Spin-glass phase transitions on real-world graphs

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We use the Bethe approximation to calculate the critical temperature for the transition from a paramagnetic to a glassy phase in spin-glass models on real-world graphs. Our criterion is based on the marginal stability of the minimum of the Bethe free energy. For uniform degree random graphs (equivalent to the Viana-Bray model) our numerical results, obtained by averaging single problem instances, are in agreement with the known critical temperature obtained by use of the replica method. Contrary to the replica method, our method immediately generalizes to arbitrary (random) graphs. We present new results for Bárabasi-Albert scale-free random graphs, for which no analytical results are known. We investigate the scaling behavior of the critical temperature with graph size for both the finite and the infinite connectivity limit. We compare these with the naive Mean Field results. We observe that the Belief Propagation algorithm converges only in the paramagnetic regime.

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Sparse networks with non-uniform topology occur in many contexts ranging from biology and sociology to communication systems and computer science [1]. Prominent examples of mathematical models designed to capture the topological features of these so-called "real-world" graphs are uniform degree random graphs [2], scale-free networks [3] and small-world graphs [4]. While much research has been done on topological properties of these complex networks, not much seems to be known about the properties of such networks when nodes contain dynamic variables and links represent positive or negative interaction between them. Examples of complex networks with interacting nodes are networks of neurons in the brain [5], communication in networks of sensors [6], combinatoric optimization problems [7] and protein folding [8, 9]. In this Letter, we take a statistical physics approach to study the behavior of such systems.

We study generalizations of the SK model [10] where we replace the fully connected underlying graph by complex random graphs. We use the Bethe approximation, an extension of the naive Mean Field (MF) approximation, to calculate the critical temperature corresponding to the phase transition from a paramagnetic to a spin-glass-like phase. The transition is characterized by a marginal instability of the Hessian of the Bethe free energy. For uniform degree random graphs, averaging over the interactions and the underlying graph instances yields results consistent with known analytical results obtained by use of the replica method [11]. Contrary to the replica method, our method immediately generalizes to arbitrary (random) graphs. We present results for scale-free networks, for which no analytical results are known to the best of our knowledge (however, for the ferromagnetic case on random graphs with arbitrary degree distribution, see [12]).

Another advantage of the Bethe approximation is that it yields results for finite N and for specific problem instances of the interactions. This is important for technologically relevant applications *viz.* image restoration [13], artificial vision [14], decoding of error-correcting codes [15] and medical diagnosis [16]. The problems in these applications can generally be reformulated in terms of thermodynamic systems defined on graphs, and solving them amounts to the determination of the Boltzmann distribution for these systems.

Let $G = (V, B)$ be an undirected labelled graph without self-connections, defined by a set of vertices $V = \{1, \dots, N\}$ (corresponding to the spins) and a set of edges $B \subseteq \{(i,j) \,|\, 1 \le i < j \le N\}$ (corresponding to non-zero interactions between the spins). We define the *adjacency matrix* M corresponding to G as follows: $M_{ij} = 1$ if $(ij) \in B$ or $(ji) \in B$ and 0 otherwise. Denote by N_i the set of neighbors of vertex i, and denote the degree (connectivity) of vertex i by $d_i := |N_i| = \sum_{j \in V} M_{ij}$. We define the *average degree* $d := \frac{1}{N} \sum_{i \in V} d_i$ and the *maximum degree* $\Delta := \max_{i \in V} d_i$.

To each vertex $i \in V$ we associate an Ising spin s_i, taking values in $\{-1, +1\}$. Let J be a symmetric $N \times N$ matrix representing the interactions, which we do not further specify for the moment, except for the constraint that J should be compatible with the adjacency matrix M, i.e. $J_{ij} = 0$ if $M_{ij} = 0$. For the Hamiltonian of the system we take

$$H = -\sum_{(i,j) \in B} J_{ij} s_i s_j$$

and we study the corresponding Boltzmann distribution over the configurations $s = (s_1, \dots, s_N) \in \{-1, +1\}^N$:

$$\mathbb{P}(s) = \frac{1}{Z} \exp\left(\beta \sum_{(i,j) \in B} J_{ij} s_i s_j\right).$$

Note that, because of the sign reversal symmetry, the exact magnetizations are given by $\langle s_i \rangle = 0$.

The Bethe free energy [17] can be written [18] as a function of the parameters $m = (m_1, \dots, m_N)$ and $\xi = \{\xi_{ij}\}_{(ij)\in B}$:

$$F_{Be}(m,\xi) := -\beta \sum_{(ij)\in B} J_{ij}\xi_{ij} + \sum_{i=1}^{N}(1-d_i)\sum_{s_i=\pm 1}\eta\left(\frac{1+m_i s_i}{2}\right) + \sum_{(ij)\in B}\sum_{s_i,s_j=\pm 1}\eta\left(\frac{1+m_i s_i + m_j s_j + s_i s_j \xi_{ij}}{4}\right)$$

where $\eta(x) := x\log x$. The Bethe approximation consists of minimizing the Bethe free energy with respect to the parameters m and ξ under the following constraints:

$$\begin{aligned} &-1 \le m_i \le 1 \\ &-1 \le \xi_{ij} \le 1 \\ &1 + m_i\sigma + m_j\sigma' + \xi_{ij}\sigma\sigma' \ge 0 \quad \text{for all } \sigma,\sigma' = \pm 1. \end{aligned}$$

The parameters m_i are then approximations for the means $\langle s_i\rangle$, while the ξ_{ij} are approximations for the moments $\langle s_i s_j\rangle$ for $(ij)\in B$; if G is a tree, these approximations are exact [19]. It is straightforward to check that $m_i = 0$ and $\xi_{ij} = \tanh(\beta J_{ij})$ is a stationary point of F_{Be}, which we will call the *paramagnetic* solution. For this solution to be a minimum, the Hessian of F_{Be} has to be positive definite. Defining $\xi_{ji} := \xi_{ij}$ for $(i,j)\in B$ and $\xi_{ij} := 0$ if $(i,j)\notin B$ and $(j,i)\notin B$, this is equivalent to the matrix

$$(A_{Be})_{ik} := \frac{\partial^2 F_{Be}}{\partial m_k \partial m_i}\Big|_{m=0,\xi=\tanh(\beta J)} = \delta_{ik}\left(1 + \sum_{j\in N_i}\frac{\xi_{ij}^2}{1-\xi_{ij}^2}\right) - \frac{\xi_{ik}}{1-\xi_{ik}^2} \tag{1}$$

being positive definite, since the $\partial F_{Be}/\partial m_k \partial \xi_{ij}$ part vanishes and the other block $\partial F_{Be}/\partial\xi_{ij}\partial\xi_{kl}$ is positive definite for all possible parameter values.

We will compare the results with the naive Mean Field approximation. The MF free energy is given by

$$F_{MF}(m) := -\beta\sum_{(i,j)\in B} J_{ij} m_i m_j + \sum_{i=1}^{N}\sum_{s_i=\pm 1}\eta\left(\frac{1+m_i s_i}{2}\right)$$

and has to be minimized. The Hessian is simply

$$(A_{MF})_{ij} := \frac{\partial^2 F_{MF}}{\partial m_i \partial m_j} = -\beta J_{ij} + \delta_{ij}\frac{1}{1-m_i^2}. \tag{2}$$

Note that $m = 0$ is a stationary point of the MF free energy—not necessarily a minimum—which we also call the *paramagnetic* solution.

The stability of the paramagnetic MF solution implies the stability of the paramagnetic Bethe solution, as we shall now demonstrate. Define $A := A_{Be} - A_{MF}$; we have to show that A is positive semidefinite. Substituting (1), (2) and the relation $\xi_{ij} = \tanh(\beta J_{ij})$:

$$A_{ij} = -\frac{\xi_{ij}}{1-\xi_{ij}^2} + \operatorname{arctanh}\xi_{ij} + \delta_{ij}\sum_{k=1}^{N}\frac{\xi_{ik}^2}{1-\xi_{ik}^2}.$$

Note that A is symmetric and that all its diagonal entries are nonnegative. Furthermore, A is diagonally dominant, i.e. for all $i = 1,\dots,N$:

$$A_{ii} - \sum_{\substack{j=1\\ j\neq i}}^{N} |A_{ij}|\,, \ge 0$$

which immediately follows from the following inequality:

$$\frac{x^2}{1-x^2} - \left|\operatorname{arctanh} x - \frac{x}{1-x^2}\right| \ge 0$$

that holds for all $x \in (-1,1)$. A simple application of Gerschgorin's Circle Theorem yields the desired result.

Before we embark on spin-glasses, let us first shortly discuss the purely ferromagnetic case, where we take all nonzero interactions to be equal and positive, i.e. $J = M$. Both approximations are stable for high temperature (i.e. small β) but break down at some critical β_c, where the Hessians develop negative eigenvalues and the unique minimum of the free energy splits into two minima. For MF, this critical β_c^{MF} is given by $\beta_c^{MF} = 1/\lambda_1$, where λ_1 is the principal eigenvalue of the adjacency matrix M, as easily follows from (2). Since $d \le \lambda_1 \le \Delta$, we immediately get the following bound on the ferromagnetic MF critical temperature:

$$\frac{1}{\Delta} \le \beta_c^{MF} \le \frac{1}{d}.$$

For the Bethe approximation, the critical value β_c^{Be} at which A_{Be} develops a negative eigenvalue can be shown to satisfy the following bound:

$$\frac{1}{\Delta - 1} \le \frac{1}{\lambda_1 - 1} \le \tanh\beta_c^{Be} \le \frac{1}{d-1}.$$

In practice, for the graph topologies that we investigated, the critical values β_c^{MF} and β_c^{Be} differ only slightly. This is not the case for spin-glass like interactions, where the Bethe approximation clearly outperforms the MF approximation, as we shall discuss shortly.

In the following, we take the nonzero interactions $\{J_{ij}\,|\,M_{ij} = 1, i > j\}$ to be independent Gaussian random variables with mean 0 and variance 1. We first discuss the typical single-instance behavior. Fig. 1(a) shows how the minimal eigenvalues of the stability matrices A_{MF} and A_{Be} typically depend on the inverse temperature β. Varying the graph topology only scales the axes (except for tree-like or even sparser graphs), but qualitatively the picture remains the same. For the Mean Field

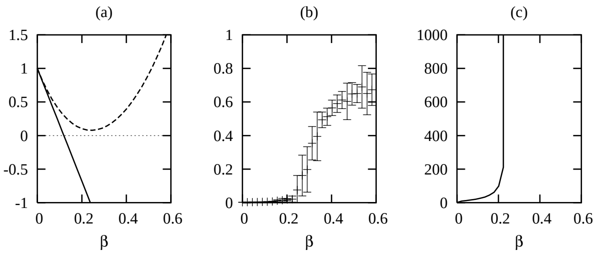

FIG. 1: Transition from paramagnetic to spin-glass phase for an ER graph with $N = 100$ and $d = 20$ and Gaussian interactions. From left to right: (a) minimal eigenvalues of A_{MF} (solid) and of A_{Be} (dashed); (b) Edwards-Anderson order parameter q_{EA}; (c) number of Belief Propagation iterations before convergence.

method, the paramagnetic solution becomes unstable for $\beta > \beta_c^{MF} := \sup\{\beta > 0; A_{MF} > 0\}$. For the Bethe approximation however, we typically find that with increasing β, the smallest eigenvalue $\lambda_{\min}(A_{Be})$ first decreases until it becomes approximately zero at some critical β_c^{Be}, after which it starts increasing again. At this critical β_c^{Be}, which we define as

$$\beta_c^{Be} := \operatorname*{argmin}_{\beta>0} \lambda_{\min}(A_{Be}),$$

the paramagnetic solution is *marginally* stable. Our numerical experiments show that in the thermodynamic limit $N \to \infty$, the minimal eigenvalue $\lambda_{\min}(A_{Be})$ evaluated at β_c^{Be} converges to 0. Furthermore, Monte Carlo simulations using the Metropolis algorithm show that the Edwards-Anderson parameter $q_{EA} := \frac{1}{N}\sum_{i=1}^N \langle s_i \rangle^2$ becomes positive at the transition (see Fig. 1(b)). We therefore interpret this marginal instability as a phase transition to a spin-glass like state [20].

In the remainder of this article we study the dependence of the Bethe and MF critical temperatures on the graph topology and its size N. Until now, everything is valid for single instances (consisting of a specific choice of G and of J), which is obviously very useful in applications. In the following we will average over graph instances and over interactions in order to get an average-case analysis. We start with the uniform degree random graphs introduced and studied by Erdős and Rényi [2] (ER graphs in short). The ensemble consists of graphs with N vertices, where each pair of vertices is independently connected with probability p. The degree distribution is approximately Poisson for large N and the expected average degree is $\langle d \rangle = p(N-1)$. The resulting model is also known in statistical physics as the Viana-Bray model of diluted spin-glasses [11]. Numerical results are shown in Fig. 2.a and 2.b.

For $N \to \infty$, we can state rigorous results about the scaling behavior of the MF critical temperature. There are (at least) two ways to take the limit $N \to \infty$, which result in different scaling behavior: the *sparse* (or finite connectivity) limit in which we fix the average degree d and let $N \to \infty$, and the *dense* (infinite connectivity) limit in which we fix p and take $N \to \infty$. In the dense limit (Fig. 2.a), $\beta_c^{MF} \sim 1/2\sqrt{d}$, which follows from a result of Khorunzhy [21] stating that the principal eigenvalue of J is asymptotically equal to $2\sqrt{Np}$, if $d(N) \gg \log N$. On the other hand, for $d(N) \ll \log N$, the spectral norm of J is asymptotically much larger than $\sqrt{Np}$, which implies that the MF β_c^{MF} converges to zero in the sparse limit (c.f. Fig. 2.b).

For the Bethe approximation, we were not able to obtain rigorous results about the scaling behavior of β_c^{Be}, but our numerical results turn out to be in agreement with the known phase boundary derived using the replica method. In [11], the following equation is derived for the critical inverse temperature β_c^{VB} corresponding to paramagnetic–spin-glass phase transition:

$$\int \tanh^2(\beta_c^{VB} x)\, dP(x) = \frac{1}{d}, \tag{3}$$

where P is the probability distribution of the weights, which is Gaussian with mean 0 and variance 1 in our case. For large d, this yields a critical inverse temperature of approximately $\beta_c^{VB} \approx 1/\sqrt{d}$. As illustrated in Fig. 2.a and Fig. 2.b, the average Bethe critical β_c^{Be} perfectly agrees with the value β_c^{VB} obtained by Viana and Bray, in the dense as well as in the sparse limit. This confirms our interpretation of the marginal instability as a phase transition to a spin-glass like phase. In sharp contrast with MF, the Bethe critical β_c^{Be} converges to a positive constant in the sparse limit. In the dense limit the Bethe β_c^{Be} is twice as large as the MF β_c^{MF}.

We now present numerical results on Barabási-Albert scale-free networks, for which no results have been published before as far as we know. A phenomenon often observed in real-world networks is that the degree distribution behaves like a power law [1], i.e. the number of vertices with degree δ is proportional to $\delta^{-\alpha}$ for some $\alpha > 0$. The first and intensely studied random graph model showing this behavior is due to Barabási and Albert [3]. The degree distribution has a power-law dependence for $N \to \infty$: the probability that a randomly chosen vertex has a particular degree δ is proportional to δ^{-3}. The difference between the maximum degree Δ and the average degree d becomes quite large for the BA model compared with ER random graphs. A natural question to ask is what quantity will govern the spin-glass transition: the average degree d or the maximum degree Δ.

In the dense limit (see Fig. 2.c), we find $\beta_c^{MF} \propto 1/2\sqrt{d}$ and $\beta_c^{Be} \propto 1/\sqrt{d}$. This is very similar to the ER case, up to a constant factor of order 1. Thus it appears that in the dense limit, the critical temperatures are almost independent of graph topology, except for the d-dependence. In the sparse limit (see Fig. 2.d, note the rescaled vertical axis), the two approximations show clearly different scal-

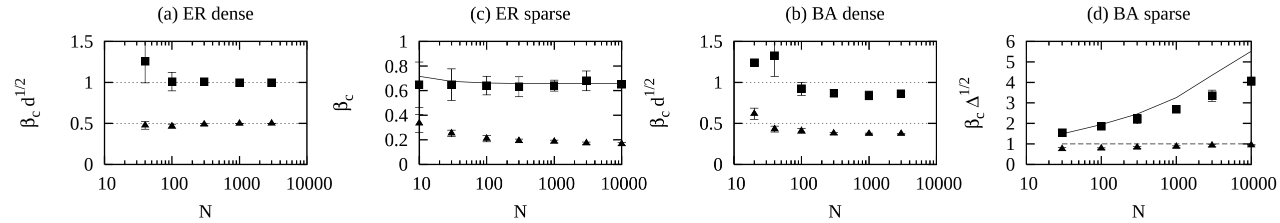

FIG. 2: Critical inverse temperatures β_c^{MF} (MF approximation, triangles) and β_c^{Be} (Bethe approximation, squares) for the spin-glass transition vs. graph size N, averaged over interactions and over graph instances. From left to right: (a) ER, dense limit, $p = 0.1$ (the vertical axis is rescaled by $1/\sqrt{d}$); (b) ER, sparse limit, $d = 4$; the solid line shows β_c^{VB} according to eqn. (3); (c) BA, dense limit, $p = 0.1$ (the vertical axis is rescaled by $1/\sqrt{d}$); (d) BA, sparse limit, $d = 10$ (the vertical axis is rescaled by $1/\sqrt{\Delta}$); the solid line is $1/\sqrt{d}$ and the dashed line is $1/\sqrt{\Delta}$.

ing behavior: the MF critical β_c^{MF} apparently scales like $1/\sqrt{\Delta}$, wherease the Bethe critical β_c^{MF} more closely follows $1/\sqrt{d}$. With increasing graph size, the difference between both approximation methods becomes larger and larger. For the BA model, we have not found any theoretical results concerning phase transitions in the literature, but based on the analysis for ER graphs and on Monte Carlo experiments we believe that the Bethe approximation correctly describes the phase transitions.

In conclusion, we have applied the Bethe approximation to spin-glass systems on random graphs. We have shown that the Bethe approximation is more powerful than the naive Mean Field approximation and that our approach agrees with previous results using replica methods. The advantage of our approach is that it extends to arbitrary graph topologies and interactions and works for single instances, which is important for applications. In this light we would like to mention the connection with the *Belief Propagation* (BP) algorithm [22], also known under the names *Sum-Product algorithm* and *Loopy Belief Propagation*. BP is a currently very popular algorithm used in diverse applications to minimize the Bethe free energy [17, 23]. As illustrated in Fig. 1(c), and what we in fact have observed in all our numerical experiments, the BP algorithm converges only in the paramagnetic regime. At the transition to a spin-glass phase, the number of iterations before convergence explodes. Details are beyond the scope of this Letter and will be explored in a forthcoming article.

A possible generalization of this work would be the incorporation of local fields h_i. Based on (preliminary) numerical experiments, we expect that adding local fields *increases* the Bethe critical inverse temperature β_c^{Be}, thereby extending the paramagnetic regime (it is easy to see that the Mean Field critical β_c^{MF} increases).

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