Solution of the 2-star model of a network

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The $p$-star model or exponential random graph is among the oldest and best-known of network models. Here we give an analytic solution for the particular case of the 2-star model, which is one of the most fundamental of exponential random graphs. We derive expressions for a number of quantities of interest in the model and show that the degenerate region of the parameter space observed in computer simulations is a spontaneously symmetry broken phase separated from the normal phase of the model by a conventional continuous phase transition.

I. INTRODUCTION

There has in recent years been a surge of interest within the physics community in the properties of networks, including the Internet, the world wide web, and social and biological networks of various kinds [1, 2, 3, 4]. Work has been divided between studies of specific real-world networks, along with the development of measures and algorithms for their analysis, and the creation of models to predict and explain network behavior. It is on models that we focus here.

Network modeling goes back at least as far as the well-known random graph or Bernoulli graph, studied by Solomonoff and Rapoport in the early 1950s [5] and famously by Erdős and Rényi [6] a decade later. The random graph however is a poor model for most real-world networks, as has been argued by many authors [1, 4, 7], and so other models have been developed. Recent attention has focused particularly on generalized random graphs such as the configuration model [8, 9, 10] and on generative models, particularly models of growing networks [2, 4, 11, 12]. There is, however, another class of network models that, while widely used and valuable, has attracted little attention in the physics community, namely the class of “exponential random graphs” or “p-star models.” Building on early statistical work by Besag [13], exponential random graphs were first studied in the 1980s by Holland and Leinhardt [14], and later developed extensively by Strauss and others [15, 16]. Today, they are commonly used as a practical tool by statisticians and social network analysts [17, 18, 19].

Despite their widespread adoption, few analytic results are known for exponential random graphs: most work has made use of computer simulation to fit models to observational data and evaluate model predictions. Exponential random graphs however are ideally suited to study using the techniques of statistical physics. Recently, physicists have examined exponential random graph models of network assortativity [20, 21] and transitivity [22]. Here we take a different approach and show how physics techniques can be used to derive analytically the behavior of one of the most fundamental of exponential random graph models, the 2-star model. We view this solution not only as a calculation of interest in its own right, but also as a demonstration of the way in which physics techniques can be fruitfully applied to problems from other fields.

II. THE MODEL

The exponential random graph is an ensemble model. One defines an ensemble consisting of the set of all simple undirected graphs with $n$ vertices and no self-edges (i.e., networks with either zero or one edge between each pair of distinct vertices) and one specifies a probability $P(G)$ for each graph $G$ in this ensemble. Properties of the model are calculated as averages over the ensemble. Let us define the graph Hamiltonian, also referred to by statisticians as a log odds ratio, to be $H(G) = F - \ln P(G)$. Here $F$ (usually called the free energy) is any convenient origin for the measurement of the Hamiltonian, such as, for instance, the log of the probability of the empty graph (i.e., the probability of $n$ vertices with no edges). Then

$$P(G) = \frac{e^{-H(G)}}{Z}, \quad Z = e^{-F} = \sum_G e^{-H(G)}.$$  \hspace{1cm} (1)

$Z$ is the graph partition function and many quantities of interest can be calculated from it, or alternatively from the free energy.

So far, this model is entirely general, but progress is made by assuming the Hamiltonian to be a linear combination of scalar graph observables, such as number of edges, degree sequences, or clustering coefficients. In this paper we study one of the simplest nontrivial cases, the 2-star model, for which $H(G) = \theta_1 m(G) + \theta_2 s(G)$, where $\theta_1$ and $\theta_2$ are independent parameters, $m(G)$ is the number of edges in the graph and $s(G)$ is the number of “2-stars.” A 2-star is a pair of edges that share a common vertex.

Let us denote by $k_i$ the degree of vertex $i$. Then $m(G) = \frac{1}{2} \sum_i k_i$ and $s(G) = \frac{1}{4} \sum_i k_i(k_i - 1)$, and hence we can write the Hamiltonian in the form

$$H = -\frac{J}{n - 1} \sum_i k_i^2 - B \sum_i k_i,$$ \hspace{1cm} (2)

where the “coupling constant” $J = -\frac{1}{2}(n - 1)\theta_2$ and the “field” $B = \frac{1}{4}(\theta_2 - \theta_1)$. The factor $(n - 1)$ in the definition of $J$ is not strictly necessary, but it makes the equations simpler later on.
There are two analytic approaches from statistical mechanics that can be brought to bear on problems like this. The first is to use perturbation theory \cite{22} and the second is to use non-perturbative techniques, usually based on the Hubbard–Stratonovich transform and saddle-point expansions \cite{20}. Here we make use of the latter to solve the 2-star model.

III. ANALYTIC APPROACH

Our goal is to calculate the partition function $Z$, Eq. (11), or equivalently the free energy. First, we introduce auxiliary fields $\phi_i$ on the vertices of the graph using the Hubbard–Stratonovich relation

$$
\exp\left(\frac{Jk_i^2}{(n-1)}\right) = \sqrt{\frac{(n-1)J}{\pi}} \times \int_{-\infty}^{\infty} d\phi_i \exp\left(-(n-1)J\phi_i^2 + 2J\phi_i k_i\right),
$$

which gives

$$
Z = \left[\frac{(n-1)J}{\pi}\right]^{n/2} \int \mathcal{D}\phi \exp\left(-\frac{n}{2}J\sum_i \phi_i^2\right) \times \sum_G \exp\left(\sum_i (2J\phi_i + B)k_i\right),
$$

where $\mathcal{D}\phi$ indicates the path integral over the fields $\{\phi_i\}$ and we have interchanged the order of the integral and the sum over graphs $G$.

The sum over graphs can now be performed by defining the symmetric adjacency matrix $\sigma_{ij}$ equal to 1 if there is an edge between vertices $i$ and $j$ and zero otherwise. Then, noting that $k_i = \sum_j \sigma_{ij}$, we can write

$$
\sum_i (2J\phi_i + B)k_i = \sum_{ij} (2J\phi_i + B)\sigma_{ij} = \sum_{i<j} [2J(\phi_i + \phi_j) + 2B] \sigma_{ij}.
$$

Since $\sigma_{ij}$ is symmetric, its values for $i < j$ completely define the graph, and hence

$$
\sum_{G} \exp\left(\sum_i (2J\phi_i + B)k_i\right) = \prod_{i<j} \sum_{\sigma_{ij}=0} e^{2J(\phi_i + \phi_j) + 2B} = \prod_{i<j} (1 + e^{2J(\phi_i + \phi_j) + 2B}).
$$

Substituting this result into Eq. (11), we then get

$$
Z = \int \mathcal{D}\phi \exp^{-\mathcal{H}(\phi)},
$$

where the effective Hamiltonian $\mathcal{H}$ is

$$
\mathcal{H}(\phi) = (n-1)J \sum_i \phi_i^2 - \frac{1}{2} \sum_{i \neq j} \ln(1 + e^{2J(\phi_i + \phi_j) + 2B}) - \frac{1}{2} n \ln((n-1)J).
$$

Thus we have transformed our network model into a field theory of a continuous scalar field on $n$ sites, which can be solved using a variety of methods. The simplest mean-field approach is to ignore fluctuations and assume $\phi_i$ always to be equal to its most probable value, which occurs at the saddle point

$$
\frac{\partial \mathcal{H}}{\partial \phi_i} = 0 = 2(n-1)J\phi_i - J \sum_{j(\neq i)} [\tanh(J(\phi_i + \phi_j) + B) + 1].
$$

This has a symmetric solution $\phi_i = \phi_0$ for all $i$ with

$$
\phi_0 = \frac{1}{2} [\tanh(2J\phi_0 + B) + 1].
$$

This quantity has a simple physical interpretation. The mean degree $\langle k \rangle$ of a vertex in the graph is given by the derivative of the free energy thus:

$$
\langle k \rangle = \frac{1}{n} \sum_i \langle k_i \rangle = \frac{1}{n} \frac{\partial F}{\partial B} = \frac{1}{2n} \sum_{i \neq j} \langle \tanh(J(\phi_i + \phi_j) + B) + 1 \rangle_{\phi},
$$

where $\langle \ldots \rangle_{\phi}$ indicates an average in the $\phi$ ensemble of Eq. (7). Making the mean-field assumption of Eq. (10), this becomes $\langle k \rangle = (n-1)\phi_0$ and hence $\phi_0$ is simply proportional to the mean degree of a vertex, within the mean-field approximation. The quantity $\langle k \rangle / (n-1)$ is called the “connectance” of the graph—it is the fraction of possible edges that are actually present and is a measure of the mean density. So we could also say that $\phi_0$ is equal to the connectance. This allows us to interpret Eq. (10) very directly. For $J \leq 1$, this equation has only a single solution, but for $J > 1$ we have three coexisting solutions when $B$ is sufficiently close to $-J$. Only the outer two solutions are stable, giving us a bifurcation at $J_c = 1$ corresponding to a continuous phase transition at this point to a symmetry broken state exhibiting two phases, one of high density (typically nearly a complete graph) and one of low density. We show a plot of the solution of (10) in the main panel of Fig. 1.

Along the line $B = -J$ the Hamiltonian (12) is symmetric with respect to the interchange of edges and “holes”—the absence of edges between vertex pairs. In the inset to Fig. 1 we show the solution for the connectance as a function of $J$ along this symmetric line and the plot shows the bifurcation clearly.

To move beyond the mean-field result, we make use of the method of stationary phase. Expanding the effective Hamiltonian (8) about the mean-field solution to leading order we have $\mathcal{H} = \mathcal{H}(\phi_0) + \phi^T M \phi' + O(\phi^3)$, where $\phi' = \phi - \phi_0$ and $M$ is the Hessian matrix of second derivatives of $\mathcal{H}$ with respect to $\phi$, evaluated at $\phi_0$. Changing variables to $\xi = Q\phi'$, where $Q$ is the matrix of eigenvectors of $M$, $M$ is diagonalized and $\mathcal{H} = \mathcal{H}(\phi_0) + \sum_i \lambda_i \xi_i^2 + O(\xi^3)$, with $\lambda_i$ being the $i$th eigenvalue of $M$. Substituting into Eq. (11) and observing that the Jacobian of the variable change $|Q| = 1$, the path integral becomes
a product of independent Gaussian integrals and $Z = e^{-\mathcal{H}(\phi_0)/\sqrt{|\mathbf{M}|}}$, or equivalently $F = \mathcal{H}(\phi_0) + \frac{1}{2} \ln |\mathbf{M}|$, where $|\mathbf{M}|$ is the determinant of $\mathbf{M}$.

The elements of the Hessian matrix have the values:

$$M_{ij} = \begin{cases} -4J^2\phi_0(1-\phi_0) & \text{for } i \neq j, \\ (n-1)[2J-4J^2\phi_0(1-\phi_0)] & \text{for } i = j, \end{cases} \quad (12)$$

giving

$$|\mathbf{M}| = (2(n-1)J)^n(1-2J\phi_0(1-\phi_0))^{n-1}(1-4J\phi_0(1-\phi_0)). \quad (13)$$

Then, making use of Eqs. (8) and (10), we arrive at the solution for the free energy

$$F = n(n-1)J\phi_0^2 - \frac{1}{2}n(n-1)\ln(1 + e^{4J\phi_0+2B})$$
$$+ \frac{1}{2}(n-1)\ln(1 - 2J\phi_0(1 - \phi_0)), \quad (14)$$

where we have kept leading order corrections to the mean-field result but dropped terms of order a constant and smaller that vanish in the large $n$ limit.

From the free energy we can calculate expected values of a variety of properties of the model. For instance the mean degree $\langle k \rangle$ and the mean squared degree $\langle k^2 \rangle$ are given by derivatives with respect to $B$ and $J$ and are equal to

$$\langle k \rangle = (n-1)\phi_0 + \frac{2J\phi_0(1-\phi_0)(1-2\phi_0)}{(1-4J\phi_0(1-\phi_0))(1-2J\phi_0(1-\phi_0))}. \quad (15)$$

$$\langle k^2 \rangle = (n-1)^2\phi_0^2 + \frac{(n-1)\phi_0(1-\phi_0)(1-4J\phi_0^2)}{(1-4J\phi_0(1-\phi_0))(1-2J\phi_0(1-\phi_0))}. \quad (16)$$

The leading order term in each case is the same as the mean-field result, so that in the limit of large $n$ both $\langle k \rangle$ and $\langle k^2 \rangle$ take their mean-field values. The variance of the degree $\langle k^2 \rangle - \langle k \rangle^2$ on the other hand is zero within the mean-field approximation because of the cancellation of the leading terms but non-zero beyond mean-field:

$$\langle k^2 \rangle - \langle k \rangle^2 = (n-1)\frac{\phi_0(1-\phi_0)}{1-2J\phi_0(1-\phi_0)}. \quad (17)$$

From consideration of Fig. 1 one might expect this quantity to diverge at the phase transition, but in fact it does not, having merely a cusp at that point. In Fig. 2 we show the form of this function along the symmetric line $B = -J$ as a function of $J$. The figure also shows the results of Monte Carlo simulations of the 2-star model for the same parameter values and, as we can see, agreement between the simulations and the analytic solution is excellent.

A divergence does occur in the variance of the number of edges in the network at the phase transition. This quantity, which plays the role of a susceptibility for the model, is given to leading order by

$$\langle m^2 \rangle - \langle m \rangle = \frac{\partial^2 F}{\partial B^2} = (n-1)\frac{2\phi_0(1-\phi_0)}{1-4J\phi_0(1-\phi_0)}. \quad (18)$$

This diverges as $|J-J_c|^{-1}$ as we approach the transition along the symmetric line $B = -J$.

One can also ask whether the network described by the 2-star model possesses a giant component. Molloy and Reed [3] have demonstrated that a network without degree correlations possesses a giant component if and only if $\langle k^2 \rangle > 2\langle k \rangle$. We can evaluate this criterion using
In this paper, we have given a non-perturbative analytic solution of one of the oldest of network models, the 2-star model, which is perhaps the simplest nontrivial model of the class known as exponential random graphs and has been long studied in the social sciences. The model turns out to be perfectly suited to solution by the methods of statistical physics, and among other things the solution shows the degenerate behavior of the model in certain parameter regimes to be the result of a symmetry breaking between high- and low-density phases, which are separated from the “normal” region of the model by a continuous phase transition.

The exponential random graphs are, we believe, an important class of network models, which have largely been neglected despite the high level of interest in networks in the last few years. We hope that others will also take up the study of these models, either using methods like those discussed here or other methods yet to be described.

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