

Ground states for exponential random graphs

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We propose a perturbative method to estimate the normalization constant in exponential random graph models as the weighting parameters approach infinity. As an application, we give evidence of discontinuity in natural parametrization along the critical directions of the edge-triangle model. Joint work with Rajinder Mavi.

Outline

- Exponential random graphs; Graph limit theory
- The edge-triangle model; Perturbation analysis

Erdős-Rényi graph $G(n, \rho)$: n vertices; include edges independently with probability ρ .

Empirical study of network structure shows that “**transitivity** is the outstanding feature that differentiates observed data from a pattern of random ties”. Modeling transitivity (or lack thereof) in a way that makes statistical inference feasible however has proved to be rather difficult.

One direction is using **exponential random graph** models. They are particularly useful when one wants to construct models that resemble observed networks as closely as possible, but without going into detail of the specific process underlying network formation.

Probability space: The set $\mathcal{G}_n$ of all simple graphs G_n on n vertices.
Probability mass function:

$$\mathbb{P}_n^\beta(G_n) = \exp \left(n^2(\beta_1 t(H_1, G_n) + \dots + \beta_k t(H_k, G_n) - \psi_n^\beta) \right).$$

- $\beta_1, \dots, \beta_k$ are real parameters and $H_1, \dots, H_k$ are pre-chosen finite simple graphs. Each H_i has vertex set $V(H_i) = \{1, \dots, k_i\}$ and edge set $E(H_i)$. By convention, we take H_1 to be a single edge.
- Graph homomorphism $\text{hom}(H_i, G_n)$ is a random vertex map $V(H_i) \rightarrow V(G_n)$ that is edge-preserving. Homomorphism density $t(H_i, G_n) = \frac{|\text{hom}(H_i, G_n)|}{|V(G_n)|^{|V(H_i)|}}$.
- Normalization constant:

$$\psi_n^\beta = \frac{1}{n^2} \log \sum_{G_n \in \mathcal{G}_n} \exp \left(n^2(\beta_1 t(H_1, G_n) + \dots + \beta_k t(H_k, G_n)) \right).$$

$\beta_i = 0$ for $i \geq 2$:

$$\begin{aligned}\mathbb{P}_n^\beta(G_n) &= \exp\left(n^2(\beta_1 t(H_1, G_n) - \psi_n^\beta)\right) \\ &= \exp\left(2\beta_1 |E(G_n)| - n^2 \psi_n^\beta\right).\end{aligned}$$

Erdős-Rényi graph $G(n, \rho)$,

$$\mathbb{P}_n^\rho(G_n) = \rho^{|E(G_n)|} (1 - \rho)^{\binom{n}{2} - |E(G_n)|}.$$

Include edges independently with probability $\rho = e^{2\beta_1} / (1 + e^{2\beta_1})$.

$$\exp(n^2 \psi_n^\beta) = \sum_{G_n \in \mathcal{G}_n} \exp(2\beta_1 |E(G_n)|) = \left(\frac{1}{1 - \rho}\right)^{\binom{n}{2}}.$$

What happens with general β_i ?

Problem: Graphs with different numbers of vertices belong to different probability spaces!

Solution: Theory of graph limits (graphons)! (Lovász and coauthors; earlier work of Aldous and Hoover)

Graphon space $\mathcal{W}$ is the space of all symmetric measurable functions $h(x, y)$ from $[0, 1]^2$ into $[0, 1]$. The interval $[0, 1]$ represents a 'continuum' of vertices, and $h(x, y)$ denotes the probability of putting an edge between x and y .

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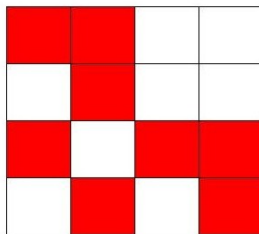
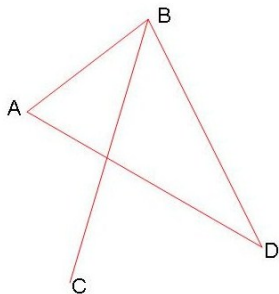
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Example: Erdős-Rényi graph $G(n, \rho)$, $h(x, y) = \rho$.

Example: Any $G_n \in \mathcal{G}_n$,

$$h(x, y) = \begin{cases} 1, & \text{if } (\lceil nx \rceil, \lceil ny \rceil) \text{ is an edge in } G_n; \\ 0, & \text{otherwise.} \end{cases}$$



Large deviation and Concentration of measure:

$$\psi^\beta = \lim_{n \rightarrow \infty} \psi_n^\beta = \max_{h \in \mathcal{W}} \left(\beta_1 t(H_1, h) + \dots + \beta_k t(H_k, h) - \int_{[0,1]^2} I(h) dx dy \right),$$

where:

$$t(H_i, h) = \int_{[0,1]^{k_i}} \prod_{(i,j) \in E(H_i)} h(x_i, x_j) dx_1 \dots dx_{k_i},$$

and $I : [0, 1] \rightarrow \mathbb{R}$ is the function

$$I(u) = \frac{1}{2} u \log u + \frac{1}{2} (1 - u) \log(1 - u).$$

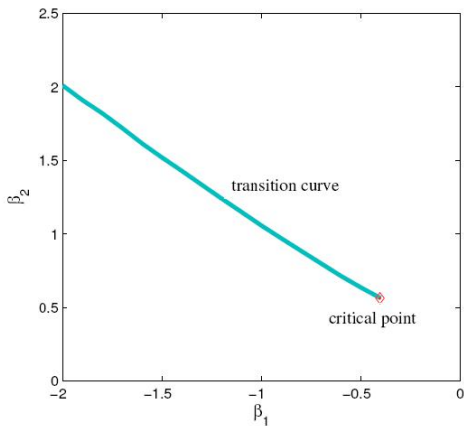
Let F^* be the set of maximizers. G_n lies close to F^* with high probability for large n .

$\beta_2, \dots, \beta_k \geq 0$: G_n behaves like the Erdős-Rényi graph $G(n, u^*)$, where $u^* \in [0, 1]$ maximizes

$$\beta_1 u + \dots + \beta_k u^{|E(H_k)|} - \frac{1}{2} u \log u - \frac{1}{2} (1 - u) \log(1 - u).$$

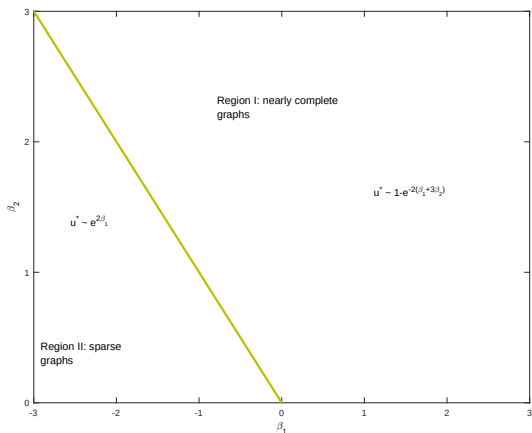
(Chatterjee and Varadhan; Chatterjee and Diaconis; Häggström and Jonasson; Bhamidi, Bresler, and Sly)

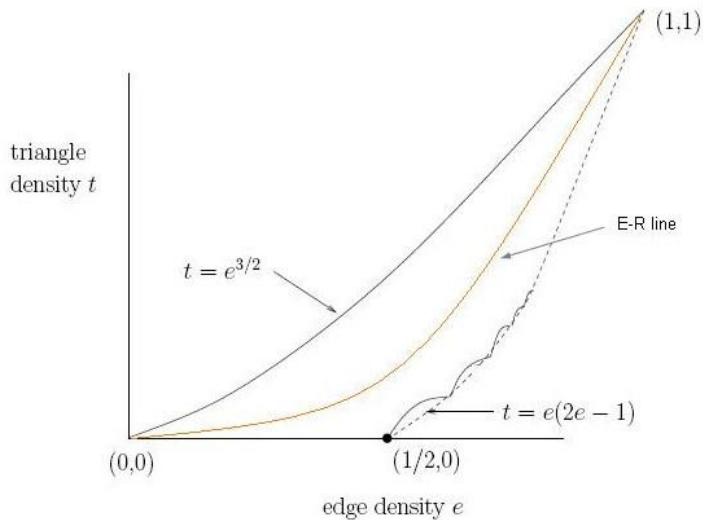
Take H_1 a single edge and H_2 a triangle. Fix the edge parameter β_1 . Let the triangle parameter β_2 vary from 0 to ∞ . Then ψ^{β_1, β_2} loses its analyticity at at most one value of β_2 . (Radin and Y)
 Gas/liquid transition:



Critical point is $(\frac{1}{2} \log 2 - \frac{3}{4}, \frac{9}{16})$.

The line $\beta_1 = -\beta_2$ is of particular importance. The edge-triangle model **transitions** from an Erdős-Rényi type almost complete graph ($\beta_1 > -\beta_2$) to an Erdős-Rényi type almost empty graph ($\beta_1 \leq -\beta_2$). (Y)





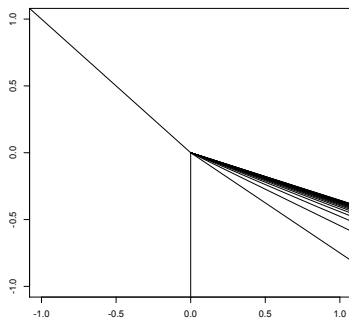
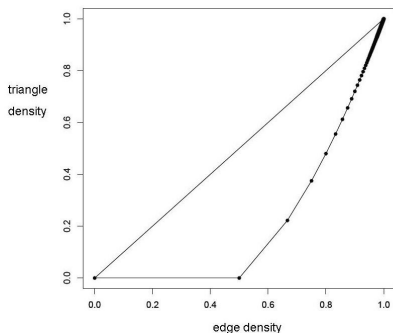
Feasible edge-triangle densities.

Upper bound: complete subgraph on $e^{1/2}n$ vertices.

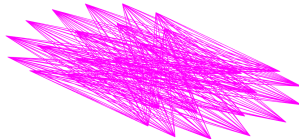
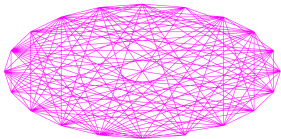
Lower bound for $e \leq 1/2$: complete bipartite graph with $1 - 2e$ fraction of edges randomly deleted.

Lower bound for $e \geq 1/2$: complicated scallop curves where boundary points are complete multipartite graphs. (Razborov and others)

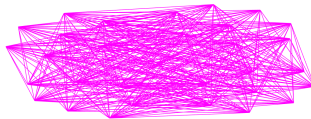
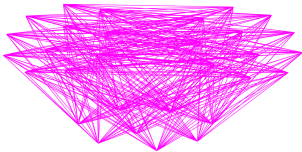
Take $\beta_1 = a\beta_2 + b$. Fix a and b . Let $n \rightarrow \infty$ and then let $\beta_2 \rightarrow -\infty$. G_n exhibits **quantized behavior**. (Y, Rinaldo, and Fadnavis; related work in Handcock; Rinaldo, Fienberg, and Zhou)



The infinite polytope.



emergence of multipartite structures



Problem: Along the critical directions o_k , a typical graph sampled from the edge-triangle model may behave like either a Turán graphon with $k + 1$ classes or a Turán graphon with $k + 2$ classes, with **no clear preference**.

Solution: Refined perturbation approximation! (Mavi and Y)

Take a finite simple graph H with vertex set $V(H)$ and edge set $E(H)$. For each $(r, s) \in E(H)$ and each pair of points $x_r, x_s \in [0, 1]$, define

$$\Delta_{H,r,s} f(x_r, x_s) = \int_{[0,1]^{|V(H) \setminus \{r,s\}|}} \prod_{\substack{(r',s') \in E(H) \\ (r',s') \neq (r,s)}} f(x_{r'}, x_{s'}) \prod_{\substack{v \in V(H) \\ v \neq r,s}} dx_v.$$

This may be identified with the homomorphism density $t(H, h)$, if we remove edge (r, s) from H and do not integrate out the associated vertices x_r and x_s .

For $(x, y) \in [0, 1]$, define

$$\Delta_H f(x, y) = \sum_{(r,s) \in E(H)} \Delta_{H,r,s} f(x, y).$$

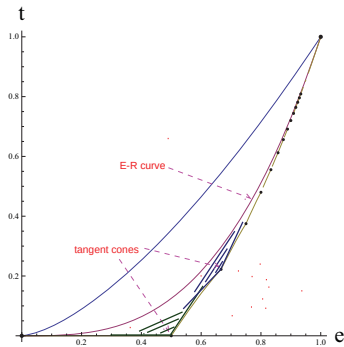
This corresponds to the total homomorphism density generated after all possible ways of removing one edge from H .

Assumption: $\Delta_H f = \alpha \chi_A + \beta \chi_B$, where A and B are complement sets.

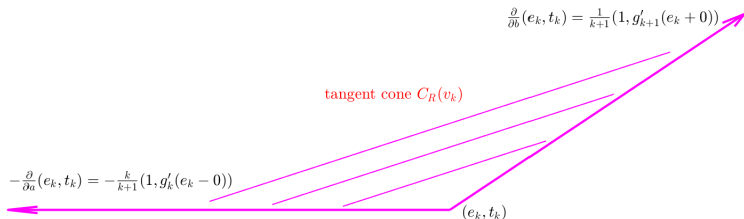
Example: Let K_k be a complete graph on k vertices. Denote $f^{K_{k+1}}$ by T_k (Turán graphon with $k+1$ classes) and $\chi_{[0,1]^2} - f^{K_{k+1}}$ by D_k . Then T_k and D_k are indicator functions associated with sets of measure $k/(k+1)$ and $1/(k+1)$, respectively.

$$\Delta_{K_2} T_k \equiv 1.$$

$$\Delta_{K_3} T_k = 3 \int_{[0,1]} T_k(x, z) T_k(y, z) dz = \frac{3(k-1)}{k+1} T_k + \frac{3k}{k+1} D_k.$$



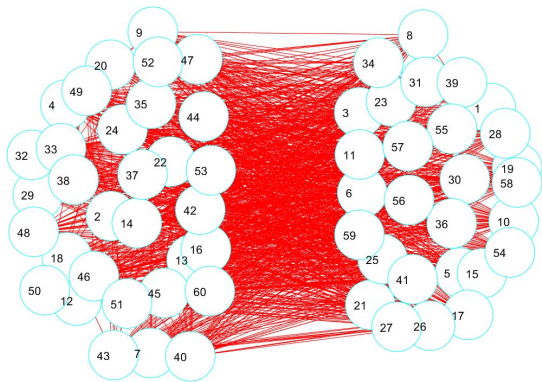
Region of attainable edge (e) and triangle (t) densities for graphons revisited. The tangent cones at complete bipartite graphon (Turán graphon with 2 classes) and complete tripartite graphon (Turán graphon with 3 classes) are displayed.



The (internal) tangent cone $C_R(v_k)$, consisting of graphons of the type $X_h = aT_k + bD_k$. Taking $a = 1, b = 0$ gives the Turán graphon with $k + 1$ classes, whose edge-triangle densities are $v_k = (e_k, t_k)$. Here $g'_k(e_k - 0)$ and $g'_k(e_k + 0)$ indicate the left and right hand side derivatives of the lower boundary curve g_k at e_k , respectively.

Let h be the true maximizing graphon for the edge-triangle model: $H_1 = K_2$ and $H_2 = K_3$. T_k and h become arbitrarily close as $|\beta| \rightarrow \infty$.

Consider the averaged graphon perturbation $X_h = aT_k + bD_k$, viewed as a **flattened out version** of h . We may justify that for suitably chosen values of a and b , $t(H_i, X_h)$ gives a better asymptotic approximation for $t(H_i, h)$ than $t(H_i, T_k)$, hence removing the ambiguity.



A simulated realization of the exponential random graph model on 60 nodes with edges and triangles as sufficient statistics, where $\beta = (10, -7.5)$ diverges along the critical direction $\alpha_1 = (1, -0.75)$. The simulated graph displays bipartite feature with edge density 0.557.

Thanks For Having Me Back!:)