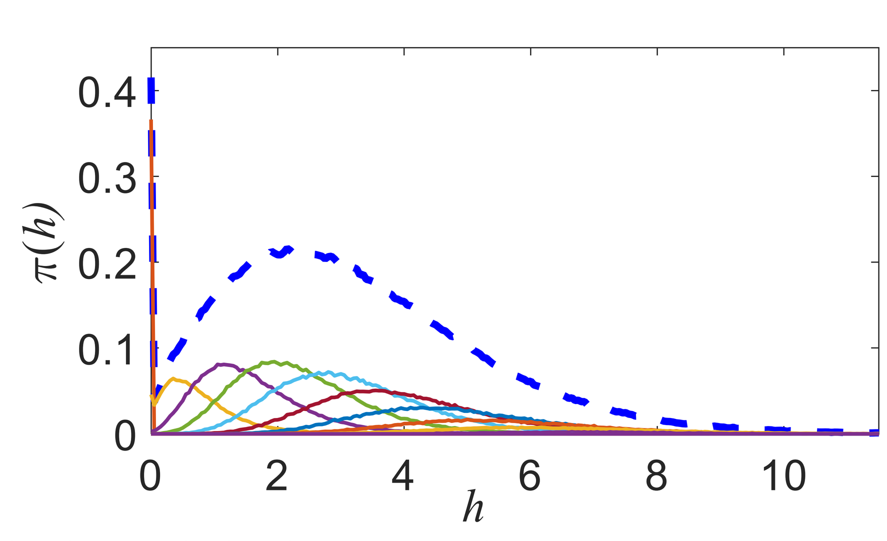
Thermodynamic limit: Population Dynamics





Erdős–Rényi connectivity with $c = 4$. A population of size $N_P = 10^6$ has been considered. The maximum degree is $s_{max} = 17$. On the left, the distribution $\rho(u)$ obtained with Pop Dyn against results from direct diagonalization of 5000 matrices 2000x2000. On the right, the distribution $\rho(u)$ obtained with Pop Dyn in thick blue line and the degree contributions $s = 0,1,2,3, \dots$





On the left panel, the marginal distribution $\pi(\omega)$ in thick dashed blue line with the degree contributions. In this case, every peak corresponds to a certain degree, increasing from right to left. On the right panel, the marginal pdf $\pi(h)$ with degree contributions.

References

[1] Y. Kabashima, H. Takahashi and O. Watanabe. "Cavity approach to the first eigenvalue problem in a family of symmetric random sparse matrices." *Journal of Physics: Conference Series*. Vol. 233. No. 1. IOP Publishing, 2010.
[2] R. Kühn, "Spectra of sparse random matrices." *Journal of Physics A: Mathematical and Theoretical.* Vol. 41. No. 29. IOP Publishing, 2008.