Fields and Flows on Random Graphs

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1. Introduction

Random graphs have become objects of increasing interest over the last thirty years. Two sets of physical models which have particularly stimulated this development are those of polymerisation and of percolation.

The early polymerisation work is associated especially with the names of Flory, Stockmayer, Gordon and Good. An approach in which one sets up a reversible Markov model of association/dissociation and analyses its equilibrium properties is set out systematically in Whittle (1986). Percolation theory is firmly associated with the name of Hammersley, who initiated and so greatly developed the subject. For reviews see Hammersley and Welsh (1980) and Kesten (1982).

Finally, largely in isolation from either of the above movements, pure mathematicians developed an interest in the subject, beginning with Erdős and co-workers, and continued notably by Stepanov and Bollobás. The work of this school is systematically presented in Bollobás (1985).

However, there are now new applications developing, which will require fundamental theoretical advances. I think especially of the study of neural networks. These are viewed as random graphs, partly because their size and complexity makes the statistical approach inevitable, and partly also because (just as in communication theory), the further one penetrates into the subject, the more one realises that the statistical approach is 'right'.

The interest of a neural network is that impulses and activity of some kind are propagated around it. One is then motivated to a study which has received only sporadic attention hitherto and of which this article can only be a token: of directed dynamics on a random graph.

The view of a neural net as a random graph is explicit in the papers of Kauffman (1969), Little and Shaw (1978) and Hopfield (1982), for example. More recent papers are those by Derrida and co-workers and by the author, listed in the references, particular aspects of which we shall refer to later.

2. Random Graphs and Reversible Dynamics

Our starting point is some earlier work of the author's (see Whittle 1986 and references quoted there) which we now summarise for convenience.

The configuration $\mathcal{C}$ of a random graph on N nodes is specified by $\mathcal{C} = \{s_{ab}; a, b = 1, 2, \ldots, N\}$ where s_{ab} is the number of arcs directed from node a to node b. In a 'first-shell' Markov model this has equilibrium distribution

$$P_N(\mathcal{C}) \propto Q_N(\mathcal{C}) = \left[\prod_{a,b} \frac{h^{s_{ab}}}{s_{ab}!}\right]\left[\prod_j H_j^{N_j}\right]. \tag{2.1}$$

Here h has the form

$$h = \frac{1}{2\kappa V} \tag{2.2}$$

where κ is a constant and V is volume. Despite the fact that distance and dimension do not enter into this description, one needs an 'extension' parameter, supplied by V. The interesting results emerge in the thermodynamic limit, when N and V become infinite in constant ratio

$$\rho = N/V$$

interpretable as the 'node density'.

The quantity N_j in (2.1) is the number of nodes which have degree j (or, in polymerisation terminology, the number of units which have formed j bonds). The final factor in (2.1) then represents the component of a Gibbs distribution dependent on 'configuration energy', this energy being supposed to be dependent on 'first-shell' effects alone in this model. One can also include the effect of differing rates of arc-formation between and within components of the graph (i.e. differing rates of inter- and intramolecular association) but, for simplicity, we shall dispense with this.

Distribution (2.1) is a *consequence* of a model, but such an immediate one that we can view (2.1) as itself constituting the assumption and the model. The quantity

$$Q_N = \sum_{\mathcal{C}} Q_N(\mathcal{C})$$

is the partition function for this statistical model. We can view it as the unnormalised 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.. (To be more specific: Q_N would be the un-normalised p.g.f. with arguments z_j if H_j were replaced by $H_j z_j$ for all j.)

Define the function

$$H(\xi) = \sum_{j=0}^{\infty} \frac{H_j \xi^j}{j!}. \tag{2.3}$$

THEOREM 1. *Suppose* $\log H(\xi)$ *of less than quadratic growth at infinity. Then for model (2.1) the partition function* Q_N *has the evaluation*

$$Q_N = \sqrt{\frac{\kappa V}{2\pi}} \int_{-\infty}^{\infty} H(\xi)^N e^{-\kappa V \xi^2/2}\, d\xi. \tag{2.4}$$

The value $\bar{\xi}$ of ξ maximising the integrand of (2.4) is, in the thermodynamic limit, that maximising

$$J(\xi) = \rho \log H(\xi) - \kappa \xi^2/2. \tag{2.5}$$

This determines the statistics of node degree in that, for example

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

The components of the random graph would be identified as the polymer molecules themselves in the polymerisation context. What is interesting is that the evaluation (2.4) of Q_N effectively determines the polymer statistics. The natural level of description of a polymer for model (2.1) is $r = \{r_j; j = 0, 1, 2, \dots\}$ where r_j is the number of nodes in the component of degree j. Let us term such a polymer an r-mer; it will contain

$$R = \sum_j r_j$$

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

$$\sum_r R n_r = N. \tag{2.6}$$

THEOREM 2. *Suppose that* $\log\left(\sum_{N=0}^{\infty} Q_N/N!\right)$ *has the formal expansion* $\sum_r \gamma_r$ *in powers of the* H_j*, where* 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* γ_r*, conditioned by the constraint (2.6).*

This theorem has an obvious analogue in all the variants of the model which follow.

The model demonstrates a phase transition, in that, as ρ increases through a critical value ρ_c, the assembly of polymers passes from the 'sol' to the 'gel' state (the graph changes from having many modest-sized components to having a dominant component, which includes most nodes). This transition is not revealed in the behaviour of $J(\xi)$ itself, which has a single non-negative maximising value $\bar{\xi}$ for all ρ. However, it is revealed in the representation

$$J(\xi) = \min_{\theta} \left[\theta H(\xi) - \frac{\kappa \xi^2}{2} - \rho \log \theta \right]. \tag{2.7}$$

The square bracket possesses a saddle-point (min-max in (θ, ξ)) only for $\rho \ \leq \ \rho_c$.

Suppose now that the nodes of the graph can be 'coloured' in that there is a variable α at each node which can take values $\alpha = 1, 2, \ldots, p$. Let $c(a)$ denote the value of α at node a; this can be regarded as the value at a of a field defined on the graph. The configuration $\mathcal{C}$ of the graph will now specify both the arc multiplicities $s = \{s_{ab}\}$ and the field $c = \{c(a)\}$. Under probability transition rules for $\mathcal{C}$ which are Markov and reversible but otherwise rather general one deduces the generalisation of the equilibrium distribution (2.1)

$$P_N(\mathcal{C}) \propto Q_N(\mathcal{C}) = \left(\prod_{\alpha} \sigma_{\alpha}^{M_{\alpha}} \right) \left(\prod_{a,b} \frac{h_{ab}^{s_{ab}}}{s_{ab}!} \right) \left(\prod_j \prod_{\alpha} H_{\alpha j}^{N_{\alpha j}} \right). \tag{2.8}$$

Here M_{α} is the number of nodes at which the field takes the value α, and h_{ab} depends on field values at a and b in that

$$h_{ab} = \frac{1}{2V \kappa_{c(a)c(b)}}.$$

The 'degree' j is now a vector of integers $j = (j_1, j_2, \ldots, j_p)$ and $N_{\alpha j}$ is the number of nodes with state value α from which j_{β} arcs are directed to nodes of state value β $(\beta = 1, 2, \ldots, p)$.

Model (2.8) allows field dynamics on the graph, but two points should be noted. First, these dynamics are reversible, in that (2.8) is deduced from a reversible model. Second, the model is one that allows field value and graph configuration to interact, in that each affects the transition rules of the other. This is exactly what is desired for some applications (e.g. the Ising and socio-economic models discussed in Whittle 1986). However, if one were seeking to represent a neural network then (i) dynamics on the network would not be reversible, and (ii) the interaction mentioned would be an interaction of form and function. It is natural that form (the network) should influence function (the field). However, for function to influence form represents adaptation, or learning, which is a feature one may or may not wish to incorporate.

The generalisation of the partition function evaluation (2.4) is interesting. Suppose all field values are possible, so that distribution (2.8) is subject only to the constraint

$$\sum_{\alpha} \sum_{j} N_{\alpha j} = N.$$

Define the functions of a p-vector variable $\xi = (\xi_1, \xi_2, \ldots, \xi_p)$

$$H_\alpha(\xi) = \sum_j H_{\alpha j} \prod_\beta \frac{\xi_\beta^{j_\beta}}{j_\beta!}.$$

THEOREM 3. *Suppose* $\log\left(\sum_\alpha \sigma_\alpha H_\alpha(\xi)\right)$ *of less than quadratic growth at infinity. Then for model (2.8) the partition function* Q_N *has the evaluation*

$$Q_N = \left(\prod_{\alpha,\beta} \frac{\kappa_{\alpha\beta} V}{2\pi}\right)^{1/2} \int \left[\sum_\alpha \sigma_\alpha H_\alpha(\xi)\right]^N \exp\left[-\frac{V}{2} \sum_\alpha \sum_\beta \xi_{\alpha\beta}\xi_{\beta\alpha}\right] d\eta \tag{2.9}$$

where the integral is over all real η*, and* ξ, η *are related by*

$$\xi_{\alpha\beta} = \begin{cases} \frac{1}{\sqrt{2}}(\eta_{\alpha\beta} + i\eta_{\beta\alpha}) & (\beta < \alpha) \\ \eta_{\alpha\alpha} & (\beta = \alpha) \\ \frac{1}{\sqrt{2}}(\eta_{\alpha\beta} - i\eta_{\beta\alpha}) & (\beta > \alpha). \end{cases} \tag{2.10}$$

The complex form of these integrals has considerable significance, as we shall see in part.

One may now ask whether the contribution to the integral (2.9) comes essentially from a single value $\bar{\xi}$ of ξ in the thermodynamic limit, as in the 'fieldless' case $p = 1$. Indeed, this seems to be true, at a *real* value $\bar{\xi}$ derived in the following manner. Consider the real form of transformation (2.10)

$$\xi_{\alpha\beta} = \begin{cases} \frac{1}{\sqrt{2}}(\zeta_{\alpha\beta} + \zeta_{\beta\alpha}) & (\beta < \alpha) \\ \zeta_{\alpha\alpha} & (\beta = \alpha) \\ \frac{1}{\sqrt{2}}(\zeta_{\alpha\beta} - \zeta_{\beta\alpha}) & (\beta > \alpha) \end{cases} \tag{2.11}$$

and seek for the real values of the $\zeta_{\alpha\beta}$ that maximise the integrand of (2.9) for $\alpha \geq \beta$ and minimise it for $\alpha < \beta$. Relations (2.11) determine $\bar{\xi}$ in terms of the saddle-point $\bar{\zeta}$ thus located.

It is interesting that for the case $p = 2$, when nodes can adopt exactly two states (particle and antiparticle?), one is then led to consider a function of four variables, and to seek for a value at which this is maximal with respect to three of the variables, and minimal with respect to one. That is, one has three local 'space-like' axes and one local 'time-like' axis.

Criticality shows itself as before, in that the form analogous to (2.7) may or may not possess a saddle-point of the required type. However, the integrand of (2.9) may now itself possess several saddle-points of the required type. The fact that the effective saddle-point may switch as parameters change leads to new phase transitions (see Section 3).

The spin-glass models of memory considered by various authors (see e.g. Amit et al. 1985) could also be regarded as the specification of reversible dynamics upon a random graph. A comparison deserves fuller discussion than we can afford here.

3. The 'Locally Tree-Like' Property

If we view the arcs as bonds, then models (2.1) and (2.8) permit multiple bonding, self-bonding and the formation of cycles. All these effects become less probable as one approaches the thermodynamic limit. Roughly speaking, the V^{-1} dependence in (2.2) and its vector analogue ensures that the number of bonds a node forms is roughly independent of V, for given ρ. As V increases, the probability that these bonds take place with *assigned* other nodes tends to zero.

This effect also manifests itself in that the γ_r of Theorem 2 depends upon V by a factor V^{R-L}, where

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

is the number of bonds in the polymer (arcs in the component). For a polymer of given size R, polymers with cycles (i.e. $L > R-1$) are discouraged relative to the tree-form (for which $L = R-1$) as V increases. This effect can be countervailed by the combinatorial fact that the number of ways of introducing cycles increases rapidly with R.

However, one can certainly establish the following property. Consider a given node, and its *neighbourhood* of radius D (i.e. the set of nodes which are connected to the initial node by paths of length not exceeding D). Consider the subgraph $\mathcal{G}_D$ of the full graph $\mathcal{G}$ in this neighbourhood.

THEOREM 4. *$\mathcal{G}_D$ is, for given D, a tree with probability one in the thermodynamic limit.*

This we shall speak of as the 'locally tree-like' (LTL) property. The property could be stated (and will indeed be required) in stronger forms, the mildest of these being that Theorem 4 should continue to hold if D is allowed to increase to infinity at a suitable rate as the thermodynamic limit is approached.

Several authors have made an effective appeal to this property in the neural network context (see the four papers listed by Derrida and co-authors, and Hilhorst and Nijmeijer 1987). Suppose, for example, that one has directed dynamics on the graph, which do not show long-range order, in that the field values at nodes far apart on the graph are independent. Then one consequence of the LTL property and short-range order is (very roughly expressed) that field-statistics are the same whether the graph is fixed (although randomly chosen) or randomly evolving (by rules independent of the field) — the so-called *quenched* and *annealed* cases.

However, a consequence to which we shall make more explicit appeal is that, if we consider the dynamic inputs to a node via the arcs entering that node, then these will be statistically independent. This is because the subgraphs which these inputs have traversed are, with probability approaching unity, mutually disjoint out to any given radius.

As an example of this effect, suppose we consider a simplification of model (2.8) in which graph-statistics are uninfluenced by field values to the extent that the factor $\prod_j \prod_\alpha H_{j\alpha}^{N_{j\alpha}}$ is simply replaced by $\prod_j H_j^{N_j}$, as in (2.1). Let us also set

$$\kappa_{\alpha\beta}^{-1} = \psi_{\alpha\beta}$$

and define the symmetric matrix $\Psi = (\psi_{\alpha\beta})$. One can then deduce (Whittle 1989c) the following simplification of Theorem 3.

THEOREM 5. *Under the conditions stated the partition function Q_N has the evaluation*

$$Q_N \propto |\Psi|^{-1} \int \left[\sum_\alpha \sigma_\alpha H(\xi_\alpha) \right]^N \exp\left[-\tfrac{1}{2} V \xi' \Psi^{-1} \xi \right] \, d\xi. \tag{3.1}$$

Here $\xi = (\xi_1, \xi_2, \dots, \xi_p)$, the function H has the definition (2.3), and the integral in (3.1) is the complex integral ensuring the u-identity

$$\int \exp\left(u'\xi - \tfrac{1}{2}\xi' \Psi^{-1} \xi \right) \, d\xi \propto \exp\left(\tfrac{1}{2} u' \Psi u \right). \tag{3.2}$$

We can be explicit about this integral. The symmetric matrix Ψ will have a diagonal representation

$$\Psi = U' \Lambda U$$

where U is a real orthogonal matrix and Λ a diagonal matrix, with diagonal $(\lambda_1, \lambda_2, \dots, \lambda_p)$. Define $\eta = U\xi$. Then the integral in (3.1), (3.2) is along the whole real η_α axis if $\lambda_\alpha > 0$, and the whole imaginary η_α axis if $\lambda_\alpha < 0$ $(\alpha = 1, 2, \dots, p)$.

We can write the integrand of (3.1) as $\exp(VJ)$ where

$$J(\xi) = \rho \log\left(\sum_\alpha \sigma_\alpha H(\xi_\alpha) \right) - \tfrac{1}{2} \xi' \Psi^{-1} \xi.$$

One can show (op. cit.) that the principal contribution to the integral comes from a *real* value $\bar{\xi}$ where $\bar{\xi}$ is an appropriate saddle-point of J. Further,

$$\rho_\alpha \propto \sigma_\alpha H(\bar{\xi}_\alpha) \tag{3.3}$$

where ρ_α is the expected density of nodes at which the field takes value α.

Consider now the symmetric two-state case

$$\psi_{11} = \psi_{22} = \psi_1$$
$$\psi_{12} = \psi_{21} = \psi_2$$
$$\sigma_1 = \sigma_2.$$

These states could represent two possible orientations of spin at the nodes of a random lattice. The quantities ψ_1 and ψ_2 then represent strengths of bonding between nodes of like or unlike spin respectively. Let us also suppose that

$$H_j = \begin{cases} 1 & j = r+1 \\ 0 & j \neq r+1. \end{cases}$$

We are then effectively considering an Ising model on a random graph whose nodes are all constrained to have degree $r+1$. Let us also define

$$\mu = \left(\bar{\xi}_1/\bar{\xi}_2\right)^r.$$

Then the saddle-point characterisation gives the equation

$$\mu = \left(\frac{\psi_1\mu + \psi_2}{\psi_1 + \psi_2\mu}\right)^r \tag{3.4}$$

for μ, and equation (3.3) gives the characterisation

$$\mu = \left(\frac{\rho_1}{\rho_2}\right)^{r/(r+1)}. \tag{3.5}$$

But equation (3.4) is exactly the equation which occurs in Spitzer's treatment (1975) of an Ising model on an r-branching tree. The fact that we recover it is a stronger manifestation of the LTL property: a graph of constant degree $r+1$ which is a tree will be an r-branching tree.

In Spitzer's case μ had the interpretation

$$\mu = \rho_1'/\rho_2' \tag{3.6}$$

where ρ_α' is proportional to the probability that the field value at the *root* of the tree is α. The difference between (3.5), (3.6) comes from the fact that ρ_α is proportional to the probability that the field value at a *randomly chosen* node is α.

As is known from Spitzer's work, equation (3.4) can have one or several real solutions, depending upon parameter values. The transition corresponds to the transition of *magnetisation*: of alignment of spins.

4. Directed Graphs

Actual neural dynamics are directed and irreversible. Consideration of directed dynamics certainly implies that one must consider a directed graph. Models (2.1), (2.8) may have seemed to be models for a directed graph, in that s_{ab} is specified as the number of arcs from a to b. However, the distribution $P_N(\mathcal{C})$ is invariant under permutation of s_{ab} and s_{ba}, and in this sense there is no real directionality.

To achieve directionality, we modify model (2.1) to

$$P_N(\mathcal{C}) \propto Q_N(\mathcal{C}) = \left(\prod_{a,b} \frac{h^{s_{ab}}}{s_{ab}!}\right)\left(\prod_{j,k} H_{jk}^{N_{jk}}\right) \tag{4.1}$$

where h has evaluation (2.2) as before, and N_{jk} is the number of nodes of degree (j,k). By this double degree we mean that j arcs leave the node and k enter it.

We now give two of the most important conclusions from Whittle (1989b). Define the function

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

THEOREM 6. *Suppose* $\log H(\xi_1,\xi_2)$ *of less than quadratic growth at infinity. Then the partition function* Q_N *has the evaluation*

$$Q_N = \frac{2\kappa V}{\pi} \iint_{-\infty}^{\infty} H(\eta_1+i\eta_2, \eta_1-i\eta_2)^N \exp\left[-2\kappa V(\eta_1^2+\eta_2^2)\right] d\eta_1\, d\eta_2. \tag{4.2}$$

The complex form of the integral is interesting and essential. It enforces the constraint

$$\sum_j \sum_k N_{jk}(j-k) = 0 \tag{4.3}$$

that the total numbers of outgoing and incoming arcs should be equal.

THEOREM 7. *In the thermodynamic limit, the dominant contribution to integral (4.2) comes from the value* $\bar\xi = (\bar\xi_1, \bar\xi_2)$, *this being the real value that simultaneously maximises*

$$J(\xi) = \rho \log H(\xi_1,\xi_2) - 2\kappa V \xi_1 \xi_2$$

with respect to $\xi_1\xi_2$ *and minimises it with respect to* ξ_1/ξ_2.

So we find, for example, that

$$E(N_{jk}) \propto H_{jk} \frac{\bar\xi_1^j \bar\xi_2^k}{j!\,k!} \tag{4.4}$$

to within terms of smaller order in V. Expression (4.4) then defines the distribution p_{jk} of the random variable (j,k), where this is the degree of a randomly chosen node. Relation (4.3) will have the implication

$$E(j-k)=0.$$

5. Directed Dynamics

The study of directed dynamics is not yet advanced. Consider, for example, the case of a purely linear graph, for which $a=1,2,3,\ldots$ represent the consecutive nodes. This might constitute a discrete model of a nerve fibre. As ever, $c(a)$ is the value of field at node a.

A simple specification of directed dynamics would be to say that transitions in $c(a)$ were conditioned by the values of $c(a)$ and $c(a-1)$. Suppose now one wishes to evaluate the equilibrium distribution of $c(a)$ conditional on $c(1)$ for large a. This evaluation is not simple, because the relevant Markov process is infinite-dimensional, not p-dimensional. Might one expect $c(a)$ to become independent of $c(1)$ as a becomes infinite? In other words, is there long-range order or not? If one is speaking of the nerve fibre model then one would hope for long-range order, for faithful propagation along the fibre of impulses injected at $a=1$ would imply dependence at all distances.

One model for which one can conjecture conclusions is a random Jackson network. Let us consider the simplest form of such a network, for which $c(a)$ represents the number of 'quanta' at node a, and the transition $(c(a),c(b))\to(c(a)-1,c(b)+1)$, in which a quantum passes from node a to node b has intensity $c(a)s_{ab}$. In a large, fixed, closed network the stream of quanta from node a to node b will then be a Poisson stream of rate $f_{ab}=w_a s_{ab}$. Here the parameters w_a are subject to the balance conditions

$$\sum_b (f_{ab}-f_{ba})=0 \qquad (a=1,2,\ldots,N).$$

Suppose we consider a random such network with directed network statistics specified by (4.1).

Conjecture. *In the thermodynamic limit the quantum stream along a randomly chosen arc is Poisson with random rate f, where the characteristic function $\phi(\zeta)=E(e^{\zeta f})$ of f satisfies*

$$\phi(\zeta)=\frac{\sum_j\sum_k jp_{jk}\phi(\zeta/j)^k}{\sum_j\sum_k jp_{jk}}. \tag{5.1}$$

Here p_{jk} is the distribution of node degree (j, k) determined in Section 3, and both summations exclude $j = 0$.

'PROOF': Suppose the arc chosen emanates from a node of degree (j, k). By the LTL property the inputs to the node will be independent, each Poisson with a rate having characteristic function $\phi(\zeta)$. Since the sum of the k independent inputs is then divided into j streams of equal rate, this rate on the output arcs will have characteristic function $\phi(\zeta/j)^k$. Averaging over j, k we deduce the identity (5.1). In averaging we use a distribution proportional to jp_{jk}, because the fact that we have chosen an arc randomly will weight the distribution p_{jk} by the factor j. In particular, the value $j = 0$ is excluded — a point worth making, since inverse powers of j will occur if we consider coefficients of powers of ζ in expression (5.1).

Relation (5.1) gives determining equations for the moments of f. One finds that $f = 0$ unless $P(j = 0) = 0$; nodes should have zero probability of being 'absorbing' if there is to be a continuing flow. If this condition is satisfied then there is an undetermined parameter in the f-distribution: the number of quanta contained in the graph component in which the chosen arc lies.

Our 'proof' is of course not a proof, because it appeals to a stronger form of the LTL property than has been established.

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