RECIPROCITY IN DIRECTED NETWORKS

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Abstract. Reciprocity is an important statistics in directed networks and has been widely used in the modeling of World Wide Web, email, social, and other complex networks. In this paper, we take a statistical physics point of view and study the limiting entropy and free energy densities from the microcanonical ensemble, the canonical ensemble, and the grand canonical ensemble whose sufficient statistics are given by edge and reciprocal densities. The sparse case is also studied for the grand canonical ensemble. Further results concerning reciprocal triangle and star densities will likewise be discussed.

1. Introduction

Reciprocity measures the tendency of vertex pairs to form mutual connections between each other and is an important object to study in complex networks, such as email networks, see e.g. Newman et al. [25], World Wide Web, see e.g. Albert et al. [1], World Trade Web, see e.g. Gleditsch [14], social networks, see e.g. Wasserman and Faust [34], and cellular networks, see e.g. Jeong et al. [16]. In networks that aggregate temporal information such as email or social networks, reciprocity provides a measure of the simplest feed-back process occurring in the network, i.e., the tendency of one stimulus, a vertex, to respond to another stimulus, another vertex. In general, reciprocity is the main quantity characterizing feasible dyadic patterns, namely possible types of connections between two vertices. Reciprocity is important because most complex networks are directed. One example is the email network. Just because user B's email address appears in user A's address book does not necessarily mean that the reverse is also true, although it often is, see e.g. Newman et al. [25]. Another example is the social network. Reciprocity captures a basic way in which different forms of interaction take place on a social network like Twitter. When two users A and B interact as peers, one expects that messages will be exchanged between them in both directions. However, if user A sends messages to user B, who is a celebrity or news source, it is likely that user B will not send messages in return, see e.g. Cheng et al. [8]. Therefore, it is not enough to just understand the *edge density* of a directed network, the *reciprocal density* needs to be studied as well. In Garlaschelli and Loffredo [12], it was discovered that detecting nontrivial patterns of reciprocity can reveal mechanisms and organizing principles that help understand the topology of the observed network. They also proposed a measure of reciprocity and studied how strong the reciprocity is for different complex networks and found that reciprocity is strongest in the World Trade Web. People often treat complex networks as undirected ones for simplicity.

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Reciprocity can help quantify the information loss induced by projecting a directed network into an undirected one. Using the knowledge of reciprocity, significant directed information can be retrieved from an undirected projection, and the error introduced when a directed network is treated as undirected may be estimated, see e.g. Garlaschelli and Loffredo [13].

Directed networks consisting of n nodes can be modeled by directed graphs on n vertices, where a graph is represented by a matrix $X = (X_{ij})_{1\leq i,j\leq n}$ with each $X_{ij} \in \{0,1\}$. Here, $X_{ij} = 1$ means there is a directed edge from vertex i to vertex j; otherwise, $X_{ij} = 0$. We assume that $(X_{ii})_{1\leq i\leq n} = 0$ so that there are no self loops. Denote by $\mathbb{P}$ the uniform probability measure under which $(X_{ij})_{1\leq i\neq j\leq n}$ are i.i.d. Bernoulli random variables taking values 1 and 0 each with probability $\frac{1}{2}$. The corresponding expectation is denoted by $\mathbb{E}$. Give the set of such graphs the probability

$$\mathbb{P}_n^{\beta_1,\beta_2}(X) = Z_n(\beta_1,\beta_2)^{-1} \exp\left[n^2\left(\beta_1 e(X) + \beta_2 r(X)\right)\right], \tag{1.1}$$

where

$$e(X) := n^{-2} \sum_{1\leq i,j\leq n} X_{ij}, \quad r(X) := n^{-2} \sum_{1\leq i,j\leq n} X_{ij}X_{ji}, \tag{1.2}$$

and $Z_n(\beta_1,\beta_2)$ is the appropriate normalization. Note that $e(X)$ and $r(X)$, defined in (1.2), respectively represent the directed *edge density* and the *reciprocal density*.

In the literature, X_{ij} and $X_{ij}X_{ji}$ are sometimes referred to as the *single edge* and the *reciprocal edge*. This belongs to class of exponential random graph models called p_1 models of Holland and Leinhardt [15]. Further extensions include p_2 models, see e.g. Lazega and Van Duijin [19] and Van Duijin et al. [33]. More general types of exponential models have also been introduced and studied. See Besag [4], Newman [24], Rinaldo et al. [30], Robins et al. [31], Snijders et al. [32], Wasserman and Faust [34], and Fienberg [10, 11] for history and a review of developments. The exponential random graph models have popular counterparts in statistical physics: a hierarchy of models ranging from the *grand canonical ensemble*, the *canonical ensemble*, to the *microcanonical ensemble*, with particle density and energy density in place of $e(X)$ and $r(X)$, and temperature and chemical potential in place of β_1 and β_2. In the grand canonical ensemble, the reciprocal model (1.1) in this case, no prior knowledge of the graph is assumed. In the canonical ensemble, partial information of the graph is given. For instance, the edge density of the graph is close to 1/2 or the reciprocal density is close to 1/4. In the microcanonical ensemble, complete information of the graph is observed beforehand, say in the reciprocal model, both the edge density and the reciprocal density are specified.

It is well-known that models in this hierarchy have a very simple relationship involving Legendre transforms and, more importantly, the free energy density (of the grand canonical ensemble), the conditional free energy density (of the canonical ensemble), and the entropy density (of the microcanonical ensemble) encode important information of a random graph drawn from the model. Since real-world networks are often very large in size, this justifies our interest in studying the asymptotics of these quantities, which have received exponentially growing attention in recent years. See e.g. Aristoff and Zhu [2, 3], Chatterjee and Dembo [5], Chatterjee and Diaconis [6], Kenyon et al. [17], Kenyon and Yin [18], Lubetzky and Zhao [22, 23], Radin and Sadun [27, 28], Radin et al. [26], Radin and Yin [29], Yin [35], Yin et al. [36], and Zhu [38]. It may be worth pointing out that most of these papers utilize the theory of graph limits as developed by Lovász and coworkers [20, 21].

The rest of this paper is organized as follows. In Section 2 we derive the exact expression for the normalization constant (partition function) of the reciprocal model (the grand canonical ensemble) and analyze the asymptotic features of its associated microcanonical ensemble. Our main results are: an exact expression for the limiting entropy density (Theorem 4), a joint central limit theorem describing convergence of the edge density and the reciprocal density (Proposition 5), and some discussions on the monotonicty of the limiting entropy density (Remark 9). In Section 3 we investigate the asymptotic features of two canonical ensembles associated with the reciprocal model, one conditional on the edge density and the other conditional on the reciprocal density. Our main results are: exact expressions for the two limiting conditional free energy densities (Theorem 10) and some discussions on their monotonicity (Remark 11). In Section 4 we take another look at the reciprocal model and examine its asymptotic features in the sparse regime. Our main results are: exact scalings for the limiting normalization constant (Theorem 12), the mean (Proposition 13) and variance (Remark 14) of the limiting probability distribution. Lastly, in Section 5 we extend our analysis to more general reciprocal models whose sufficient statistics, besides single edge and reciprocal edge, also include reciprocal p-star and reciprocal triangle. Large deviations techniques are used throughout this paper. We refer the readers to the works of Chatterjee and Diaconis [6] and Chatterjee and Varadhan [7] for more details of this framework.

2. The microcanonical ensemble

Theorem 1.

$$\frac{1}{\binom{n}{2}}\log Z_n(\beta_1,\beta_2)=\log\left(\frac{1}{4}+\frac{1}{2}e^{\beta_1}+\frac{1}{4}e^{2\beta_1+2\beta_2}\right)+2\log 2. \tag{2.1}$$

Proof of Theorem 1.

$$\begin{aligned}
Z_n(\beta_1,\beta_2) &= 2^{n(n-1)}\mathbb{E}\left[e^{\beta_1\sum_{1\le i,j\le n}X_{ij}+\beta_2\sum_{1\le i,j\le n}X_{ij}X_{ji}}\right] \qquad (2.2)\\
&= 2^{n(n-1)}\mathbb{E}\left[e^{\frac{\beta_1}{2}\sum_{1\le i,j\le n}(X_{ij}+X_{ji})+\frac{\beta_2}{2}\sum_{1\le i,j\le n}[(X_{ij}+X_{ji})^2-(X_{ij}+X_{ji})]}\right]\\
&= 2^{n(n-1)}\mathbb{E}\left[e^{\frac{\beta_1-\beta_2}{2}\sum_{1\le i,j\le n}(X_{ij}+X_{ji})+\frac{\beta_2}{2}\sum_{1\le i,j\le n}(X_{ij}+X_{ji})^2}\right]\\
&= 2^{n(n-1)}\mathbb{E}\left[e^{(\beta_1-\beta_2)\sum_{1\le i<j\le n}(X_{ij}+X_{ji})+\beta_2\sum_{1\le i<j\le n}(X_{ij}+X_{ji})^2}\right]\\
&= 2^{n(n-1)}\prod_{1\le i<j\le n}\mathbb{E}\left[e^{(\beta_1-\beta_2)(X_{ij}+X_{ji})+\beta_2(X_{ij}+X_{ji})^2}\right]\\
&= \left[4\left(\frac{1}{4}+\frac{1}{2}e^{\beta_1}+\frac{1}{4}e^{2\beta_1+2\beta_2}\right)\right]^{\binom{n}{2}}.
\end{aligned}$$

Hence we draw the conclusion. □

Define

$$\psi_{n,\delta}(\epsilon,r)=\frac{1}{n^2}\log\mathbb{P}\left(e(X)\in(\epsilon-\delta,\epsilon+\delta),\, r(X)\in(r-\delta,r+\delta)\right).$$

We are interested in the limit

$$\psi(\epsilon,r):=\lim_{\delta\to 0}\lim_{n\to\infty}\psi_{n,\delta}(\epsilon,r). \tag{2.3}$$

The quantity in (2.3) will be called the *limiting entropy density.*

Corollary 2.

$$\psi(\epsilon,r)=-\sup_{\beta_1,\beta_2\in\mathbb{R}}\left\{\beta_1\epsilon+\beta_2 r-\frac{1}{2}\log\left(\frac{1}{4}+\frac{1}{2}e^{\beta_1}+\frac{1}{4}e^{2\beta_1+2\beta_2}\right)\right\}. \tag{2.4}$$

Proof of Corollary 2. Note that from the proof of Theorem 1,

$$\lim_{n\to\infty}\frac{1}{n^2}\log\mathbb{E}\left[e^{\beta_1\sum_{1\leq i,j\leq n}X_{ij}+\beta_2\sum_{1\leq i,j\leq n}X_{ij}X_{ji}}\right]=\frac{1}{2}\log\left(\frac{1}{4}+\frac{1}{2}e^{\beta_1}+\frac{1}{4}e^{2\beta_1+2\beta_2}\right), \tag{2.5}$$

which is finite for any $\beta_1,\beta_2\in\mathbb{R}$ and is differentiable in both β_1 and β_2. The result then follows from Gärtner-Ellis theorem in large deviations theory, see e.g. Dembo and Zeitouni [9]. □

Remark 3. *(i) Note that* $0\leq\frac{1}{n^2}\sum_{1\leq i,j\leq n}X_{ij}\leq 1$ *and* $0\leq\frac{1}{n^2}\sum_{1\leq i,j\leq n}X_{ij}X_{ji}\leq 1$, *which implies that* $\psi(\epsilon,r)=-\infty$ *if* $\epsilon\notin[0,1]$ *or* $r\notin[0,1]$.

(ii) Note that $\sum_{1\leq i,j\leq n}X_{ij}X_{ji}\leq\sum_{1\leq i,j\leq n}X_{ij}$, *which implies that* $\psi(\epsilon,r)=-\infty$ *if* $r>\epsilon$.

(iii) Note that

$$\begin{aligned}\sum_{1\leq i,j\leq n}[X_{ij}X_{ji}+1]-2\sum_{1\leq i,j\leq n}X_{ij}&=\sum_{1\leq i,j\leq n}[X_{ij}X_{ji}+1-X_{ij}-X_{ji}]\\&=\sum_{1\leq i,j\leq n}(X_{ij}-1)(X_{ji}-1)\geq 0,\end{aligned}$$

which implies that $\psi(\epsilon,r)=-\infty$ *if* $1+r-2\epsilon<0$.

Theorem 4. *For* $\epsilon,r\in[0,1]$, $\epsilon\geq r$ *and* $1+r-2\epsilon\geq 0$,

$$\begin{aligned}\psi(\epsilon,r)=-\epsilon\log\left(\frac{\epsilon-r}{1+r-2\epsilon}\right)-\frac{r}{2}\log\left(\frac{r(1+r-2\epsilon)}{(\epsilon-r)^2}\right)\\+\frac{1}{2}\log\left(\frac{1}{4(1+r-2\epsilon)}\right),\end{aligned} \tag{2.6}$$

and otherwise $\psi(\epsilon,r)=-\infty$.

Proof of Theorem 4. Under the assumption that $\epsilon,r\in[0,1]$, it is easy to see that supremum in (2.4) can not be obtained at $\beta_1,\beta_2=\pm\infty$, and $\psi(\epsilon,r)$ must attain its extremum at finite β_1,β_2. At optimality,

$$\epsilon=\frac{\frac{1}{4}e^{\beta_1}+\frac{1}{4}e^{2\beta_1+2\beta_2}}{\frac{1}{4}+\frac{1}{2}e^{\beta_1}+\frac{1}{4}e^{2\beta_1+2\beta_2}}, \tag{2.7}$$

$$r=\frac{\frac{1}{4}e^{2\beta_1+2\beta_2}}{\frac{1}{4}+\frac{1}{2}e^{\beta_1}+\frac{1}{4}e^{2\beta_1+2\beta_2}}. \tag{2.8}$$

Dividing (2.8) into (2.7), we get

$$\frac{\epsilon}{r}=1+e^{-\beta_1-2\beta_2}. \tag{2.9}$$

Substitute this back into (2.7),

$$\epsilon=\frac{e^{-\beta_1-2\beta_2}+1}{e^{-2\beta_1-2\beta_2}+2e^{-\beta_1-2\beta_2}+1}=\frac{\frac{\epsilon}{r}}{e^{-\beta_1}(\frac{\epsilon}{r}-1)+\frac{2\epsilon}{r}-1}, \tag{2.10}$$

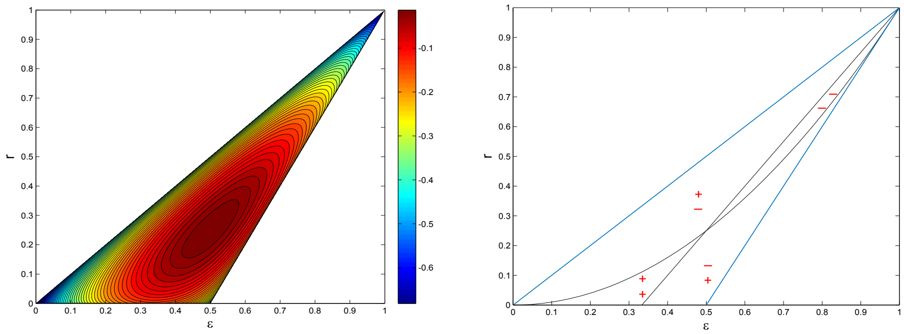

FIGURE 1. On the left hand side, we have the contour plot of the limiting entropy density $\psi(\epsilon, r)$ obtained from Theorem 4. On the right hand side, we specify the regions of monotonicity as obtained in Remark 9. In region $\substack{-\\-}$, ψ is decreasing in both ϵ and r; in region $\substack{+\\-}$, ψ is increasing in ϵ and decreasing in r; in region $\substack{+\\+}$, ψ is increasing in both ϵ and r; in region $\substack{-\\+}$, ψ is decreasing in ϵ and increasing in r. The boundaries are given by $1 + 2r = 3\epsilon$ and $r = \epsilon^2$.

which implies that

$$e^{\beta_1} = \frac{\epsilon - r}{1 + r - 2\epsilon}, \qquad e^{2\beta_2} = \frac{r(1 + r - 2\epsilon)}{(\epsilon - r)^2}. \tag{2.11}$$

The conclusion thus follows. □

The entropy $\psi(\epsilon, r)$ in the microcanonical model is essentially the negation of the rate function from the large deviation principle. In the microcanonical model, the averaged edge density is $\frac{1}{2}$ and the averaged reciprocal density is $\frac{1}{4}$. One can further study the fluctuations of the edge and reciprocal densities, i.e., the central limit theorem.

Proposition 5. *In the microcanonical model,*

$$n\left(e(X) - \frac{1}{2}, r(X) - \frac{1}{4}\right) \to N(\mu, \Sigma), \tag{2.12}$$

in distribution as $n \to \infty$, where

$$\mu := \begin{pmatrix} -\frac{1}{2} \\ -\frac{1}{4} \end{pmatrix}, \qquad \Sigma := \begin{pmatrix} \frac{3}{4} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix}. \tag{2.13}$$

Remark 6. *The drift term μ in Proposition 5 is due to the definition of $e(X)$ and $r(X)$ in (1.2). If one defines $e(X)$ and $r(X)$ as*

$$e(X) = \frac{1}{n(n-1)} \sum_{1 \le i,j \le n} X_{ij}, \quad r(X) = \frac{1}{n(n-1)} \sum_{1 \le i,j \le n} X_{ij} X_{ji} \tag{2.14}$$

instead, then Proposition 5 will hold with minor modifications:

$$(n-1)\left(e(X) - \frac{1}{2}, r(X) - \frac{1}{4}\right) \to N(0, \Sigma). \tag{2.15}$$

Though definitions (1.2) and (2.14) *lead to a difference of the drift term in the central limit theorem, they are indistinguishable for the limiting entropy and free energy densities.*

Proof of Proposition 5. Let us recall that the edge density and the reciprocal density are given by (1.2). For any $\theta_1, \theta_2 \in \mathbb{R}$,

$$\begin{aligned}
&\mathbb{E}\left[e^{\theta_1 n(e(X)-\frac{1}{2})+\theta_2 n(r(X)-\frac{1}{4})}\right] \qquad (2.16)\\
&=\mathbb{E}\left[e^{\frac{\theta_1}{n}\sum_{1\leq i,j\leq n}X_{ij}+\frac{\theta_2}{n}\sum_{1\leq i,j\leq n}X_{ij}X_{ji}}\right]e^{-\frac{\theta_1}{2}n-\frac{\theta_2}{4}n}\\
&=\left(\frac{1}{4}+\frac{1}{2}e^{\frac{\theta_1}{n}}+\frac{1}{4}e^{\frac{2\theta_1}{n}+\frac{2\theta_2}{n}}\right)^{\frac{n(n-1)}{2}}e^{-\frac{\theta_1}{2}n-\frac{\theta_2}{4}n}\\
&=\left(1+\frac{\theta_1}{n}+\frac{\theta_2}{2n}+\frac{3\theta_1^2}{4n^2}+\frac{\theta_1\theta_2}{n^2}+\frac{\theta_2^2}{2n^2}+O(n^{-3})\right)^{\frac{n(n-1)}{2}}e^{-\frac{\theta_1}{2}n-\frac{\theta_2}{4}n}\\
&\to\exp\left\{-\frac{\theta_1}{2}-\frac{\theta_2}{4}+\frac{1}{2}\left(\frac{3\theta_1^2}{4}+\frac{2\theta_1\theta_2}{2}+\frac{\theta_2^2}{2}\right)\right\}
\end{aligned}$$

as $n \to \infty$. Since convergence of moment generating functions implies convergence in distribution, the proof is complete. □

Remark 7. *It is straightforward to compute that*

$$\psi\left(\frac{1}{2},\frac{1}{4}\right)=-\frac{1}{2}\log\left(\frac{\frac{1}{4}}{\frac{1}{4}}\right)-\frac{1}{8}\log\left(\frac{\frac{1}{4}\cdot\frac{1}{4}}{(\frac{1}{4})^2}\right)+\frac{1}{2}\log\left(\frac{1}{4\cdot\frac{1}{4}}\right)=0. \qquad (2.17)$$

This is consistent with the law of large numbers that the averaged edge density is $\frac{1}{2}$ *and the averaged reciprocal density is* $\frac{1}{4}$.

Remark 8. *Along the Erdős-Rényi curve* $r = \epsilon^2$, $0 \leq \epsilon \leq 1$,

$$\psi(\epsilon,\epsilon^2)=-\epsilon\log\epsilon-(1-\epsilon)\log(1-\epsilon)-\log 2, \qquad (2.18)$$

which is the entropy of a Bernoulli random variable and is the negation of the rate function of the large deviations for the edge density.

Remark 9. *We can compute that*

$$\frac{\partial\psi}{\partial\epsilon}=-\log\left(\frac{\epsilon-r}{1+r-2\epsilon}\right). \qquad (2.19)$$

Therefore $\frac{\partial\psi}{\partial\epsilon} \geq 0$ *if and only if* $\epsilon - r \leq 1 + r - 2\epsilon$*, which is equivalent to* $1 + 2r \geq 3\epsilon$.

We can also compute that

$$\frac{\partial\psi}{\partial r}=-\frac{1}{2}\log\left(\frac{r(1+r-2\epsilon)}{(\epsilon-r)^2}\right). \qquad (2.20)$$

Therefore, $\frac{\partial\psi}{\partial r} \geq 0$ *if and only if* $r(1 + r - 2\epsilon) \leq (\epsilon - r)^2$*, which is equivalent to* $r \leq \epsilon^2$*, i.e.,* $\psi(\epsilon, r)$ *is increasing in* r *below the Erdős-Rényi curve* $r = \epsilon^2$ *and* $\psi(\epsilon, r)$ *is decreasing in* r *above the Erdős-Rényi curve* $r = \epsilon^2$*. (See* [28] *for a similar phenomenon across the Erdős-Rényi curve in the (undirected) edge-triangle model.)*

3. The canonical ensemble

As in Aristoff and Zhu [3], Kenyon and Yin [18], Zhu [38], we can also study constrained exponential random graph models. More precisely, we can study the exponential random graph model conditional on the edge density

$$\psi_{n,\delta}(\epsilon,\beta_2)=\frac{1}{n^2}\log\mathbb{E}\left[\exp\left\{\beta_2\sum_{1\leq i,j\leq n}X_{ij}X_{ji}\right\}1_{|e(X)-\epsilon|<\delta}\right], \tag{3.1}$$

and the exponential random graph model conditional on the reciprocal density

$$\psi_{n,\delta}(\beta_1,r)=\frac{1}{n^2}\log\mathbb{E}\left[\exp\left\{\beta_1\sum_{1\leq i,j\leq n}X_{ij}\right\}1_{|r(X)-r|<\delta}\right]. \tag{3.2}$$

The corresponding conditional probability measure to (3.1) is given by

$$\mathbb{P}^{\epsilon,\beta_2}_{n,\delta}(X)=\frac{1}{2^{n(n-1)}}\exp\left\{-n^2\psi_{n,\delta}(\epsilon,\beta_2)+\beta_2\sum_{1\leq i,j\leq n}X_{ij}X_{ji}\right\}1_{|e(X)-\epsilon|<\delta}. \tag{3.3}$$

and the corresponding conditional probability measure to (3.2) is given by

$$\mathbb{P}^{\beta_1,r}_{n,\delta}(X)=\frac{1}{2^{n(n-1)}}\exp\left\{-n^2\psi_{n,\delta}(\beta_1,r)+\beta_1\sum_{1\leq i,j\leq n}X_{ij}\right\}1_{|r(X)-r|<\delta}. \tag{3.4}$$

We can shrink the interval around ϵ (or r) by letting δ go to zero:

$$\psi(\epsilon,\beta_2):=\lim_{\delta\to0}\lim_{n\to\infty}\psi_{n,\delta}(\epsilon,\beta_2), \tag{3.5}$$

$$\psi(\beta_1,r):=\lim_{\delta\to0}\lim_{n\to\infty}\psi_{n,\delta}(\beta_1,r). \tag{3.6}$$

The quantities in (3.5) will be called the *limiting conditional free energy densities.*

Theorem 10. *For any $\beta_2\in\mathbb{R}$, $0\leq\epsilon\leq1$,*

$$\psi(\epsilon,\beta_2)=-\epsilon\log\left(\frac{\epsilon-r^*}{1+r^*-2\epsilon}\right)+\frac{1}{2}\log\left(\frac{1}{4(1+r^*-2\epsilon)}\right), \tag{3.7}$$

where

$$r^*=\begin{cases}\frac{(2\epsilon e^{2\beta_2}-2\epsilon+1)-\sqrt{(2\epsilon e^{2\beta_2}-2\epsilon+1)^2-4\epsilon^2e^{2\beta_2}(e^{2\beta_2}-1)}}{2(e^{2\beta_2}-1)} & \text{if } \beta_2\neq0\\ \epsilon^2 & \text{if } \beta_2=0\end{cases}, \tag{3.8}$$

and for any $\beta_1\in\mathbb{R}$, $0\leq r\leq1$,

$$\psi(\beta_1,r)=-\frac{r}{2}\log r-\log2-\frac{1+r}{2}\log\left(\frac{1-r}{2e^{\beta_1}+1}\right)+r\log\left(\frac{e^{\beta_1}(1-r)}{2e^{\beta_1}+1}\right). \tag{3.9}$$

Proof of Theorem 10. By using Varadhan's lemma, see e.g. Dembo and Zeitouni [9],

$$\psi(\epsilon,\beta_2)=\sup_{2\epsilon-1\leq r\leq\epsilon}\{\beta_2r+\psi(\epsilon,r)\}, \tag{3.10}$$

$$\psi(\beta_1,r)=\sup_{r\leq\epsilon\leq\frac{r+1}{2}}\{\beta_1\epsilon+\psi(\epsilon,r)\}. \tag{3.11}$$

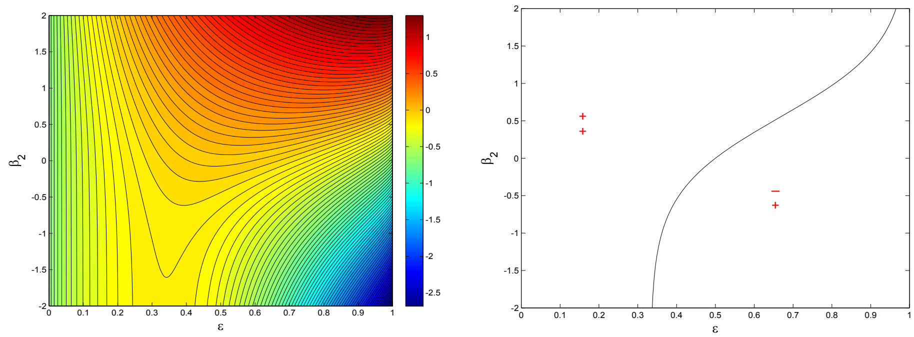

FIGURE 2. On the left hand side, we have the contour plot of the limiting conditional free energy density $\psi(\epsilon, \beta_2)$ obtained from Theorem 10. On the right hand side, we specify the regions of monotonicity as obtained in Remark 11. ψ is always increasing in β_2. In region $\substack{+\\+}$, ψ is increasing in ϵ and in region $\substack{-\\+}$, ψ is decreasing in ϵ. The boundary is specified in Remark 11.

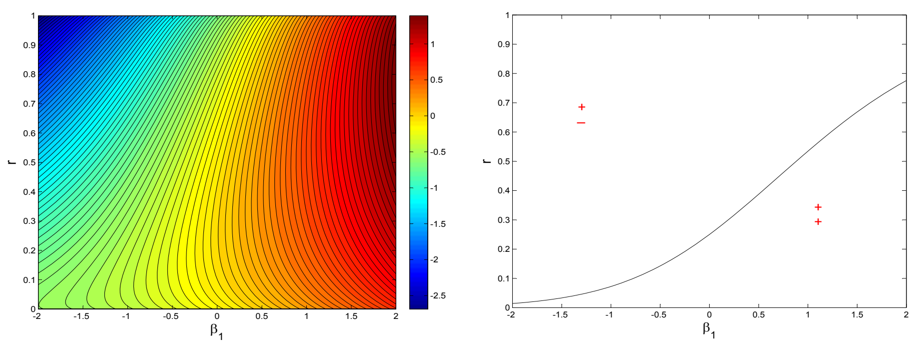

FIGURE 3. On the left hand side, we have the contour plot of the limiting conditional free energy density $\psi(\beta_1, r)$ obtained from Theorem 10. On the right hand side, we specify the regions of monotonicity as obtained in Remark 11. ψ is always increasing in β_1. In region $\substack{+\\-}$, ψ is decreasing in r and in region $\substack{+\\+}$, ψ is increasing in r. The boundary is specified in Remark 11.

By (2.20), the optimal r in (3.10) satisfies

$$0 = \beta_2 + \frac{\partial\psi}{\partial r} = \beta_2 - \frac{1}{2}\log\left(\frac{r(1+r-2\epsilon)}{(\epsilon-r)^2}\right), \tag{3.12}$$

since we can easily check that $\frac{\partial\psi}{\partial r}|_{r=\epsilon-} = -\infty$ and $\frac{\partial\psi}{\partial r}|_{r=(2\epsilon-1)+} = +\infty$. Moreover, (3.12) must have a solution on $(2\epsilon-1, \epsilon)$ by the mean value theorem.

Note that (3.12) is equivalent to

$$(e^{2\beta_2}-1)r^2 - (2\epsilon e^{2\beta_2} - 2\epsilon + 1)r + \epsilon^2 e^{2\beta_2} = 0. \tag{3.13}$$

When $\beta_2 = 0$, (3.12) has one solution

$$r^* = \epsilon^2, \tag{3.14}$$

and when $\beta_2 \neq 0$, (3.12) has two solutions

$$r^{\pm} = \frac{(2\epsilon e^{2\beta_2} - 2\epsilon + 1) \pm \sqrt{(2\epsilon e^{2\beta_2} - 2\epsilon + 1)^2 - 4\epsilon^2 e^{2\beta_2}(e^{2\beta_2} - 1)}}{2(e^{2\beta_2} - 1)}, \tag{3.15}$$

since we can easily check that

$$\begin{aligned}(2\epsilon e^{2\beta_2} - 2\epsilon + 1)^2 - 4\epsilon^2 e^{2\beta_2}(e^{2\beta_2} - 1) &= 4\epsilon^2 + 1 - 4\epsilon + 4\epsilon e^{2\beta_2} - 4\epsilon^2 e^{2\beta_2} \\ &= (2\epsilon - 1)^2 + 4\epsilon(1-\epsilon)e^{2\beta_2} \geq 0.\end{aligned} \tag{3.16}$$

When $\beta_2 < 0$, we have $e^{2\beta_2} - 1 < 0$ and one solution of (3.12) is positive and the other is negative. It is easy to check that $r^- > 0$ and $r^+ < 0$ and thus the optimal $r^* = r^-$. When $\beta_2 > 0$, both solutions $r^{\pm}$ of (3.12) are positive and

$$r^+ + r^- = \frac{(2\epsilon e^{2\beta_2} - 2\epsilon + 1)}{(e^{2\beta_2} - 1)} > 2\epsilon. \tag{3.17}$$

Thus $r^+ \geq \frac{r^+ + r^-}{2} > \epsilon$ and $\psi(\epsilon, r^+) = -\infty$. Hence the optimal $r^* = r^-$.

By (2.19), the optimal ϵ in (3.11) satisfies

$$0 = \beta_1 + \frac{\partial \psi}{\partial \epsilon} = \beta_1 - \log\left(\frac{\epsilon - r}{1 + r - 2\epsilon}\right), \tag{3.18}$$

which yields that the optimizer is $\epsilon^* = \frac{e^{\beta_1}(1+r)+r}{2e^{\beta_1}+1}$. This is indeed the optimizer following the mean value theorem, since $\frac{\partial \psi}{\partial \epsilon}|_{\epsilon=r^+} = \infty$ and $\frac{\partial \psi}{\partial \epsilon}|_{\epsilon=(\frac{1+r}{2})^-} = -\infty$. ☐

Remark 11. *Let us recall that*

$$\psi(\epsilon, \beta_2) = \sup_{2\epsilon - 1 \leq r \leq \epsilon} \{\beta_2 r + \psi(\epsilon, r)\} = \beta_2 r^* + \psi(\epsilon, r^*), \tag{3.19}$$

$$\psi(\beta_1, r) = \sup_{r \leq \epsilon \leq \frac{r+1}{2}} \{\beta_1 \epsilon + \psi(\epsilon, r)\} = \beta_1 \epsilon^* + \psi(\epsilon^*, r), \tag{3.20}$$

where r^* and ϵ^* are the optimizers that satisfy $\beta_2 + \frac{\partial \psi}{\partial r}|_{r=r^*} = 0$ and $\beta_1 + \frac{\partial \psi}{\partial \epsilon}|_{\epsilon=\epsilon^*} = 0$. Hence,

$$\begin{aligned}\frac{\partial \psi(\epsilon, \beta_2)}{\partial \beta_2} &= r^* + \left[\beta_2 + \frac{\partial \psi(\epsilon, r^*)}{\partial r^*}\right]\frac{\partial r^*}{\partial \beta_2} = r^*, \\ \frac{\partial \psi(\beta_1, r)}{\partial \beta_1} &= \epsilon^* + \left[\beta_1 + \frac{\partial \psi(\epsilon^*, r)}{\partial \epsilon^*}\right]\frac{\partial \epsilon^*}{\partial \beta_1} = \epsilon^*.\end{aligned} \tag{3.21}$$

$\psi(\epsilon, \beta_2)$ and $\psi(\beta_1, r)$ are increasing in β_2 and β_1 respectively.

Moreover, we have

$$\begin{aligned}\frac{\partial \psi(\epsilon, \beta_2)}{\partial \epsilon} &= \left[\beta_2 + \frac{\partial \psi(\epsilon, r^*)}{\partial r^*}\right]\frac{\partial r^*}{\partial \epsilon} + \frac{\partial \psi(\epsilon, r^*)}{\partial \epsilon} \\ &= -\log\left(\frac{\epsilon - r^*}{1 + r^* - 2\epsilon}\right).\end{aligned} \tag{3.22}$$

Therefore, $\psi(\epsilon,\beta_2)$ is increasing in ϵ if and only if $1+2r^*\geq 3\epsilon$. This is equivalent to $\epsilon\leq\frac{1}{2}$ when $\beta_2=0$; while for $\beta_2\neq 0$, this is equivalent to

$$\frac{(2\epsilon e^{2\beta_2}-2\epsilon+1)-\sqrt{(2\epsilon e^{2\beta_2}-2\epsilon+1)^2-4\epsilon^2 e^{2\beta_2}(e^{2\beta_2}-1)}}{(e^{2\beta_2}-1)}\geq 3\epsilon-1, \tag{3.23}$$

which can be simplified to

$$\begin{aligned} &-\epsilon e^{2\beta_2}+\epsilon+e^{2\beta_2}\geq\sqrt{(2\epsilon e^{2\beta_2}-2\epsilon+1)^2-4\epsilon^2 e^{2\beta_2}(e^{2\beta_2}-1)} \qquad \text{if } \beta_2>0, \\ &-\epsilon e^{2\beta_2}+\epsilon+e^{2\beta_2}\leq\sqrt{(2\epsilon e^{2\beta_2}-2\epsilon+1)^2-4\epsilon^2 e^{2\beta_2}(e^{2\beta_2}-1)} \qquad \text{if } \beta_2<0. \end{aligned} \tag{3.24}$$

This can be further simplified to

$$\begin{aligned} (1-\epsilon)e^{4\beta_2}-2\epsilon e^{2\beta_2}+(3\epsilon-1)\geq 0 \qquad \text{if } \beta_2>0, \\ (1-\epsilon)e^{4\beta_2}-2\epsilon e^{2\beta_2}+(3\epsilon-1)\leq 0 \qquad \text{if } \beta_2<0 \end{aligned} \tag{3.25}$$

or alternatively

$$\epsilon\leq\frac{e^{2\beta_2}+1}{e^{2\beta_2}+3}. \tag{3.26}$$

Similarly,

$$\begin{aligned} \frac{\partial\psi(\beta_1,r)}{\partial r}&=\left[\beta_1+\frac{\partial\psi(\epsilon^*,r)}{\partial\epsilon^*}\right]\frac{\partial\epsilon^*}{\partial r}+\frac{\partial\psi(\epsilon^*,r)}{\partial r} \\ &=-\frac{1}{2}\log\left(\frac{r(1+r-2\epsilon^*)}{(\epsilon^*-r)^2}\right). \end{aligned} \tag{3.27}$$

Therefore, $\psi(\beta_1,r)$ is increasing in r if and only if $r\leq(\epsilon^*)^2$, which is equivalent to

$$\sqrt{r}\leq\frac{e^{\beta_1}(1+r)+r}{2e^{\beta_1}+1}, \tag{3.28}$$

which is equivalent to

$$\beta_1\geq\log\left(\frac{\sqrt{r}}{1-\sqrt{r}}\right). \tag{3.29}$$

4. Another look at the grand canonical ensemble

Similar to the analysis in Yin and Zhu [37], we can also study sparse exponential random graph models whose sufficient statistics are given by edge and reciprocal densities. We allow $\beta_1^{(n)}$ and $\beta_2^{(n)}$ to depend on n and assume that $\beta_1^{(n)}=\beta_1\alpha_n$ and $\beta_2^{(n)}=\beta_2\alpha_n$, where α_n is positive and $\alpha_n\to\infty$ as $n\to\infty$. With some abuse of notation we will still denote the associated normalization constant, probability measure, and expectation by $Z_n(\beta_1,\beta_2)$, $\mathbb{P}_n^{\beta_1,\beta_2}$, and $\mathbb{E}_n^{\beta_1,\beta_2}$ respectively. From the proof of Theorem 1, we have

$$Z_n(\beta_1,\beta_2)^{1/\binom{n}{2}}=4\left(\frac{1}{4}+\frac{1}{2}e^{\beta_1^{(n)}}+\frac{1}{4}e^{2\beta_1^{(n)}+2\beta_2^{(n)}}\right), \tag{4.1}$$

which yields the following result.

Proposition 12. *(i) When* $\beta_1 < 0$ *and* $\beta_1 + \beta_2 < 0$, $\lim_{n\to\infty}(Z_n(\beta_1,\beta_2))^{\frac{1}{n^2}} = 1$.

(ii) When $\beta_1 < 0$ *and* $\beta_1 + \beta_2 = 0$, $\lim_{n\to\infty}(Z_n(\beta_1,\beta_2))^{\frac{1}{n^2}} = \sqrt{2}$.

(iii) When $\beta_1 \leq 0$ *and* $\beta_1 + \beta_2 > 0$, $\lim_{n\to\infty}\frac{(Z_n(\beta_1,\beta_2))^{\frac{1}{n^2}}}{e^{\alpha_n(\beta_1+\beta_2)}} = 1$.

(iv) When $\beta_1 = 0$ *and* $\beta_2 < 0$, $\lim_{n\to\infty}(Z_n(\beta_1,\beta_2))^{\frac{1}{n^2}} = \sqrt{3}$.

(v) When $\beta_1 = 0$ *and* $\beta_2 = 0$, $\lim_{n\to\infty}(Z_n(\beta_1,\beta_2))^{\frac{1}{n^2}} = 2$.

(vi) When $\beta_1 > 0$ *and* $\beta_1 + 2\beta_2 < 0$, $\lim_{n\to\infty}\frac{(Z_n(\beta_1,\beta_2))^{\frac{1}{n^2}}}{e^{\frac{1}{2}\alpha_n\beta_1}} = \sqrt{2}$.

(vii) When $\beta_1 > 0$ *and* $\beta_1 + 2\beta_2 = 0$, $\lim_{n\to\infty}\frac{(Z_n(\beta_1,\beta_2))^{\frac{1}{n^2}}}{e^{\frac{1}{2}\alpha_n\beta_1}} = \sqrt{3}$.

(viii) When $\beta_1 > 0$ *and* $\beta_1 + 2\beta_2 > 0$, $\lim_{n\to\infty}\frac{(Z_n(\beta_1,\beta_2))^{\frac{1}{n^2}}}{e^{\alpha_n(\beta_1+\beta_2)}} = 1$.

Proposition 13. *Let* $i \in \mathbb{N}$, $2 \leq i \leq n$.

(i) When $\beta_1 < 2(\beta_1+\beta_2) < 0$, $\lim_{n\to\infty}\frac{\mathbb{P}_n^{\beta_1,\beta_2}(X_{1i}=1)}{e^{2\alpha_n(\beta_1+\beta_2)}} = \frac{1}{4}$.

(ii) When $2(\beta_1+\beta_2) < \beta_1 < 0$, $\lim_{n\to\infty}\frac{\mathbb{P}_n^{\beta_1,\beta_2}(X_{1i}=1)}{e^{\alpha_n\beta_1}} = \frac{1}{4}$.

(iii) When $\beta_1 = 2(\beta_1+\beta_2) < 0$, $\lim_{n\to\infty}\frac{\mathbb{P}_n^{\beta_1,\beta_2}(X_{1i}=1)}{e^{\alpha_n\beta_1}} = \frac{1}{2}$.

Proof of Proposition 13.

$$\begin{aligned}
\mathbb{P}_n^{\beta_1,\beta_2}(X_{1i}=1) &= \mathbb{E}_n^{\beta_1,\beta_2}[X_{1i}] \\
&= \frac{\mathbb{E}\left[X_{1i}e^{\beta_1\alpha_n\sum_{1\leq i,j\leq n}X_{ij}+\beta_2\alpha_n\sum_{1\leq i,j\leq n}X_{ij}X_{ji}}\right]}{\mathbb{E}\left[e^{\beta_1\alpha_n\sum_{1\leq i,j\leq n}X_{ij}+\beta_2\alpha_n\sum_{1\leq i,j\leq n}X_{ij}X_{ji}}\right]} \\
&= \frac{\mathbb{E}\left[X_{1i}e^{(\beta_1-\beta_2)\alpha_n\sum_{1\leq i<j\leq n}(X_{ij}+X_{ji})+\beta_2\alpha_n\sum_{1\leq i<j\leq n}(X_{ij}+X_{ji})^2}\right]}{\mathbb{E}\left[e^{(\beta_1-\beta_2)\alpha_n\sum_{1\leq i<j\leq n}(X_{ij}+X_{ji})+\beta_2\alpha_n\sum_{1\leq i<j\leq n}(X_{ij}+X_{ji})^2}\right]} \\
&= \frac{\mathbb{E}\left[X_{1i}e^{(\beta_1-\beta_2)\alpha_n(X_{1i}+X_{i1})+\beta_2\alpha_n(X_{1i}+X_{i1})^2}\right]}{\mathbb{E}\left[e^{(\beta_1-\beta_2)\alpha_n(X_{1i}+X_{i1})+\beta_2\alpha_n(X_{1i}+X_{i1})^2}\right]} \\
&= \frac{\frac{1}{4}e^{\beta_1\alpha_n}+\frac{1}{4}e^{2(\beta_1+\beta_2)\alpha_n}}{\frac{1}{4}+\frac{1}{2}e^{\beta_1\alpha_n}+\frac{1}{4}e^{2(\beta_1+\beta_2)\alpha_n}}
\end{aligned} \tag{4.2}$$

Therefore, when $\beta_1 < 0$ and $\beta_1+\beta_2 < 0$, $\mathbb{P}_n^{\beta_1,\beta_2}(X_{1i}=1) \to 0$ as $n \to \infty$. The rest of the proof easily follows. □

Remark 14. *For any $i \neq j$ and $i,j \neq 1$,*

$$\begin{aligned}
&\mathbb{P}_n^{\beta_1,\beta_2}(X_{1i}=1,X_{1j}=1) \qquad (4.3)\\
&=\mathbb{E}_n^{\beta_1,\beta_2}[X_{1i}X_{1j}]\\
&=\frac{\mathbb{E}\left[X_{1i}X_{1j}e^{\beta_1^{(n)}\sum_{1\leq i,j\leq n}X_{ij}+\beta_2^{(n)}\sum_{1\leq i,j\leq n}X_{ij}X_{ji}}\right]}{\mathbb{E}\left[e^{\beta_1^{(n)}\sum_{1\leq i,j\leq n}X_{ij}+\beta_2^{(n)}\sum_{1\leq i,j\leq n}X_{ij}X_{ji}}\right]}\\
&=\frac{\mathbb{E}\left[X_{1i}X_{1j}e^{(\beta_1^{(n)}-\beta_2^{(n)})\sum_{1\leq i<j\leq n}(X_{ij}+X_{ji})+\beta_2^{(n)}\sum_{1\leq i<j\leq n}(X_{ij}+X_{ji})^2}\right]}{\mathbb{E}\left[e^{(\beta_1^{(n)}-\beta_2^{(n)})\sum_{1\leq i<j\leq n}(X_{ij}+X_{ji})+\beta_2^{(n)}\sum_{1\leq i<j\leq n}(X_{ij}+X_{ji})^2}\right]}\\
&=\frac{\mathbb{E}\left[X_{1i}X_{1j}e^{(\beta_1^{(n)}-\beta_2^{(n)})(X_{1i}+X_{i1}+X_{1j}+X_{j1})+\beta_2^{(n)}[(X_{1i}+X_{i1})^2+(X_{1j}+X_{j1})^2]}\right]}{\mathbb{E}\left[e^{(\beta_1^{(n)}-\beta_2^{(n)})(X_{1i}+X_{i1}+X_{1j}+X_{j1})+\beta_2^{(n)}[(X_{1i}+X_{i1})^2+(X_{1j}+X_{j1})^2]}\right]}\\
&=\frac{\mathbb{E}\left[X_{1i}e^{(\beta_1^{(n)}-\beta_2^{(n)})(X_{1i}+X_{i1})+\beta_2^{(n)}(X_{1i}+X_{i1})^2}\right]}{\mathbb{E}\left[e^{(\beta_1^{(n)}-\beta_2^{(n)})(X_{1i}+X_{i1})+\beta_2^{(n)}(X_{1i}+X_{i1})^2}\right]}\frac{\mathbb{E}\left[X_{1j}e^{(\beta_1^{(n)}-\beta_2^{(n)})(X_{1j}+X_{j1})+\beta_2^{(n)}(X_{1j}+X_{j1})^2}\right]}{\mathbb{E}\left[e^{(\beta_1^{(n)}-\beta_2^{(n)})(X_{1j}+X_{j1})+\beta_2^{(n)}(X_{1j}+X_{j1})^2}\right]}\\
&=\mathbb{P}_n^{\beta_1,\beta_2}(X_{1i}=1)\mathbb{P}_n^{\beta_1,\beta_2}(X_{1j}=1).
\end{aligned}$$

5. Further discussions

We have studied the edge and reciprocal densities for a directed graph. We can generalize these ideas to study densities of *reciprocal p-star* and *reciprocal triangle*. Reciprocal triangles are sometimes called *cyclic triads* in the literature, see e.g. Robins et al. [31]. They are used to model the situation where you have three vertices i, j and k and there are bilateral relations between i and j, j and k, and k and i, i.e., $X_{ij}=X_{ji}=X_{jk}=X_{kj}=X_{ki}=X_{ik}=1$. Similarly, reciprocal p-stars have generated significant interest as well. We define the density of reciprocal triangle and reciprocal p-star respectively as

$$t(X):=\frac{1}{n^3}\sum_{1\leq i,j,k\leq n}X_{ij}X_{ji}X_{jk}X_{kj}X_{ki}X_{ik}, \qquad (5.1)$$

and

$$s(X):=\frac{1}{n^{p+1}}\sum_{i=1}^n\left(\sum_{j=1}^n X_{ij}X_{ji}\right)^p. \qquad (5.2)$$

We are interested in the *limiting free energy density*

$$\psi(\beta_1,\beta_2,\beta_3,\beta_4):=\lim_{n\to\infty}\frac{1}{n^2}\log 2^{n(n-1)}\mathbb{E}\left[e^{n^2(\beta_1 e(X)+\beta_2 r(X)+\beta_3 t(X)+\beta_4 s(X))}\right], \qquad (5.3)$$

for the grand canonical ensemble and the *limiting entropy density*

$$\psi(\epsilon,r,t,s):=\lim_{\delta\to 0}\lim_{n\to\infty}\frac{1}{n^2}\log\mathbb{P}\left(e(X)\in B_\delta(\epsilon),r(X)\in B_\delta(r),t(X)\in B_\delta(t),s(X)\in B_\delta(s)\right), \qquad (5.4)$$

for the microcanonical ensemble, where $B_\delta(x):=\{y:|y-x|<\delta\}$.

The key observation here is that we can define $Z_{ij}=Z_{ji}=X_{ij}X_{ji}$ so that $(Z_{ij})_{1\leq i<j\leq n}$ are i.i.d. random variables with $\mathbb{P}(Z_{ij}=1)=\frac{1}{4}$ and $\mathbb{P}(Z_{ij}=0)=\frac{3}{4}$.

Then

$$r(X) = \frac{1}{n^2} \sum_{1 \leq i,j \leq n} Z_{ij}, \tag{5.5}$$

$$t(X) = \frac{1}{n^3} \sum_{1 \leq i,j,k \leq n} Z_{ij} Z_{jk} Z_{ki}, \tag{5.6}$$

$$s(X) = \frac{1}{n^{p+1}} \sum_{i=1}^{n} \left(\sum_{j=1}^{n} Z_{ij} \right)^p,$$

respectively.

From Chatterjee and Varadhan's large deviations results for the Erdős-Rényi random graph, see [7],

$$\begin{aligned} &\lim_{\delta \to 0} \lim_{n \to \infty} \frac{1}{n^2} \log \mathbb{P} \left(r(X) \in B_\delta(r), t(X) \in B_\delta(t), s(X) \in B_\delta(s) \right) \\ &= - \inf_{\substack{g:[0,1]^2 \to [0,1], g(x,y)=g(y,x) \\ r(g)=r, t(g)=t, s(g)=s}} \frac{1}{2} I_{\frac{1}{4}}(g), \end{aligned} \tag{5.7}$$

where

$$\begin{aligned} r(g) &:= \iint_{[0,1]^2} g(x,y) dx dy, \\ t(g) &:= \iiint_{[0,1]^3} g(x,y) g(y,z) g(z,x) dx dy dz, \\ s(g) &:= \int_0^1 \left(\int_0^1 g(x,y) dy \right)^p dx, \end{aligned} \tag{5.8}$$

and $I_{\frac{1}{4}}(g) := \iint_{[0,1]^2} I_{\frac{1}{4}}(g(x,y)) dx dy$, where

$$\begin{aligned} I_{\frac{1}{4}}(x) :&= x \log \left(\frac{x}{1/4} \right) + (1-x) \log \left(\frac{1-x}{1-\frac{1}{4}} \right) \\ &= x \log 3 + x \log x + (1-x) \log (1-x) - \log(3/4). \end{aligned} \tag{5.9}$$

We examine the *limiting entropy density* (5.4) first. Another key observation is that the distribution of $e(X)$ conditional on $(Z_{ij})_{1 \leq i,j \leq n}$ is the same as conditional on $r(X)$. Thus, the distribution of $e(X)$ conditional on $r(X), t(X), s(X)$ is the same as conditional on $r(X)$. We already proved that

$$\begin{aligned} &\lim_{\delta \to 0} \lim_{n \to \infty} \frac{1}{n^2} \log \mathbb{P}(e(X) \in B_\delta(\epsilon), r(X) \in B_\delta(r)) \\ &= -\epsilon \log \left(\frac{\epsilon - r}{1 + r - 2\epsilon} \right) - \frac{r}{2} \log \left(\frac{r(1 + r - 2\epsilon)}{(\epsilon - r)^2} \right) \\ &\qquad + \frac{1}{2} \log \left(\frac{1}{4(1 + r - 2\epsilon)} \right). \end{aligned} \tag{5.10}$$

It is easy to see that

$$\begin{aligned} &\lim_{\delta \to 0} \lim_{n \to \infty} \frac{1}{n^2} \log \mathbb{P}(r(X) \in B_\delta(r)) \\ &= -\frac{1}{2} r \log \left(\frac{r}{1/4} \right) - \frac{1}{2} (1-r) \log \left(\frac{1-r}{1-1/4} \right). \end{aligned} \tag{5.11}$$

Therefore,

$$\begin{aligned}\phi(\epsilon,r) &:= \lim_{\delta\to 0}\lim_{n\to\infty}\frac{1}{n^2}\log\mathbb{P}(e(X)\in B_\delta(\epsilon)|r(X)\in B_\delta(r)) \\ &= -\epsilon\log\left(\frac{\epsilon-r}{1+r-2\epsilon}\right)-\frac{r}{2}\log\left(\frac{(1-r)(1+r-2\epsilon)}{3(\epsilon-r)^2}\right) \\ &\qquad +\frac{1}{2}\log\left(\frac{1-r}{3(1+r-2\epsilon)}\right).\end{aligned} \tag{5.12}$$

Together with (5.7), we conclude that

$$\psi(\epsilon,r,t,s)=\phi(\epsilon,r)-\inf_{\substack{g:[0,1]^2\to[0,1],g(x,y)=g(y,x)\\ r(g)=r,t(g)=t,s(g)=s}}\frac{1}{2}I_{\frac{1}{4}}(g). \tag{5.13}$$

Next we examine the *limiting free energy density* (5.3). By Varadhan's lemma from large deviations theory, see e.g. Dembo and Zeitouni [9],

$$\begin{aligned}&\psi(\beta_1,\beta_2,\beta_3,\beta_4) \\ &=\sup_{0\le\epsilon,r,t,s\le 1}\{\beta_1\epsilon+\beta_2 r+\beta_3 t+\beta_4 s+\psi(\epsilon,r,t,s)\}+\log 2 \\ &=\sup_{\substack{0\le\epsilon,r,t,s\le 1\\ g:[0,1]^2\to[0,1],g(x,y)=g(y,x)\\ r(g)=r,t(g)=t,s(g)=s}}\left\{\beta_1\epsilon+\beta_2 r+\beta_3 t+\beta_4 s+\phi(\epsilon,r)-\frac{1}{2}\left(I_{\frac{1}{4}}(g)-2\log 2\right)\right\}\end{aligned} \tag{5.14}$$

Let us first consider the optimization problem

$$\eta(\beta_1,r):=\sup_{0\le\epsilon\le 1}\{\beta_1\epsilon+\phi(\epsilon,r)\}. \tag{5.15}$$

Note that at optimality

$$\frac{\partial\phi(\epsilon,r)}{\partial\epsilon}=\frac{\partial\psi(\epsilon,r)}{\partial\epsilon}=-\log\left(\frac{\epsilon-r}{1+r-2\epsilon}\right)=-\beta_1, \tag{5.16}$$

which implies that $\epsilon=\frac{(1+r)e^{\beta_1}+r}{1+2e^{\beta_1}}$. Therefore, we have

$$\eta(\beta_1,r)=\beta_1\frac{(1+r)e^{\beta_1}+r}{1+2e^{\beta_1}}+\phi\left(\frac{(1+r)e^{\beta_1}+r}{1+2e^{\beta_1}},r\right). \tag{5.17}$$

Hence, we have

$$\begin{aligned}&\psi(\beta_1,\beta_2,\beta_3,\beta_4) \\ &=\sup_{\substack{0\le r,t,s\le 1\\ g:[0,1]^2\to[0,1],g(x,y)=g(y,x)\\ r(g)=r,t(g)=t,s(g)=s}}\left\{\eta(\beta_1,r)+\beta_2 r+\beta_3 t+\beta_4 s-\frac{1}{2}\left(I_{\frac{1}{4}}(g)-2\log 2\right)\right\} \\ &=\sup_{\substack{g:[0,1]^2\to[0,1]\\ g(x,y)=g(y,x)}}\left\{\eta(\beta_1,r(g))+\beta_2 r(g)+\beta_3 t(g)+\beta_4 s(g)-\frac{1}{2}\left(I_{\frac{1}{4}}(g)-2\log 2\right)\right\},\end{aligned} \tag{5.18}$$

which is a complicated variational problem that is hard to solve in general, however we can proceed further in two special situations.

The first special situation is when $\beta_1 = 0$,

$$\psi(0,\beta_2,\beta_3,\beta_4) \tag{5.19}$$
$$= \sup_{\substack{g:[0,1]^2\to[0,1]\\ g(x,y)=g(y,x)}} \left\{\beta_2 r(g) + \beta_3 t(g) + \beta_4 s(g) - \frac{1}{2}\left(I_{\frac{1}{4}}(g) - 2\log 2\right)\right\}$$
$$= \sup_{\substack{g:[0,1]^2\to[0,1]\\ g(x,y)=g(y,x)}} \left\{\left(\beta_2 - \frac{\log 3}{2}\right) r(g) + \beta_3 t(g) + \beta_4 s(g) - \frac{1}{2} I_0(g)\right\} + \frac{1}{2}\log 3,$$

where $I_0(g) := \iint_{[0,1]^2} I_0(g(x,y))dxdy$ and $I_0(x) := x\log x + (1-x)\log(1-x)$. This shows that $\psi(0,\beta_2,\beta_3,\beta_4)$ may be equivalently viewed as the *limiting free energy density* of an undirected model whose sufficient statistics are given by (undirected) edge, triangle, and p-star densities. The 3 parameters β_2,β_3,β_4 allow one to adjust the influence of these different local features on the limiting probability distribution and thus expectedly should impact the global structure of a random graph drawn from the model. It is therefore important to understand if and when the supremum in (5.19) is attained and whether it is unique. Many people have delved into this area. A particularly significant discovery was made by Chatterjee and Diaconis [6], who showed that the supremum in (5.19) is always attained and a random graph drawn from the model must lie close to the maximizing set with probability vanishing in n. When $\beta_3,\beta_4 \geq 0$, Yin [35] further showed that the 3-parameter space would consist of a single phase with first order phase transition(s) across one (or more) surfaces, where all the first derivatives of ψ exhibit (jump) discontinuities, and second order phase transition(s) along one (or more) critical curves, where all the second derivatives of ψ diverge.

The second special situation is when $\beta_3 = 0$,

$$\psi(\beta_1,\beta_2,0,\beta_4) \tag{5.20}$$
$$= \sup_{\substack{g:[0,1]^2\to[0,1]\\ g(x,y)=g(y,x)}} \left\{\eta(\beta_1, r(g)) + \beta_2 r(g) + \beta_4 s(g) - \frac{1}{2}\left(I_{\frac{1}{4}}(g) - 2\log 2\right)\right\}.$$

We can derive the Euler-Lagrange equation for this variational problem, and it is given by

$$2\frac{\partial\eta}{\partial r}(\beta_1, r(g)) + 2\beta_2 + \beta_4 p d(x)^{p-1} + \beta_4 p d(y)^{p-1} = \log\left(\frac{g(x,y)}{1-g(x,y)}\right) + \log 3, \tag{5.21}$$

where $d(x) := \int_0^1 g(x,y)dy$. Solving for $g(x,y)$ and then integrating over y, we get

$$d(x) = \int_0^1 \frac{dy}{1 + 3e^{-2\frac{\partial\eta}{\partial r}(\beta_1,r(g)) - 2\beta_2 - \beta_4 p d(x)^{p-1} - \beta_4 p d(y)^{p-1}}}. \tag{5.22}$$

Following the same arguments as in Kenyon et al. [17], we conclude that $d(x)$ can take only finitely many values and hence so is the optimal g. The optimal graph is thus multipodal.

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