Journal of Statistical Physics, Vol. 56, Nos. 3/4, 1989

The Statistics of Random Directed Graphs

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Received September 2, 1988; final February 28, 1989

The analysis of random graphs developed by the author, principally as a model for polymerization processes, is extended to the case of directed random graphs, with models of neural nets in mind. The principal novelty of the directed case is the representation of the partition function by a complex rather than a real integral, and the replacement of simple maxima in asymptotic evaluations by an interesting form of saddle point.

KEY WORDS: Random graphs; directed graphs; polymerization; neural nets.

1. INTRODUCTION

The study of random graphs can be said to have been pursued by two fairly distinct schools: one constituted by those working with physical models (notably of polymerization) and the other constituted by the pure graph theorists. Accounts of the work of these two schools up to about 1985 are effectively summarized in Whittle[10] and Bollobás,[1] respectively.

Both approaches have been concerned almost entirely with undirected graphs. The principal exception to this assertion would have been the study of polymers constructed of several types of unit, when a bond between units of different type (i.e., an arc between nodes of different color) is intrinsically asymmetric.

However, there is a need to study the directed case. Random graphs with field variables defined at the nodes are being increasingly used as models for neural networks, and realism requires that the dynamics of this field be directed and irreversible.[2–7,11] A general theory for such models is still lacking, but a first step is certainly the study of random directed graphs.

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0022-4715/89/0800-0499$06.00/0

The model considered by Whittle (see ref. 10 and papers quoted there) may seem to be a directed formulation, in that a graph ("configuration") $\mathscr{C}$ on N given nodes is specified by $\mathscr{C} = \{s_{ab}; a, b = 1, 2,..., N\}$, where s_{ab} is the number of arcs directed from node a to node b. The equilibrium distribution deduced for this configuration on statistical mechanical grounds is

$$P_N(\mathscr{C}) \propto Q_N(\mathscr{C}) = \left(\prod_{a,b} \frac{h^{s_{ab}}}{s_{ab}!}\right) e^{-E(\mathscr{C})/T} \tag{1}$$

where $E(\mathscr{C})$ is the potential energy associated with configuration $\mathscr{C}$ and T is a normalized temperature. The quantity h is inversely proportional to "volume" V

$$h = \frac{1}{2\kappa V} \tag{2}$$

Distance and dimensionality do not enter into this model, but volume can be regarded as an "extension" parameter, significant in that the essential results emerge in the thermodynamic limit, when N and V tend to infinity in constant ratio

$$\rho = N/V$$

We can thus regard ρ as the "density" of nodes.

Distribution (1) is just a Gibbs distribution, obeying a detailed balance condition if the rates λ, λ' for the transitions $s_{ab} \rightleftharpoons s_{ab} + 1$ are in the ratio

$$\frac{\lambda}{\lambda'} = \frac{(2\kappa V)^{-1}}{s_{ab} + 1} e^{-\Delta E/T}$$

where ΔE is the increment in potential energy under the transition $s_{ab} \to s_{ab} + 1$. This ratio is plausible: the V^{-1} term represents the fact that the association rate between two *given* nodes will decrease as V^{-1} with increasing V, and the $s_{ab} + 1$ term represents an assumption that all of the $s_{ab} + 1$ ab-bonds are equally likely to break. The factor κ could be incorporated in ΔE, but is useful to retain separately.

In the so-called "first-shell" model distribution (1) is specialized to

$$P_N(\mathscr{C}) \propto Q_N(\mathscr{C}) = \left(\prod_{a,b} \frac{h^{s_{ab}}}{s_{ab}!}\right)\left(\prod_j H_j^{N_j}\right) \nu^{B+C-N} \tag{3}$$

where N_j is the number of nodes of degree j (that is, nodes at which j arcs meet, or units which have formed j bonds; $j=0, 1, 2,...$). Further,

$$B=\tfrac{1}{2}\sum_j jN_j \tag{4}$$

is the number of bonds, and C is the number of components in the graph (polymers in the mix). We can regard $-T\log H_j$ as the potential energy associated with a j-bond unit: it is the fact that E is largely made up of these contributions which constitutes the "first-shell" assumption. The term in ν in (3) represents a difference in interpolymer and intrapolymer bond function rates. If a new bond is formed, this term contributes $-T\log\nu$ to ΔE if the new bond is within an existing polymer (graph component), but contributes nothing if the bond links two previously separate polymers. So, if $\nu=1$, then inter- and intrapolymer association rates are equal; if $\nu=0$, then the polymers are constrained to be trees.

Distribution (3) is a consequence of a reversible Markov model, but such an immediate one that we may as well regard prescription of (3) as the model itself. The model may seem to allow directional effects, in that it distinguishes between s_{ab} and s_{ba}. Such a distinction is mathematically natural, but the fact that distribution (3) is invariant under permutation of s_{ab} and s_{ba} implies that the model exhibits no real directional effect.

To achieve a truly directed specification, let us say that a node has degree (j,k) if it has j outgoing arcs and k incoming arcs, and let N_{jk} be the (random) number of such nodes. We shall then modify model (3) to

$$P_N(\mathscr{C})\propto Q_N(\mathscr{C})=\left(\prod_{a,b}\frac{h^{s_{ab}}}{s_{ab}!}\right)\left(\prod_{j,k}H_{jk}^{N_{jk}}\right)\nu^{B+C-N} \tag{5}$$

We continue to use the notation H, but H_j and H_{jk} are of course completely different quantities. The directed model (5) would reduce to the undirected model (3) in the case

$$H_{jk}=H_{j+k} \tag{6}$$

Analysis of the directed case can be seen both as a useful extension of the polymerization model and as a preparatory study for the analysis of neural nets.

2. SUMMARY OF RESULTS FOR THE UNDIRECTED CASE

It is helpful to begin by summarizing the results for the undirected case, which we hope to generalize to the directed case. Corresponding theorems (quoted) for the undirected case and (proved) for the directed case will be denoted U and D. So, Theorems U1 and D1 are corresponding. The assertions of this section will refer to the undirected case alone.

The quantity

$$Q_N = \sum_{\mathscr{C}} Q_N(\mathscr{C}) \tag{7}$$

is the partition function of the model. It can also be viewed as the unnormalized probability generating function (p.g.f.) of the random variables N_j, with the quantities H_j serving both as parameters of the model and as marker variables for the N_j in the p.g.f.

Define the function

$$H(\xi) = \sum_{j=0}^{\infty} \frac{H_j \xi^j}{j!} \tag{8}$$

Theorem U1. Suppose log $H(\xi)$ of less than quadratic growth at infinity. Then for model (1) with $v=1$ the partition function Q_N has the evaluation

$$Q_N = \frac{\kappa V}{2\pi} \int_{-\infty}^{\infty} H(\xi)^N e^{-\kappa V \xi^2/2}\, d\xi \tag{9}$$

The growth condition on $\log H(\xi)$ is imposed in order to make integral (9) convergent for all positive N, V. We shall assume this satisfied in the sequel.

Evaluation (9) determines node statistics, at least in the case $v=1$. For example, by extracting the term in $\prod_j H_j^{N_j}$ we obtain the distribution of $N_. = \{N_0, N_1, N_2, \ldots\}$ as

$$P(N_.) \propto \left(B - \frac{1}{2}\right)! \left(\frac{2}{\kappa V}\right)^B \left[\prod_j \frac{1}{N_j!}\left(\frac{H_j}{j!}\right)^{N_j}\right] \tag{10}$$

where $(B-1/2)! = \Gamma(B+1/2)$.

However, evaluation (9) also determines the statistics of the graph components (the *polymer molecules*) for any v. The natural level of description of a component for model (1) is $r = \{r_j; j=0, 1, 2, \ldots\}$, where r_j is the number of nodes in the component of degree j (i.e., the number of units in the polymer which have formed exactly j bonds). Let us term such a component (polymer) an *r-mer*; it will contain

$$R = \sum_j r_j$$

nodes and

$$L=\tfrac{1}{2}\sum_j jr_j$$

arcs. Let n_r be the number of r-mers, so that necessarily

$$\sum_r Rn_r = N \tag{11}$$

Theorem U2. Suppose that $\log[\sum_{N=0}^{\infty}(Q_N/N!)]$ has the formal expansion $\sum_r \gamma_r$ in powers of the H_j, where Q_N has the evaluation (9) valid for $v=1$ and γ_r is the term in $\prod_j H_j^{r_j}$. Then the n_r are distributed as independent Poisson variables with respective expectations $\gamma_r v^{L-R+1}$, conditioned by the constraint (11).

The integrand in (9) can be written e^{VJ}, where

$$J(\xi)=\rho\log H(\xi)-\kappa\xi^2/2 \tag{12}$$

The value $\bar{\xi}$ of ξ maximizing $J(\xi)$ largely characterizes behavior in the thermodynamic limit, in that if we define

$$I(\phi)=\int \phi(\xi)\, e^{VJ(\xi)}\alpha\xi \tag{13}$$

then evidently we have the following result.

Theorem U3. For sufficiently regular ϕ

$$I(\phi)\propto\phi(\bar{\xi}) \tag{14}$$

in the thermodynamic limit, where the constant of proportionality is independent of ϕ.

A sufficient regularity condition would, for example, be that ϕ be continuous and integral (13) exist for sufficiently large V.

Since $E(N_j)\propto I(H_j\xi^j/j!\ H(\xi))$, an immediate corollary of this result is the following.

Theorem U4. Suppose $v=1$. Then in the thermodynamic limit

$$E(N_j)\propto\frac{H_j\bar{\xi}^j}{j!} \tag{15}$$

Expression (15) when normalized determines p_j, the distribution of the degree j of a randomly chosen node.

There is then the important question of *criticality*. Below a critical value ρ_C of ρ the components are mostly small; for $\rho > \rho_C$ most nodes lie in a single "giant component." In polymerization terms, there are the two regimes of the *sol state* and the *gel state*. The regime *at* the critical density ρ_C may be sol or gel or transitional; see the comments at the end of Section 6.

The best way to test which regime prevails is to test for the breaking of replica symmetry: for whether matter in communicating replicas of the model tends to equidistribute itself statistically between replicas or to concentrate in some single replica. The assumption that two replicas communicate would be expressed by saying that the configurations $\mathscr{C}_1$, $\mathscr{C}_2$ in the two replicas would have joint distribution

$$P(\mathscr{C}_1, \mathscr{C}_2) \propto Q_{M_1}(\mathscr{C}_1)\, Q_{M_2}(\mathscr{C}_2) \qquad (M_1 + M_2 = 2N)$$

where $Q_N(\mathscr{C})$ is given by expression (3), M_i is the number of nodes (units) in replica i, and the condition $M_1 + M_2 = 2N$ is the only constraint upon the distribution. Integrating this joint distribution over configurations $\mathscr{C}_i$ and permutations of nodes for given M_1, M_2, we deduce the distribution of M_1, M_2 to be

$$P(M_1, M_2) \propto \frac{Q_{M_1} Q_{M_2}}{M_1!\; M_2!} \qquad (M_1 + M_2 = 2N)$$

One will be in the subcritical regime if matter equidistributes itself between the two regimes, i.e., if $P(N+n, N-n)$ is maximal at $n = 0$. It is shown in ref. 10, Chapter 15, that this is equivalent to requiring that

$$[H(\xi_1) + H(\xi_2)]^{2N} e^{-\kappa V(\xi_1^2 + \xi_2^2)/2}$$

should be maximal at $\xi_1 = \xi_2$ (the common maximizing value necessarily being $\bar{\xi}$), and that this is in turn equivalent to the condition that in the representation

$$J(\xi) = \min_{\theta} \left[\theta H(\xi) - \frac{\kappa \xi^2}{2} - \rho \log \theta \right] \tag{16}$$

of J the square bracket should possess a saddle point [min-max in (θ, ξ)].

Otherwise expressed, let $\bar{\xi}(\theta)$ be the value of ξ maximizing the square bracket in (16), with ρ expressed parametrically in terms of θ by $\rho = \theta H(\bar{\xi}(\theta))$. As θ (and so ρ) increases from zero, a point is reached at which $\partial \bar{\xi}(\theta)\, \partial \theta$ becomes infinite; this point marks criticality. This characterization leads to following the conclusion.

Theorem U5. Suppose $v = 1$ and consider ρ increasing from zero. Then the regime is subcritical exactly so long as

$$\xi \frac{\partial^2 H}{\partial \xi^2} - \frac{\partial H}{\partial \xi} < 0 \tag{17}$$

where ξ has the value $\bar{\xi}$ maximizing $J(\xi)$.

This criterion in fact locates the critical point for all values of v, but as v increases, the sol solution becomes metastable rather than unconditionally stable for values of ρ less than ρ_C (ref. 10, p. 346).

In virtue of Theorem U4, we can rephrase the criticality condition immediately in terms of degree statistics.

Theorem U6. The regime is subcritical exactly so long as

$$E(j(j-1)) < E(j) \tag{18}$$

or, equivalently,

$$E^*(j-1) < 1 \tag{19}$$

where E, E^* are expectations based upon the distributions p_j and $p_j^* \propto jp_j$, respectively.

Relation (19) states that, if one considers the nodes at the ends of a randomly chosen arc, then the expected numbers of *further* nodes to which each of these nodes is connected is less than unity. This is related to the branching process view of a random graph: the total progeny of an ancestor will be finite with probability one iff the expected number of his sons is less than unity.

3. THE EVALUATION OF THE PARTITION FUNCTION

From now on we shall consider the directed case, based on (5) rather than on (1). In this case the partition function Q_N is effectively the unnormalised p.g.f. of the variables N_{jK}, and we seek an evaluation analogous to (9). Corresponding to (8), let us define the double generating function

$$H(\xi_1, \xi_2) = \sum_j \sum_k H_{jk} \frac{\xi_1^j \xi_2^k}{j!\,k!} \tag{20}$$

Theorem D1. Suppose $\log H(\xi_1, \xi_2)$ of less than quadratic growth at infinity. Then for model (5) with $v = 1$, the partition function Q_N has the evaluation

$$Q_N = \frac{2\kappa V}{\pi} \iint_{-\infty}^{\infty} H(\eta_1 + i\eta_2, \eta_1 - i\eta_2)^N \exp[-2\kappa V(\eta_1^2 + \eta_2^2)]\, d\eta_1\, d\eta_2 \tag{21}$$

Proof. Suppose that H_{jk} has the formal integral representation

$$H_{jk} = \iint x^j y^k \, m(dx, dy) \tag{22}$$

so that

$$H(\xi_1, \xi_2) = \iint \exp(x\xi_1 + y\xi_2) \, m(dx, dy)$$

We see from (5), (22) that Q_N can be written

$$\begin{aligned} Q_N &= \int \cdots \int \left[\sum_s \prod_{a,b} \frac{(hx_a y_b)^{s_{ab}}}{s_{ab}!} \right] \prod_a m(dx_a, dy_a) \\ &= \int \cdots \exp\left[h\left(\sum_a x_a\right)\left(\sum_a y_a\right)\right] \prod_a m(dx_a, dy_a) \end{aligned} \tag{23}$$

Consider now the identity

$$e^{h\Sigma_1\Sigma_2} = \frac{1}{\pi h} \iint \exp[\Sigma_1(\eta_1 + i\eta_2) + \Sigma_2(\eta_1 - i\eta_2) - (\eta_1^2 + \eta_2^2)/h] \, d\eta_1 \, d\eta_2 \tag{24}$$

Making this substitution under the integral in (23) with the identifications $\Sigma_1 = \sum x_a$, $\Sigma_2 = \sum y_a$, and $h = (2\kappa V)^{-1}$, we deduce the asserted expression (21) for Q_N. ▌

We know that the directed specification reduces to the undirected one if (6) holds, i.e., if

$$H(\xi_1, \xi_2) = H(\xi_1 + \xi_2)$$

In this case it follows routinely that expression (21) reduces to (9).

The analogue of Eq. (10) is important enough to be stated as a theorem. Let us define the vector random variable $N_{..} = \{N_{jk}; j, k = 0, 1, 2, \ldots\}$ and the quantities

$$B_1 = \sum_j \sum_k jN_{jk} \tag{25}$$

$$B_2 = \sum_j \sum_k kN_{jk} \tag{26}$$

$$A_{jk} = \frac{H_{jk}}{j!\,k!} \tag{27}$$

Theorem D2. The vector $N_{..} = \{N_{jk}\}$ has the distribution

$$P(N_{..}) \propto \frac{B!}{(2\kappa V)^B}\left[\prod_{j,k} \frac{A_{jk}^{N_{jk}}}{N_{jk}!}\right] \tag{28}$$

this being confined to nonnegative integers N_{jk} such that

$$\sum_j \sum_k N_{jk} = N \tag{29}$$

$$\sum_j \sum_k (j-k)\, N_{jk} = 0 \tag{30}$$

The quantity B is the common value of B_1 and B_2.

Proof. $P(N_{..})$ is proportional to the term in $\prod_{j,k} H_{jH}^{N_{jk}}$ in the expansion of expression (18) in powers of the H_{jk}, and so to

$$I \prod_{j,k} \frac{A_{jk}^{N_{jk}}}{N_{jk}!}$$

where

$$I = \iint_{-\infty}^{\infty} (\eta_1 + i\eta_2)^{B_1} (\eta_1 - i\eta_2)^{B_2} \exp[-2\kappa V(\eta_1^2 + \eta_2^2)]\, d\eta_1\, d\eta_2$$

A transformation to polar coordinates shows that

$$I \propto \begin{cases} B_1!\,(2\kappa V)^{-B_1} & (B_1 = B_2) \\ 0 & (B_1 \neq B_2) \end{cases}$$

whence expression (28) and condition (30) follow. ∎

Condition (29) simply expresses the fact that there are N nodes in total. Condition (30) expresses the fact that the total number of outgoing and incoming arcs must be equal. This is a fundamental assertion, for all its obviousness, and it is interesting that this assertion should follow from the general form of the integral (21).

A node now has the double degree (j, k), where j and k are, respectively, the numbers of outgoing and incoming arcs. The natural level of description of a component (polymer) for model (5) is $r = \{r_{jk}; j, k = 0, 1, 2, \ldots\}$, where r_{jk} is the number of nodes of degree (j, k) it contains. There are no new features in the deduction of polymer statistics from the evaluation of Q_N; the only differences are the obvious points of definition.

Theorem D3. As for Theorem U2, except that r, R, and L have the revised definitions $r = \{r_{jk}\}$, $R = \sum_j \sum_k r_{jk}$, and $L = \sum_j \sum_k j r_{jk} = \sum_j \sum_k k r_{jk}$.

4. ASYMPTOTICS OF THE THERMODYNAMIC LIMIT

The integral (21) is of the form $Q_N \propto \int e^{VJ}\, d\eta$, where J now has the definition

$$J(\xi_1, \xi_2) = \rho \log H(\xi_1, \xi_2) - 2\kappa\xi_1\xi_2 \tag{31}$$

[see the undirected version (12)]. Note that J occurs in the integral with complex arguments: $J(\eta_1 + i\eta_2, \eta_1 - i\eta_2)$. One wonders now if there is a value $\bar{\xi} = (\bar{\xi}_1, \bar{\xi}_2)$ which is dominating in the thermodynamic limit in that, if we define

$$I(\phi) = I(\phi(\xi_1, \xi_2)) = \int \phi(\eta_1 + i\eta_2, \eta_1 - i\eta_2)\, e^{VJ}\, d\eta \tag{32}$$

then

$$I(\phi) \propto \phi(\bar{\xi}_1, \bar{\xi}_2) \tag{33}$$

in the thermodynamic limit (see Theorem U3). We shall find this to be the case, with $\bar{\xi} = (\bar{\xi}_1, \bar{\xi}_2)$ having the *real* saddle-point characterization stated below in Theorems D4 and D4′. We regard Theorem D4 as preparatory, in that it provides a constructive path to the asymptotic results. Once one knows where the path leads, conclusions can easily be strengthened; cf. Theorem D4′.

Theorem D4. Suppose H_{jk} zero for j, k greater than some prescribed finite value. The most probable value of $N_{..} = \{N_{jk}\}$ in the thermodynamic limit is given by

$$\bar{N}_{jk} \propto A_{jk}\bar{\xi}_1^j \bar{\xi}_2^k \tag{34}$$

where $(\bar{\xi}_1, \bar{\xi}_2)$ is the real value of (ξ_1, ξ_2) maximizing $J(\xi_1, \xi_2)$ with respect to $\xi_1\xi_2$ and minimizing it with respect to ξ_1/ξ_2.

Proof. In the more probable part of distribution (28) the N_{jk} will all be of order N, and $N_{jk}!$ can be approximated by Stirling's formula. As far as the term in B is concerned, this is equivalent to making the substitution

$$\frac{B!}{(2\kappa V)^B} \sim \max_U e^{-2\kappa V U^2} U^{2B}$$

$$= \max_U e^{-2\kappa V U^2} U^{B_1 + B_2}$$

The maximization of log $P(N_{..})$ with respect to the N_{jk} is then equivalent to maximization of the Lagrangian form

$$N \log N - N + \sum_j \sum_k N_{jk}[\log(A_{jk}/N_{jk}) - 1] - 2\kappa V U^2$$
$$+ (B_1 + B_2) \log U + \lambda \left(N - \sum_j \sum_k N_{jk} \right) + \mu(B_1 - B_2) \qquad (35)$$

with respect to $N_{..}$ and U. Here λ, μ are Lagrangian multipliers associated with the constraints (29), (30) and B_1, B_2 have the definitions (25), (26). The value of N_{jk} maximizing (35) is

$$\bar{N}_{jk} = A_{jk} e^{-\lambda + \mu(j-k)} U^{j+k} \qquad (36)$$

This substitution leaves a reduced Lagrangian form

$$\mathscr{L} = N \log N - N - 2\kappa V U^2 + \lambda N + e^{-\lambda} H(Ue^{\mu}, Ue^{-\mu})$$

to be maximized with respect to U and minimized with respect to λ, μ (since the multipliers λ, μ are the dual variables of a convex programming problem). Minimization with respect to λ yields

$$\lambda = \log H/N$$

and the further reduced Lagrangian form

$$\mathscr{L}' = N \log H(Ue^{\mu}, Ue^{-\mu}) - 2\kappa V U^2$$
$$= VJ(\xi_1, \xi_2) \qquad (37)$$

if we define

$$\xi_1 = Ue^{\mu}, \qquad \xi_2 = Ue^{-\mu}$$

Expression (37) is to be maximized with respect to $U^2 = \xi_1 \xi_2$ and minimized with respect to $2 \log \mu = \xi_1/\xi_2$. Expression (36) and these determinations of U and μ imply the assertion of the theorem. ∎

The proportionality constant in (36) is to be chosen so that $\bar{N}_{..}$ satisfies condition (29). Condition (30) should be satisfied by construction. However, a direct verification takes us over some useful ground. The saddle point $(\bar{\xi}_1, \bar{\xi}_2)$ will be located by the stationarity conditions

$$\theta \frac{\partial H}{\partial \xi_1} = 2\kappa \xi_2, \qquad \theta \frac{\partial H}{\partial \xi_2} = 2\kappa \xi_1 \qquad (38)$$

Here

$$\theta = \rho/H \tag{39}$$

and arguments $(\bar{\xi}_1, \bar{\xi}_2)$ are understood throughout. On the other hand, in virtue of (34) (with proportionality constant $e^{-\lambda}$), we have

$$\bar{B}_1 = e^{-\lambda}\xi_1 \frac{\partial H}{\partial \xi_1} = 2\kappa e^{-\lambda}\bar{\xi}_1\bar{\xi}_2$$

and the same evaluation for $\bar{B}_2$.

Theorem D4′. Supose $\log H(\xi_1, \xi_2)$ of less than quadratic growth at infinity. Then relation (33) holds for sufficiently regular ϕ in the thermodynamic limit, with $(\bar{\xi}_1, \bar{\xi}_2)$ being the real value of (ξ_1, ξ_2) that maximizes $J(\xi_1, \xi_2)$ with respect to $\xi_1\xi_2$ and minimizes it with respect to ξ_1/ξ_2.

Proof. In integral (32) let us change variables from (η_1, η_2) to the polar form (U, ψ) or to (U, z), where

$$\eta_1 \pm i\eta_2 = Ue^{\pm i\psi} = Uz^{\pm 1}$$

We then have

$$I(\phi) \propto \int_0^\infty dU \frac{dz}{z} \phi(Uz, Uz^{-1})\, H(Uz, Uz^{-1})^N e^{-2\kappa V U^2} \tag{40}$$

where the z integration is around the unit circle. Consider the z integral for fixed U. The z contour can be deformed until it passes through a saddle point of the function $H(Uz, Uz^{-1})$ of z. But this function is a power series in z with powers of both signs, but nonnegative coefficients. The dominant saddle point will then be on the positive real z axis, at a value of z *minimizing* the function on the real axis (which is orthogonal to the integration path).

One is then left with a real, positive integrand to be integrated with respect to U; it will be the maximizing value of U which is dominant.

The dominant contribution to integral (32) is thus from real, positive values of U and z which respectively maximize and minimize the function $J(Uz, Uz^{-1})$. This is just the assertion of the theorem. ∎

A "sufficiently regular" ϕ will be one for which this argument is justifiable, which will certainly be true if ϕ is a product of finite powers of ξ_1, ξ_2 and finite (positive or negative) powers of $H(\xi_1, \xi_2)$. Since

$$E(N_{jk}) \propto I(A_{jk}\xi_1^j\xi_k^k/H(\xi_1, \xi_2))$$

we deduce the following result from Theorem D4′.

Theorem D5. Suppose $\nu = 1$. Then in the thermodynamic limit

$$E(N_{jk}) \propto A_{jk} \xi_1^j \xi_2^k \tag{41}$$

consistently with (34).

Expression (41) when normalized provides the distribution p_{jk} of the degree (j, k) of a randomly chosen node in the thermodynamic limit. Relation (30) will have the implication

$$E(j-k) = 0 \tag{42}$$

5. CRITICALITY

Just as for the directed case, supercriticality of the regime (the presence of a giant component) manifests itself when the square bracket in the representation

$$J(\xi_1, \xi_2) = \min_\theta \left[\theta H(\xi_1, \xi_2) - \kappa \xi_1 \xi_2 - \rho \log \theta\right]$$

no longer has a saddle point of the correct form. Specifically, suppose that $\bar{\xi}_1(\theta)$, $\bar{\xi}_2(\theta)$ constitute a max-min point of the bracket with respect to $(\xi_1 \xi_2, \xi_1/\xi_2)$. Take θ as independent parameter, with ρ related to it by $\rho = \theta H$ (argument $\bar{\xi}(\theta)$ understood). As θ increases from zero, so does ρ, and criticality is reached when either of $\partial \bar{\xi}_i(\theta)/\partial \theta$ $(i = 1, 2)$ becomes infinite.

Theorem D6. Suppose $\nu = 1$, and consider ρ increasing from zero. Then the regime is subcritical exactly so long as the matrix

$$M = \begin{pmatrix} -\rho H^{-1} \dfrac{\partial^2 H}{\partial \xi_1^2} & 2\kappa - \rho H^{-1} \dfrac{\partial^2 H}{\partial \xi_1 \, \partial \xi_2} \\ 2\kappa - \rho H^{-1} \dfrac{\partial^2 H}{\partial \xi_1 \, \partial \xi_2} & -\rho H^{-1} \dfrac{\partial^2 H}{\partial \xi_2^2} \end{pmatrix} \tag{43}$$

is nonsingular, i.e., as long as the inequality

$$\rho^2 \frac{\partial^2 H}{\partial \xi_1^2} \frac{\partial^2 H}{\partial \xi_2^2} < \left(2\kappa H - \rho \frac{\partial^2 H}{\partial \xi_1 \, \partial \xi_2}\right)^2 \tag{44}$$

holds. Evaluation at the saddle point $(\bar{\xi}_1, \bar{\xi}_2)$ of J is understood in all cases.

Proof. We deduce from (38) that

$$\begin{pmatrix} \partial \bar{\xi}_1/\partial \theta \\ \partial \bar{\xi}_2/\partial \theta \end{pmatrix} = M^{-1} \begin{pmatrix} \partial H/\partial \xi_1 \\ \partial H/\partial \xi_2 \end{pmatrix}$$

whence the assertions follow. ∎

Theorem D7. The condition (44) for subcriticality can alternatively be written

$$[E(j^2-j)][E(k^2-k)] < [E(jk-j)]^2 \tag{45}$$

Proof. This reformulation follows easily from the form (41) of the unnormalized (j, k) distribution and relations (38). Relation (45) is the analogue of (18) for the undirected case. However, if there is still a branching process interpretation, it must be a strongly modified one.

6. SOME PARTICULAR CASES

One extreme case for the undirected version is what was termed the *Poisson case* in ref. 10:

$$H_j = \phi^j$$

For this case all arcs (bonds) have the same configurational energy, and one finds from Theorem U5 that the critical density is

$$\rho_C = \kappa/\phi^2$$

A modified version of this is Stockmayer's *f-functional case*, for which

$$H_j = \binom{f}{j}\phi^j$$

for some positive integer f. In this case all arcs again have the same configurational energy, but a node has just f "sites" to which an arc may attach. One finds that

$$\rho_C = \frac{\kappa(f-1)}{\phi^2 f(f-2)^2}$$

The case at the opposite extreme to the Poisson is

$$H_j = \delta_{jd} \tag{46}$$

when all nodes are required to have degree d exactly. Not surprisingly, one finds [see (18)] that the process is subcritical at all densities if $d = 0, 1$; and supercritical at all densities if $d = 2, 3, 4, \ldots, l$. The case $d = 2$ is a transitional one on which we comment at the end of the section.

The directed version of the Poisson case would be that for which

$$H_{jk} = \phi_1^j \phi_k^k$$

and so

$$H(\xi_1, \xi_2) = \exp(\phi_1 \xi_1 + \phi_2 \xi_2)$$

The stationary point $(\bar{\xi}_1, \bar{\xi}_2)$ of $J(\xi_1, \xi_2)$ yielded by

$$\rho\phi_1 = 2\kappa\xi_2, \qquad \rho\phi_2 = 2\kappa\xi_1$$

indeed has the saddle-point character required in Theorems D4 and D4'. Condition (43) yields the critical density

$$\rho_C = \frac{\kappa}{\phi_1 \phi_2}$$

corresponding to that for the undirected Poisson case with $\phi = (\phi_1 \phi_2)^{1/2}$.

The f-functional case could have several directed analogues: let us take the simplest, for which

$$H_{jk} = \binom{f_1}{j}\binom{f_2}{k} \phi_1^j \phi_2^k$$

That is, there are f_1 "outgoing" attachment sites and f_2 "incoming" sites, not mutually substitutable. We have then

$$H(\xi_1, \xi_2) = (1 + \phi_1 \xi_1)^{f_1} (1 + \phi_2 \xi_2)^{f_2}$$

It is useful to define the quantities

$$p_i = \frac{\phi_i \bar{\xi}_i}{1 + \phi_i \bar{\xi}_i}$$

which for i equal to 1 and 2 are interpretable respectively as the proportions of outgoing and incoming sites which are occupied. Indeed, it follows from Theorem D5 that j, k follow independent binomial distributions with parameters (f_1, p_1) and (f_2, p_2), respectively.

The stationarity conditions (38) for J become, in terms of the p_i,

$$f_1 p_1 = f_2 p_2 = \frac{2\kappa p_1 p_2}{\rho \phi_1 \phi_2 q_1 q_2} \tag{47}$$

where $q_i = 1 - p_i$. The subcriticality condition (45) becomes

$$(f_1 - 1)(f_2 - 1)\, p_1 p_2 < (1 - f_1 p_1)(1 - f_2 p_2) \tag{48}$$

We can best express matters in terms of the single parameter

$\alpha = f_1 p_1 = f_2 p_2$, identifiable as the common value of $E(j)$ and $E(k)$. In terms of α, relations (47) and (48) become, respectively,

$$\frac{2\kappa\alpha}{\rho\phi_1\phi_2} = (f_1 - \alpha)(f_2 - \alpha) \tag{49}$$

$$(f_1 - 1)(f_2 - 1)\,\alpha^2 < f_1 f_2 (1 - \alpha)^2 \tag{50}$$

As ρ increases from zero, then so does α, and by (50) criticality will be reached when

$$\frac{\alpha}{1-\alpha} = \sqrt{\frac{f_1 f_2}{(f_1 - 1)(f_2 - 1)}}$$

Inserting this determination of the critical α value into (49), we obtain, with some reduction, the determination of the critical density

$$\rho_C = \frac{\kappa}{\phi_1\phi_2(f_1 - 1)(f_2 - 1)} \frac{2(1 + c_1 c_2)}{(c_1 + c_2)^2} \tag{51}$$

where

$$c_i = \sqrt{\frac{f_i}{f_i - 1}}$$

In the case $f_1 = f_2 = f$ expression (51) reduces to

$$\rho_C = \frac{\kappa}{\phi_1\phi_2(f_1 - 1)(f_2 - 1)} \left(\frac{2f - 1}{2f}\right)$$

Finally, the directed analogue of the fixed-degree case (46) is

$$H_{jk} = \begin{cases} 1 & j = d_1, \quad k = d_2 \\ 0 & \text{otherwise} \end{cases}$$

when all nodes are constrained to have degree (d_1, d_2) exactly. We have then

$$J(\xi_1, \xi_2) = \text{const} + \rho \log(\xi_1^{d_1} \xi_2^{d_2}) - 2\kappa\xi_1\xi_2$$

Now this expression will not have a saddle point unless $d_1 = d_2$, which is indeed necessary if the balance conditions (30), (42) are to hold. However, with $d_1 = d_2 = d$ we are in the degenerate situation that J is a function of $P = \xi_1\xi_2$ alone. Since the matrix M is then trivially singular, conditions for criticality based on the first onset of singularity are uninformative. For example, both sides of inequality (45) are equal to $d^2(d-1)^2$. To overcome this, we consider the analogue of J for two communicating replicas, when we would have

$$J(\xi_1, \xi_2; \xi_1', \xi_2') \propto \rho \log(P^d + Q^d) - \kappa(P+Q)$$

where $P = \xi_1 \xi_2$; $Q = \xi_1' \xi_2'$. We seek values of these arguments maximizing J, and find, for $d = 0, 1$, that J is maximized by

$$P = Q = \frac{\rho d}{2\kappa}$$

but for $d = 1, 2, 3...$, J is maximized by $P = 0$, $Q = \rho d/\kappa$, or the permuted solution. This indicates that we are in the subcritical case for $d < 1$, the supercritical case for $d > 1$, and that the case $d = 1$ is transitional.

In fact, the undirected case with $d = 2$ and the directed case with $d = 1$ are identical, because in both cases the only components that can occur are simple loops of lengths $R = 1, 2, 3,...$. One finds from Theorem U2 or D3 that

$$\gamma_r \propto \frac{w^R}{R}$$

where w is a constant whose value becomes irrelevant once condition (11) is applied (ref. 9, p. 517).

A closer analysis shows that with positive probability loops of size $O(N)$ will occur, but that there will be more than one such loop. That is, there will be "giant components," but more than one single giant component.

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