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LETTER TO THE EDITOR

An approximation scheme for the density of states of the Laplacian on random graphs

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Abstract

In a number of recent papers, the spectral properties of the Laplacian on randomly connected graphs have been studied within the replica formalism. In this letter we show how the replica formalism can be unravelled and we find an approximation for calculating the density of states which substantially simplifies the numerical resolution of the equations obtained, whilst giving results in excellent accord with the exact solution.

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In this letter we develop an approximation scheme to solve the functional mean-field equations arising from the replica calculation for the density of states of the Laplacian on a random graph. Models based on random graphs are physically appealing as, although they remain mean field, each site has a finite number of neighbours thus keeping the finite connectedness of finite-dimensional systems. It was first remarked by Viana and Bray [1] that the spin-glass transition on a random graph cannot be described in terms of a sole matrix (a zero-by-zero matrix in the case of the fully connected Sherrington–Kirkpatrick model [2, 3]) order parameter and one is obliged to consider an infinite number of order parameters or equivalently the distribution function of local fields in the model (equivalent to the generating function for the hierarchy of order parameters). The price paid for this finite connectivity is therefore an additional analytic complexity which has hindered the search for the replica symmetry breaking which has been applied with much success in a large variety of problems [3]. In this letter we consider the simpler problem of the calculation of the spectrum of the Laplacian on a random graph. Random-graph problems have also found applications in computer science; see for example [4] and references therein. Bray and Rodgers [5] were the first to analyse this problem within the replica formalism and they obtained the mean-field equations arising from the replica symmetric ansatz; only recently [6] was this equation solved numerically, and then it was shown via comparison with numerical simulations that (just as in the case of the orthogonal ensemble [7]) the replica symmetric theory successfully predicts the density of states for this model. Indeed the rigorous supersymmetric approach also yields the same functional equations

as are needed to compute the density of states for this model [8]. As pointed out by the authors of [6], the numerical solution of these equations is a rather delicate affair. In addition it has been remarked that the techniques used in the resolution of these models can be used in finite dimensions to calculate the instantaneous normal modes of complex systems [6, 9]. Clearly the resulting equations are an order of magnitude more complex and it is therefore the purpose of this letter to propose an approximation scheme inspired by an unravelling of the replica equations and subsequently an approximation based on the central-limit (CL) theorem. This approximation successfully predicts the presence of oscillations in the density of states observed in [6, 9] and whilst a numerical solution is necessary the numerics are easy and the same idea should work in situations where the full functional equations become extremely difficult to solve numerically. The results are compared with the numerical simulations of [9] and we find excellent agreement.

The Laplacian on an arbitrary graph is given by the expression

$$H_{ij} = -\delta_{ij} \sum_{k \neq i} n_{ik} + n_{ij} \tag{1}$$

where $n_{ij} = n_{ji}$ is equal to one if the points i and j are neighbours and zero otherwise. A random *mean-field* graph is constructed by setting $n_{ij} = n_{ji} = 1$ with probability $p = c/N$ and 0 with probability $1 - p$; the average connectivity of each point is therefore c. Within the framework of the replica formalism, the density of states $\rho(E)$ of the Laplacian is calculated by considering the replicated partition function [5, 6, 9]:

$$Z^n = \int \mathrm{d}\phi_i^a \exp\left[-\frac{1}{2} \sum_{a,i,j} \phi_i^a (E - H)_{ij} \phi_j^a\right]. \tag{2}$$

In the limit of large N, the replicated partition function may be calculated by the saddle-point method, yielding

$$\overline{Z^n} \sim \exp(S[p(\sigma)]) \tag{3}$$

with

$$S[p(\sigma)] = -\int p(\sigma) \log(p(\sigma))\, \mathrm{d}\sigma + \mu \int p(\sigma)\, \mathrm{d}\sigma - \frac{c}{2} + \frac{c}{2} \int p(\sigma) p(\sigma') \exp\left(-\frac{1}{2}(\sigma - \sigma')^2\right) \mathrm{d}\sigma\, \mathrm{d}\sigma' \tag{4}$$

where $p(\sigma)$ is a probability distribution on $\mathbb{R}^n$ and μ is the Lagrange multiplier ensuring that $\int p(\sigma)\, \mathrm{d}\sigma = 1$ [9]. The density of states may be extracted as

$$\rho(E) = \frac{1}{\pi} \lim_{n \to 0} \mathrm{Im} \int p(\sigma) \frac{\sigma^2}{n}\, \mathrm{d}\sigma \tag{5}$$

where E is understood to have an infinitesimal imaginary component. The saddle-point equation for $p(\sigma)$ is easily obtained as

$$p(\sigma) = \exp\left(\mu + c \int p(\sigma') \exp(-\tfrac{1}{2}(\sigma - \sigma')^2)\, \mathrm{d}\sigma'\right). \tag{6}$$

In [5] the n-goes-to-zero limit was taken within the replica formalism and in a recent paper [6] an equivalent equation was solved numerically. As pointed out in [6], the numerical resolution is rather difficult in this case and its structure is rather opaque. An alternative approach is to use a single-defect approximation as introduced in [9]. Here we reformulate the problem, providing an alternative approach to the numerical resolution of the problem but most importantly a natural approximation to the density of states.

We proceed by making a replica spherical (and thus replica symmetric) ansatz for p as in [5, 6, 9]. We express p as a sum of Gaussians:

$$p(\sigma) = \int w(a) \exp\left(-\frac{\sigma^2}{2a}\right) \mathrm{d}a. \tag{7}$$

The normalization of p induces a normalization on w such that $\int w(a)\,\mathrm{d}a = 1$. With this ansatz, integrating the equation (6) over σ implies $\mu = -c$.

The resulting equation for w is

$$\int w(a) \exp\left(-\frac{\sigma^2}{2a}\right) \mathrm{d}a = \sum_{n=0}^{\infty} \rho_n \int \prod_{i=1}^{n} w(a_i)\,\mathrm{d}a_i \exp\left(-\frac{1}{2}\sigma^2 \sum_{i=1}^{n} \frac{1}{a_i+1} - \frac{1}{2}E\sigma^2\right) \tag{8}$$

where $\rho_n = \mathrm{e}^{-c}c^n/n!$. If we assume that the Gaussian transform on w can be inverted, one finds

$$w(a) = \sum_{n=0}^{\infty} \rho_n \int \prod_{i=1}^{n} w(a_i)\,\mathrm{d}a_i\, \delta\left(a - \frac{1}{E + \sum_{i=1}^{n} \frac{1}{a_i+1}}\right). \tag{9}$$

This equation is not much simpler than the original equation; however, the n-goes-to-zero limit has been taken easily and we now have a probabilistic interpretation for (9). One may interpret w as the fixed-point probability distribution for the iteration

$$a = \frac{1}{E + \sum_{i=1}^{N} \frac{1}{a_i+1}} \tag{10}$$

where N is a random variable distributed according to the distribution ρ_n, i.e. it is Poissonian of mean c. The distribution of w can be calculated numerically rather efficiently via a population dynamics (on an ensemble of complex numbers) using the recurrence (10). We have verified that doing this reproduces the numerical simulation results of [4] if one chooses a large enough population and lets the dynamics run for sufficiently long time. Note that when we are in the spectrum, a has a non-zero imaginary part.

We now proceed to an approximate treatment of this problem. It is useful to make a change of variables:

$$a = \frac{\omega}{1-\omega} \tag{11}$$

where the induced recurrence for ω is now

$$\omega = \frac{1}{N + 1 + E - \sum_{i=1}^{N} \omega_i}. \tag{12}$$

For c large, we may appeal to the CL theorem and make the approximation

$$\omega = \frac{1}{N + 1 + E - N\overline{\omega}}. \tag{13}$$

Taking the average of (13) over N then yields

$$\overline{\omega} = \sum_{n=0}^{\infty} \rho_n \frac{1}{n + 1 + E - n\overline{\omega}}. \tag{14}$$

The advantage of the approximation used here is that it gives an equation for a single complex variable, $\overline{\omega}$, which is straightforward to solve numerically. The density of states $\rho(E)$ in this notation is given as

$$\rho(E) = \frac{1}{\pi} \operatorname{Im} \overline{a} \tag{15}$$

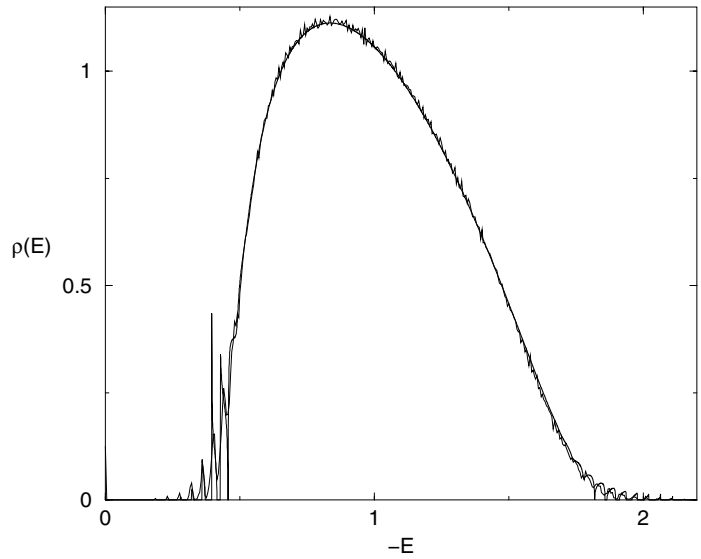

Figure 1. Comparison of the CL theorem approximation versus the numerical data of [9] for the density of states $\rho(E)$ for $c = 20$.

where the average value of a, $\overline{a}$, is given in terms of ω by

$$\overline{a} = \overline{\omega/(1-\omega)}. \tag{16}$$

One may not replace ω by $\overline{\omega}$ in equation (16), as it is not consistent with the CL-theorem-based approximation (13); using the recurrence equation for ω (12), one finds that within the context of this approximation

$$\overline{a} = \sum_{n=0}^{\infty} \rho_n \frac{1}{n + E - n\overline{\omega}}. \tag{17}$$

Shown in figure 1 (in units where E is rescaled by a factor $1/c$) is the comparison of the CL approximation with the numerical results of [9] for random graphs of mean connectivity $c = 20$; one sees that this approximation is excellent in the centre of the spectrum and at large energies. Only at small energies (corresponding to sites of small connectivity where the CL approximation should break down) does one see any appreciable deviation. At large energies the oscillations in the density of states are reproduced with a slight shift to the right with respect to the numerical simulations. The results in the centre of the spectrum are in perfect agreement with the numerical results.

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