Emergent Structures in Large Networks

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Abstract. We consider a large class of exponential random graph models and prove the existence of a region of parameter space corresponding to multipartite structure, separated by a phase transition from a region of disordered graphs.

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I. Introduction and statement of results

Complex networks, including the internet, world wide web, social networks, biological networks etc, are often modeled by probabilistic ensembles with one or more adjustable parameters; see for instance [N] and [L], and the many references therein. We will use one of these standard families, the exponential random graph models (see references in [CD], [F1], [F2], [L] and [N]), to study how multipartite structure can exist in such networks, stable against random fluctuations, in imitation of the modeling of crystalline structure of solids in thermal equilibrium.

We will be considering a large family of exponential random graph models, but for simplicity we first discuss the particular case introduced by Strauss [S] in which a graph G_N with N nodes, $E_N(G_N)$ edges and $T_N(G_N)$ triangles is probabilistically modeled with the following two-parameter probability mass function:

$$Prob_{\alpha_1,\alpha_2}(G_N) = \frac{e^{\alpha_1 E_N(G_N)+\alpha_2 T_N(G_N)}}{\text{normalization}}. \tag{1}$$

The maximum number of edges in G_N is of order N^2, and for triangles order N^3; it will be useful below if we renormalize quantities. We will work with edge and triangle *densities*, $e_N(G_N) \equiv E_N(G_N)/N^2$ and $t_N(G_N) \equiv T_N(G_N)/N^3$, and introduce new parameters β_1, β_2 so that

$$Prob_{\beta_1,\beta_2}(G_N) = \frac{e^{N^2[\beta_1 e_N(G_N)+\beta_2 t_N(G_N)]}}{\text{normalization}}. \tag{2}$$

We think of the parameters β_1, β_2 as representing mechanisms for influencing the network, as pressure and temperature do in models of materials in thermal equilibrium. Indeed it is easy to see by differentiation that if β_1 is fixed, varying β_2 will vary the mean value of the triangle density; similarly if β_2 is fixed, varying β_1 will vary the mean value of the edge density. Furthermore if the mean value $\mathbb{E}_{\beta_1,\beta_2}[e_N(G_N)]$ of $e_N(G_N)$ is fixed and $\beta_2 << 0$ then, as we will see below, the random graph will have a very low value for the mean value $\mathbb{E}_{\beta_1,\beta_2}[t_N(G_N)]$ of $t_N(G_N)$. However if $\mathbb{E}_{\beta_1,\beta_2}[e_N(G_N)]$ is fixed any variation of $\beta_2 > 0$ does not affect $\mathbb{E}_{\beta_1,\beta_2}[t_N(G_N)]$ (when N is large) [RY]. It is natural to treat separately the cases $\beta_2 < 0$ and $\beta_2 > 0$. The former is called *repulsive*, the latter *attractive*; see [RY]. The attractive case $\beta_2 > 0$ has been completely analyzed in [RY], so we concentrate here on the case with repulsion, $\beta_2 < 0$.

It is useful to analyze the phenomenon in the last paragraph, as regards $\beta_2 << 0$, in two stages. First, consider the nonprobabilistic optimization problem in which one maximizes the edge density among those graphs G_N of N nodes which have no triangles, $t_N(G_N) = 0$, corresponding intuitively to $\beta_2 = -\infty$. This was solved by Turán [T], who showed that the optimum is uniquely achieved by the complete bipartite graph with equal size parts. (The parts differ by 1 if N is odd.) One can understand the Strauss model as a two stage generalization of this optimization problem. First one considers the two-parameter set of graphs:

$$\mathcal{X}_N(e,t) \equiv \{G_N : e_N(G_N) = e, \ t_N(G_N) = t\}. \tag{3}$$

Then one studies the interaction of the two conditions, $e_N(G_N) = e$ and $t_N(G_N) = t$, through the cardinality $|\mathcal{X}_N(e,t)|$ of $\mathcal{X}_N(e,t)$. Specifically, consider the *entropy*, defined on probability mass functions ρ on the set $\mathcal{X}_N(e,t)$ by:

$$S_N(e,t)[\rho] \equiv - \sum_{j \in \mathcal{X}_N(e,t)} \rho_j \ln(\rho_j). \tag{4}$$

It is easy to prove that $S_N(e,t)$ is maximized uniquely by the uniform distribution $\tilde{\rho}(e,t)$, and that

$$S_N(e,t)[\tilde{\rho}(e,t)] = \ln(|\mathcal{X}_N(e,t)|). \tag{5}$$

If one alters the optimization so that one doesn't restrict ρ to be supported in $\mathcal{X}_N(e,t)$ but instead assumes the mean values of the two densities $e_N(G_N)$ and $t_N(G_N)$ with respect to ρ are fixed, then using Lagrange multipliers $N^2\beta_1$ for $e_N(G_N)$ and $N^2\beta_2$ for $t_N(G_N)$ in the optimization of the entropy leads to the unique optimizer given in (2), in which the β's control the mean values. It was shown in [CD] that if $\beta_2 << 0$ then in a technical sense G_N for large N looks like the complete bipartite graph with equal parts, with some edges randomly removed, but in particular $t_N(G_N) \approx 0$. On the other hand we will see that when $-1/3 < \beta_2 < 0$, the edges in G_N are roughly independent, so fixing $e_N(G_N)$ automatically fixes $t_N(G_N)$, not leaving any flexibility.

Although the networks corresponding to $\beta_2 > 0$ do not have interesting structure, there is still an interesting phenomenon in this regime, associated with sensitivity to variation of the parameters. More specifically, it was proven in [CD] that at certain values of $\beta_2 > 0$ there is a special value $\beta_1 = \beta_1(\beta_2)$ at which small changes of β_1 with β_2 fixed lead to a jump in the mean value of the density $e_N(G_N)$. Furthermore, it was shown in [RY] that *all* singular behavior of the distributions is concentrated on a certain curve $\beta_1 = q(\beta_2)$. (We will clarify the meaning of "singular" below.)

We are interested here in the more complicated case $\beta_2 < 0$. As noted above, if $|\beta_2| < 1/3$ then for large N the graph will have approximately independent edges; in particular we will show below that the difference

$$\left(\mathbb{E}_{\beta_1,\beta_2}[e_N(G_N)] \right)^3 - \mathbb{E}_{\beta_1,\beta_2}[t_N(G_N)] \tag{6}$$

has limit 0 as $N \to \infty$. However one might expect from Turán's theorem that for any fixed β_1 (or mean value of $e_N(G_N)$), once β_2 is sufficiently negative the graph should look bipartite, and so the difference should be roughly $(\mathbb{E}_{\beta_1,\beta_2}[e_N(G_N)])^3 \neq 0$. We prove this below but furthermore prove that the qualitative structural change occurs abruptly: in order to accomplish the change, for each β_1 the distribution exhibits "singular behavior" at some $\beta_2 < 0$. Before clarifying the meaning of "singular" we generalize the role played by triangles in the Strauss model to the following two-parameter *exponential random graph model*:

$$\mathbb{P}_{\beta_1,\beta_2}(G_N) = e^{N^2[\beta_1 t(H_1, G_N) + \beta_2 t(H_2, G_N) - \psi_N(\beta_1,\beta_2)]}, \tag{7}$$

where: H_1 is an edge, H_2 is any finite simple graph with $k \geq 2$ edges, and $t(H_i, G_N)$ is the density of graph homomorphisms $H \to G_N$:

$$t(H_i, G_N) = \frac{|\hom(H_i, G_N)|}{|V(G_N)|^{|V(H_i)|}}, \tag{8}$$

with $V(\cdot)$ denoting a vertex set. The term $\psi_N(\beta_1, \beta_2)$ gives the probability normalization.

Fundamental to our results are questions of analyticity of the normalization in (7), which we discuss next. (See [KP] for elementary properties of real analytic functions of several real variables.) An explicit formulation of the normalization is:

$$\psi_N(\beta_1, \beta_2) \equiv \frac{1}{N^2} \ln \Big(\sum_{G_N} e^{N^2[\beta_1 t(H_1, G_N) + \beta_2 t(H_2, G_N)]} \Big). \tag{9}$$

It is proven in [CD] that

$$\psi_\infty(\beta_1, \beta_2) \equiv \lim_{N \to \infty} \psi_N(\beta_1, \beta_2) \tag{10}$$

exists for all β_1, β_2. It is also noted in [RY] that at points where ψ_∞ is analytic,

$$\frac{\partial}{\partial \beta_j} \psi_\infty(\beta_1, \beta_2) = \lim_{N \to \infty} \frac{\partial}{\partial \beta_j} \psi_N(\beta_1, \beta_2), \tag{11}$$

that is, the partial derivatives commute with the limit $N \to \infty$. Partial derivatives of ψ_∞, when they exist, give information on the large-N mean and variance of the densities $t(H_1, G_N)$ and $t(H_2, G_N)$ (see [RY]) and it is standard in the corresponding modeling of materials, in part for this reason, to define phases and phase transitions as follows (see [FR]).

Definition. A phase is an open connected region of the parameter space $\{(\beta_1, \beta_2)\}$ which is maximal for the condition that $\psi_\infty(\beta_1, \beta_2)$ is analytic. There is a phase transition at (β_1^*, β_2^*) if (β_1^*, β_2^*) is a boundary point of an open set on which ψ_∞ is analytic, but ψ_∞ is not analytic at (β_1^*, β_2^*).

So in the above, "singular" meant nonanalytic. In this notation our main result is:

Theorem. Assume the chromatic number $\chi(H_2)$ of H_2 is at least 3. Then there is a curve $\beta_2 = s(\beta_1)$, $-\infty < \beta_1 < \infty$, in the lower half plane ($\beta_2 < 0$), such that the model exhibits a phase transition on the curve.

II. Proof of the theorem

Let k be the number of edges in H_2. We write $\mathbb{P}$ for the probability mass function $\mathbb{P}_{\beta_1, \beta_2}$ given by equation (7), and $\mathbb{E}$ for the expectation $\mathbb{E}_{\beta_1, \beta_2}$.

By Theorem 6.1 in [CD], the analyticity method of the proof of Theorem 3.10 in [RY] can be immediately extended to prove that $\psi_\infty(\beta_1, \beta_2)$ is analytic in the real variables β_1 and β_2 when $|\beta_2| < 2/[k(k-1)]$. Our proof will be by contradiction, so we assume from here on that $\psi_\infty(\beta_1, \beta_2)$ is analytic in β_1 and β_2 on the *entire* half line $L = \{(\beta_1^*, \beta_2) : \beta_2 < 0\}$, where β_1^* is arbitrary but fixed. We will find a contradiction, which will prove the existence of the curve $\beta_2 = s(\beta_1)$.

Consider the function

$$C(\beta_1, \beta_2) := \left(\frac{\partial \psi_\infty}{\partial \beta_1}(\beta_1, \beta_2) \right)^k - \frac{\partial \psi_\infty}{\partial \beta_2}(\beta_1, \beta_2) \tag{12}$$

Note that $C(\beta_1, \beta_2)$ is analytic on L, since $\psi_\infty(\beta_1, \beta_2)$ is.

Proposition 3.2 in [RY] proves, for all $\beta_2 < 0$, there is a unique solution $u^*(\beta_1, \beta_2)$ to the optimization of

$$\beta_1 u + \beta_2 u^k - \frac{1}{2} u \ln u - \frac{1}{2}(1 - u) \ln(1 - u) \tag{13}$$

for $u \in [0, 1]$. Then from Theorems 6.1 and 4.2 in [CD] we can use the same argument as used to prove equations (33) and (34) in [RY] to prove, for $-2/[k(k-1)] < \beta_2 < 0$:

$$\frac{\partial}{\partial \beta_1} \psi_\infty(\beta_1, \beta_2) = \lim_{N \to \infty} \mathbb{E}\{t(H_1, G_N)\} = t(H_1, u^*) = u^*(\beta_1, \beta_2), \tag{14}$$

$$\frac{\partial}{\partial \beta_2} \psi_\infty(\beta_1, \beta_2) = \lim_{N \to \infty} \mathbb{E}\{t(H_2, G_N)\} = t(H_2, u^*) = (u^*(\beta_1, \beta_2))^k. \tag{15}$$

It follows that $C(\beta_1^*, \beta_2) = (t(H_1, u^*))^k - t(H_2, u^*) \equiv 0$ for $|\beta_2| < 2/[k(k-1)]$. Since a function of one variable which is analytic on L and constant on a subinterval must be constant on L, it follows that

$$C(\beta_1^*, \beta_2) \equiv 0 \text{ on } L. \tag{16}$$

We next obtain a contradiction to (16), but first we need some notation; see [CD], [BCL] and [L] for discussions of the ideas behind these terms, which basically provide the framework for "infinite volume limits" for graphs, in analogy with the infinite volume limit in statistical mechanics [R].

To each graph G on N nodes we associate the following function on $[0, 1]^2$:

$$f^G(x, y) = 1 \text{ if } (\lceil Nx \rceil, \lceil Ny \rceil) \text{ is an edge of } G, \text{ and } f^G(x, y) = 0 \text{ otherwise.} \tag{17}$$

We define $\mathcal{W}$ to be the space of measurable functions $h : [0, 1]^2 \to [0, 1]$ which are symmetric: $h(x, y) = h(y, x)$, for all x, y. For $h \in \mathcal{W}$ we define

$$t(H, h) \equiv \int_{[0,1]^\ell} \prod_{(i,j) \in E(H)} h(x_i, x_j) \, dx_1 \cdots dx_\ell. \tag{18}$$

where $E(H)$ is the edge set of H, and $\ell = |V(H)|$ is the number of nodes in H, and note that for a graph G, $t(H, G)$ defined in (8) has the same value as $t(H, f^G)$. We define an equivalence relation on $\mathcal{W}$ as follows: $f \sim g$ if and only if $t(H, f) = t(H, g)$ for every simple graph H. Elements of the quotient space, $\tilde{\mathcal{W}}$, are called "graphons", and the class containing $h \in \mathcal{W}$ is denoted $\tilde{h}$. The space $\tilde{W}$ is compact [L].

On $\tilde{\mathcal{W}}$ we define a metric in steps as follows. First, on $\mathcal{W}$ we define

$$d_\square(f, g) \equiv \sup_{S,T \subseteq [0,1]} \left| \int_{S \times T} [f(x, y) - g(x, y)] \, dx dy \right|. \tag{19}$$

Let Σ be the space of measure preserving bijections σ of $[0, 1]$, and for f in $\mathcal{W}$ and $\sigma \in \Sigma$ define $f_\sigma(x, y) \equiv f(\sigma(x), \sigma(y))$. Using this we define a metric on $\tilde{W}$ by

$$\delta_\square(\tilde{f}, \tilde{g}) \equiv \inf_{\sigma_1, \sigma_2} d_\square(f_{\sigma_1}, g_{\sigma_2}). \tag{20}$$

Next we need a few terms associated with ψ_∞. Define on $[0, 1]$:

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$$I(u) \equiv \frac{1}{2} u \ln(u) + \frac{1}{2}(1-u)\ln(1-u) \tag{21}$$

and on $\tilde{\mathcal{W}}$:

$$I(\tilde{h}) \equiv \int_{[0,1]^2} I(h(x,y)) \, dxdy. \tag{22}$$

Also on $\tilde{\mathcal{W}}$ we define:

$$T(\tilde{h}) \equiv \beta_1 t(H_1, h) + \beta_2 t(H_2, h). \tag{23}$$

The above are relevant because it is proven in Theorem 3.1 of [CD] that $\psi_\infty(\beta_1, \beta_2)$ is the solution of an optimization problem:

$$\psi_\infty(\beta_1, \beta_2) = \sup_{\tilde{h} \in \tilde{\mathcal{W}}} [T(\tilde{h}) - I(\tilde{h})]. \tag{24}$$

Furthermore, from Theorem 3.2 of [CD] one has some control on the asymptotic behavior as $N \to \infty$:

$$\delta_\square[\tilde{G}_N, \tilde{F}^*(\beta_1, \beta_2)] \to 0 \text{ in probability as } N \to \infty, \tag{25}$$

where $\tilde{F}^*(\beta_1, \beta_2)$ is the (compact) subset of $\tilde{\mathcal{W}}$ on which $T - I$ is maximized, and $\tilde{G}_N \equiv \tilde{f}^{G_N}$.

We now return to our proof. Fix $\epsilon > 0$ and $i \in \{1, 2\}$. Recall $\beta_1 = \beta_1^*$ is fixed arbitrarily. Write $\tilde{F}^*(\beta_2)$ for the set $\tilde{F}^*(\beta_1, \beta_2) \subset \tilde{W}$ defined above. Using Theorem 7.1 in [CD], choose β_2' sufficiently negative so that for every $\beta_2 < \beta_2'$

$$\sup_{\tilde{f} \in \tilde{F}^*(\beta_2)} \delta_\square(\tilde{f}, p\tilde{g}) < \frac{\epsilon}{3k}. \tag{26}$$

Using Theorem 3.2 in [CD], choose $N_0(\beta_2)$ such that $N > N_0(\beta_2)$ implies

$$\mathbb{P}\left[\delta_\square(\tilde{G}_N, \tilde{F}^*(\beta_2)) \geq \frac{\epsilon}{3k}\right] < \frac{\epsilon}{3k}. \tag{27}$$

Let $A_{\epsilon,N} = \{G_N : \delta_\square(\tilde{G}_N, \tilde{F}^*(\beta_2)) < \epsilon/(3k)\}$. By compactness of $\tilde{F}^*(\beta_2)$ we may choose $\tilde{h}_{G_N} \in \tilde{F}^*(\beta_2)$ corresponding to each $G_N \in A_{\epsilon,N}$ such that

$$\delta_\square(\tilde{G}_N, \tilde{h}_{G_N}) < \frac{\epsilon}{3k}. \tag{28}$$

Write $\mathbb{E}|_A$ for the restriction of the expectation to the set A. Using (26) and (28) we have that

$$\mathbb{E}|_{A_{\epsilon,N}}[\delta_\square(\tilde{G}_N, p\tilde{g})] = \sum_{G_N \in A_{\epsilon,N}} \delta_\square(\tilde{G}_N, p\tilde{g})\mathbb{P}(G_N)$$

$$\leq \sum_{G_N \in A_{\epsilon,N}} \left[\delta_\square(\tilde{G}_N, \tilde{h}_{G_N}) + \delta_\square(\tilde{h}_{G_N}, p\tilde{g})\right]\mathbb{P}(G_N)$$

$$< \sum_{G_N \in A_{\epsilon,N}} \left[\frac{\epsilon}{3k} + \frac{\epsilon}{3k} \right] \mathbb{P}(G_N) \leq \frac{2\epsilon}{3k} \tag{29}$$

for $N > N_0(\beta_2)$. Now write $\bar{A}_{\epsilon,N}$ for the complement of $A_{\epsilon,N}$. Then by Lemma 3.12 in [RY], equation (29), and the fact that $\delta_\square(\cdot, \cdot) \leq 1$,

$$\left| \mathbb{E}\left[t(H_i, G_N) \right] - t(H_i, pg) \right|$$

$$\leq \mathbb{E}\left[|t(H_i, G_N) - t(H_i, pg)| \right]$$

$$\leq k \cdot \mathbb{E}\left[\delta_\square(\tilde{G}_N, p\tilde{g}) \right]$$

$$= k \cdot \left(\mathbb{E}|_{A_{\epsilon,n}} \left[\delta_\square(\tilde{G}_N, p\tilde{g}) \right] + \mathbb{E}|_{\bar{A}_{\epsilon,N}} \left[\delta_\square(\tilde{G}_N, p\tilde{g}) \right] \right)$$

$$\leq k \cdot \left(\frac{2\epsilon}{3k} + \frac{\epsilon}{3k} \right) = \epsilon \tag{30}$$

for $N > N_0(\beta_2)$. Using the identity

$$\frac{\partial \psi_N}{\partial \beta_i}(\beta_1^*, \beta_2) = \mathbb{E}\left[t(H_i, G_N) \right] \tag{31}$$

along with (11), we may take the limit $N \to \infty$ in (30) to obtain

$$\left| t(H_i, pg) - \frac{\partial \psi_\infty}{\partial \beta_i}(\beta_1^*, \beta_2) \right| < \epsilon. \tag{32}$$

Since $\epsilon > 0$ was arbitrary,

$$\lim_{\beta_2 \to -\infty} \frac{\partial \psi_\infty}{\partial \beta_i}(\beta_1^*, \beta_2) = t(H_i, pg). \tag{33}$$

Direct computation using equation (2.10) in [CD] yields:

$$t(H_2, pg) = 0 \quad \text{and} \quad t(H_1, pg) = \frac{e^{2\beta_1}(\chi(H) - 2)}{(1 + e^{2\beta_1})(\chi(H) - 1)} > 0. \tag{34}$$

Now, by combining (12) with (33)-(34) we find $\lim_{\beta_2 \to -\infty} C(\beta_1^*, \beta_2) > 0$, in contradiction with (16), which proves the theorem. ∎

III. Conclusion

Consider any of the two-parameter exponential random graph models with repulsion covered by our theorem. Define the 'high energy phase' of the parameter space $\{(\beta_1, \beta_2) \mid \beta_2 < 0\}$ as that domain of analyticity of $\psi_\infty(\beta_1, \beta_2)$ which contains the strip $-2/[k(k-1)] < \beta_2 < 0$. The order parameter $C(\beta_1, \beta_2)$ is identically zero in this phase (as one can see for instance by connecting by an analytic curve any given point in the open, connected phase to a point in the strip, and complexifying). We have proven that this phase is separated from the low energy regime in the sense that for each β_1 there is some β_2' such that the segment $\{(\beta_1, \beta_2) \mid \beta_2 < \beta_2'\}$ does not intersect the phase. Our proof is based on the traditional modeling of equilibrium statistical mechanics using analyticity and an order parameter [R], [K], [Y]. And we emphasize

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that this method could not have been used to prove the transition found in [RY] for attractive exponential random graph models since there is a critical point for that transition: indeed there is only one phase.

In comparison with traditional models from statistical mechanics, exponential random graph models could be thought of as either infinite range, or infinite dimensional, which suggests a relation with 'mean field theories' [K], [Y]. Mean field theories grew out of the work of van der Waals, who obtained a general description of fluids by adroitly replacing the interaction between each molecule and the rest of the fluid by an average or mean field, among other things losing track of the spatial separation of the interacting molecules. This proved to be a useful approximation to understand gas/liquid phase transitions in which the most relevant part of the particle interaction is a (long range) attraction. It is not too surprising that exponential random graph models with attractive interaction could therefore yield a phase transition like that of the liquid/gas transition, as was shown in [RY]. In the present paper we obtain a transition more like a fluid/solid transition, in which there is a change of 'symmetry' from disordered to multipartite. It is less intuitive to use a long range repulsion to model a solid/fluid transition, so the materials analogy of our models with repulsion is less compelling than for our models with attraction. Therefore the relation of these models with repulsion to mean field approximations might be particularly illuminating.

There remain many open questions. Perhaps the most pressing is the character of the singularity of $\psi_\infty(\beta_1, \beta_2)$ at the boundary of the high energy phase. In the attractive case there is only one phase but there are jump discontinuities, in the first derivatives of $\psi_\infty(\beta_1, \beta_2)$ (namely the average edge and energy densities), across a curve where two regions of the phase abut, while the edges are independent throughout the phase [RY]. We do not know the nature of the singularity at the boundary of the high energy phase for the case of repulsion studied in this paper, though we expect the first derivatives of $\psi_\infty(\beta_1, \beta_2)$ to be discontinuous across the boundary. In analogy with equilibrium materials there may be multipartite phases with different numbers of parts at low energy, though this may require more complicated interactions [CD].

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