ASYMPTOTIC STRUCTURE AND SINGULARITIES IN
CONSTRAINED DIRECTED GRAPHS

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Abstract. We study the asymptotics of large directed graphs, constrained to have certain densities of edges and/or outward p-stars. Our models are close cousins of exponential random graph models, in which edges and certain other subgraph densities are controlled by parameters. We find that large graphs have either uniform or bipodal structure. When edge density (resp. p-star density) is fixed and p-star density (resp. edge density) is controlled by a parameter, we find phase transitions corresponding to a change from uniform to bipodal structure. When both edge and p-star density are fixed, we find only bipodal structures and no phase transition.

1. Introduction

In this article we study the asymptotics of large directed graphs with constrained densities of edges and outward directed p-stars. Large graphs are often modeled by probabilistic ensembles with one or more adjustable parameters; see e.g. Fienberg [7, 8], Lovász [20] and Newman [21]. The exponential random graph models (ERGMs), in which parameters are used to tune the densities of edges and other subgraphs, are one such class of models; see e.g. Besag [2], Frank and Strauss [9], Holland and Leinhardt [12], Newman [21], Rinaldo et al. [28], Robins et al. [29], Snijders et al. [30], Strauss [31], and Wasserman and Faust [33].

It has been shown that in many ERGMs the subgraph densities actually cannot be tuned. For example, for the class of ERGMs parametrized by edges and p-stars, large graphs are essentially Erdős-Rényi for all values of the parameters. (See Chatterjee and Diaconis [8] for more complete and precise statements.) An alternative to ERGMs was introduced by Radin and Sadun [25], where instead of using parameters to control subgraph counts, the subgraph densities are controlled directly; see also Radin et al. [26], Radin and Sadun [27] and Kenyon et al. [14]. This is the approach we take in this article, with edges and (outward) p-stars as the subgraphs controlled directly. We also consider models which split the difference between the two approaches: edges (resp. p-stars) are controlled directly, while p-stars (resp. edges) are tuned with a parameter. See [15] for the undirected graph version of the latter.

We find that, in all our models, graphs have either uniform or bipodal structure as the number of nodes becomes infinite. Our approach, following refs. [14, 25, 26, 27], is to study maximizers of the entropy or free energy of the model as the number of nodes becomes infinite. When we constrain both edge and p-star densities, we

Date: 2 June 2014. Revised: 2 June 2014.
2000 Mathematics Subject Classification. 05C80, 82B26, 05C35.
Key words and phrases. dense random graphs, exponential random graphs, graph limits, entropy, phase transitions.
find only bipodal structure (except when the $p$-star density is fixed to be exactly equal to the $p$th power of the edge density). When we constrain either edge or $p$-star densities (but not both), we find both uniform and bipodal structures, with a sharp change at the interface. This is in contrast with the situation in the ERGM version of the model, in which one finds only uniform structures, albeit with sharp changes in their densities along a certain curve in parameter space; see Aristoff and Zhu [1].

These sharp changes along interfaces are called phase transitions. Phase transitions have recently been proved rigorously for ERGMs; see e.g. Yin [34] and especially Radin and Yin [24] for a precise definition of the term. Some earlier works using mean-field analysis and other approximations include Häggström and Jonasson [11] and Park and Newman [22, 23]. The terminology is apt, in that ERGMs and our models are inspired by certain counterparts in statistical physics: respectively, the grand canonical ensemble, and the microcanonical and canonical ensembles. See the discussion in Section 2.

Our directed graph models are simpler than their undirected counterparts. In particular, we can rigorously identify the asymptotic structures at all parameters, while in analogous models for undirected graphs, only partial results are known [14]. Our analysis, however, does not easily extend to directed random graph models where other subgraphs, like triangles, cycles, etc., instead of outward directed $p$-stars, are constrained.

This article is organized as follows. In Section 2, we describe our models and compare them with their statistical physics counterparts. In Section 3, we state our main results. In Section 4, we prove a large deviations principle for edge and $p$-star densities. We use the large deviations principle to give proofs, in Section 5, of our main results.

2. Description of the models

A directed graph on $n$ nodes will be represented by a matrix $X = (X_{ij})_{1 \leq i,j \leq n}$, where $X_{ij} = 1$ if there is a directed edge from node $i$ to node $j$, and $X_{ij} = 0$ otherwise. For simplicity, we allow for $X_{ii} = 1$, though this will not affect our results. Let $e(X)$ (resp. $s(X)$) be the directed edge and outward $p$-star homomorphism densities of $X$:

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

$$s(X) := n^{-p-1} \sum_{1 \leq i_1,j_1,j_2,\ldots,j_p \leq n} X_{ij_1}X_{ij_2}\cdots X_{ij_p}.$$  \hspace{1cm} (2.1)

Here, $p$ is an integer $\geq 2$. The reason for the term homomorphism density is as follows. For a given graph $X$, if $\text{hom}_e(X)$ (resp. $\text{hom}_s(X)$) are the number of homomorphisms – edge-preserving maps – from a directed edge (resp. outward $p$-star) into $X$, then

$$e(X) = \frac{\text{hom}_e(X)}{n^2}, \quad s(X) = \frac{\text{hom}_s(X)}{n^{p+1}},$$

with the denominators giving the total number of maps from a directed edge (resp. outward $p$-star) into $X$.

Let $\mathbb{P}_n$ be the uniform probability measure on the set of directed graphs on $n$ nodes. Thus, $\mathbb{P}_n$ is the uniform probability measure on the set of $n \times n$ matrices
with entries in \{0, 1\}. For \( e, s \in [0, 1] \) and \( \delta > 0 \), define
\[
\psi^\delta_n(e, s) = \frac{1}{n^2} \log P_n(e(X) \in (e - \delta, e + \delta), s(X) \in (s - \delta, s + \delta)).
\]
Throughout, \( \log \) is the natural logarithm, and we use the convention \( 0 \log 0 = 0 \).

We are interested in the limit
\[
\psi(e, s) := \lim_{\delta \to 0^+} \lim_{n \to \infty} \psi^\delta_n(e, s).
\]
(2.2)
The function in (2.2) will be called the \textit{limiting entropy density}. This is the directed graph version of the quantity studied in [14]. See also [25, 26, 27] for related work where triangles are constrained instead of \( p \)-stars.

For \( \beta_1, \beta_2 \in \mathbb{R}, e, s \in [0, 1] \) and \( \delta > 0 \), define
\[
\psi^\delta_n(e, \beta_2) = \frac{1}{n^2} \log \mathbb{E}_n \left[ e^{n^2 \beta_2 s(X)} 1_{\{e(X) \in (e - \delta, e + \delta)\}} \right],
\]
\[
\psi^\delta_n(\beta_1, s) = \frac{1}{n^2} \log \mathbb{E}_n \left[ e^{n^2 \beta_1 e(X)} 1_{\{s(X) \in (s - \delta, s + \delta)\}} \right].
\]
We will also be interested in the limits
\[
\psi(e, \beta_2) := \lim_{\delta \to 0^+} \lim_{n \to \infty} \psi^\delta_n(e, \beta_2),
\]
\[
\psi(\beta_1, s) := \lim_{\delta \to 0^+} \lim_{n \to \infty} \psi^\delta_n(\beta_1, s).
\]
(2.3)
The quantities in (2.3) will be called \textit{limiting free energy densities}. They are the directed graph versions of the quantities studied in [15]. We abuse notation by using the same symbols \( \psi \) and \( \psi^\delta_n \) to represent different functions in (2.2) and (2.3) (and in (2.4) below), but the meaning will be clear from the arguments of these functions, which will be written \((e, s), (e, \beta_2), (\beta_1, s)\) (or \((\beta_1, \beta_2)\) as below). When it is clear which function we refer to, we may simply write \( \psi \) without any arguments.

We will prove in Section 5 that the limits in (2.2) and (2.3) exist by appealing to a variational principle. Maximizers of this variational problem are associated with the asymptotic structure of the associated constrained directed graphs. See [14, 15, 24, 25, 26, 27] for discussions and related work in the undirected graph setting.

Closely related to (2.2) and (2.3) is the limit
\[
\psi(\beta_1, \beta_2) := \lim_{n \to \infty} \frac{1}{n^2} \log \mathbb{E} \left[ e^{n^2(\beta_1 e(X) + \beta_2 s(X))} \right],
\]
(2.4)
which was studied extensively in Aristoff and Zhu [1]. There it was shown that \( \psi(\beta_1, \beta_2) \) is analytic except along a certain phase transition curve \( \beta_2 = q(\beta_1) \), corresponding to an interface across which the edge density changes sharply. See Radin and Yin [24] for similar results in the undirected graph setting. Though the results in [1] and [24] will be useful in our analysis, it is not obvious how (2.4) is related to (2.2) and (2.3), as discussed below.

In this article we investigate properties of the limiting entropy density and free energy densities in (2.2) and (2.3). In statistical physics modeling there is a hierarchy analogous to (2.2)-(2.3)-(2.4), with (for example) particle density and energy density in place of \( e(X) \) and \( s(X) \), and temperature and chemical potential in place of \( \beta_1 \) and \( \beta_2 \). The statistical physics versions of (2.2)-(2.3)-(2.4) correspond to the \textit{microcanonical}, \textit{canonical} and \textit{grand canonical ensembles}, respectively. In that
setting, there are curves like $q$ along which the free energy densities are not analytic, and these correspond to physical phase transitions, for example the familiar solid/liquid and liquid gas transitions; see Gallavotti [10]. (There is no proof of this statement, though it is widely believed; see however Lebowitz et al. [17].) In statistical physics, it is well-known that the models in this hierarchy have a very simple relationship involving Legendre transforms, which arise from maximizing entropy with constraints. In statistical physics, the Legendre transforms are simple because their domains are convex. However, the domain of $\psi(e,s)$ is not convex, which complicates the relationship between $\psi(e,s)$ and $\psi(e,\beta_2)$, $\psi(\beta_1,s)$. In particular, we find singularities in $\psi(e,\beta_2)$ and $\psi(\beta_1,s)$, but not in $\psi(e,s)$. (In [1] we show $\psi(\beta_1,\beta_2)$ has singularities as well.) See Section 5 of Radin and Sadun [27] for a discussion of this general issue in a closely related random graph model.

3. Results

To state our results we need the following. For $x \in [0,1]$, define
\[
\ell(x) = \beta_1 x + \beta_2 x^p - x \log x - (1-x) \log(1-x),
\]
\[
I(x) = x \log x + (1-x) \log(1-x) + \log 2.
\]
Of course $\ell$ depends on $\beta_1$ and $\beta_2$, but we omit this to simplify notation. Clearly, $\ell$ and $I$ are analytic on $(0,1)$ and continuous on $[0,1]$. The function $\ell$ is essential to understanding the ERGM limiting free energy density [1, 24].

Theorem 1 (Radin and Yin [24], Aristoff and Zhu [1]). For each $(\beta_1,\beta_2)$ the function $\ell$ has either one or two local maximizers. There is a curve $\beta_2 = q(\beta_1)$, $\beta_1 \leq \beta_1^c$, with the endpoint $(\beta_1^c,\beta_2^c) = (\log((p-1)-\frac{p}{p-1})$, $\frac{p}{p-1})$. Such a curve will be called the phase transition curve, and its endpoint the critical point. Theorem 1 will be used extensively in most of our proofs; because of this, we will often not refer to it explicitly. (We comment that the last statement of Theorem 1, not made explicit in [24] and [1], is proved in Proposition 7 in Section 5 below.) We will sometimes write $x_1 = x_2 = (p-1)/p$ for the local maximizer of $\ell$ at the critical point. Note that the last part of the theorem implies
\[
0 < x_1 \leq \frac{p-1}{p} \leq x_2 < 1.
\]
Theorem 2. The limiting entropy density $\psi = \psi(e, s)$ is analytic in

$$D := \{(e, s) : e^p < s < e, 0 \leq e \leq 1\}$$

and equals $-\infty$ outside $\tilde{D}$. With

$$(e^c, s^c) = \left(\frac{p-1}{p}, \left(\frac{p-1}{p}\right)^p\right)$$

and

$$D^{up} = \{(e, s) : s = e\},$$

we have the semi-explicit formula

$$\psi(e, s) = \begin{cases} 
-\frac{e-x_1}{x_2-x_1} I(x_1) - \frac{e-x_2}{x_2-x_1} I(x_2), & (e, s) \in \tilde{D} \setminus (D^{up} \cup \{(e^c, s^c)\}) \\
-I(e^c), & (e, s) = (e^c, s^c) \\
-\log 2, & (e, s) \in D^{up}
\end{cases} \quad (3.2)$$

where $0 < x_1 < x_2 < 1$ are the unique global maximizers of $\ell$ along the phase transition curve $q$ which satisfy

$$\frac{x_2 - e}{x_2 - x_1} x_1^p + \frac{e - x_1}{x_2 - x_1} x_2^p = s.$$ 

Moreover, $\psi$ is continuous on $\tilde{D}$, and the first order partial derivatives of $\psi$ are continuous on $\tilde{D} \setminus D^{up}$ but diverge on $D^{up}$. When $p = 2$, we have the explicit formula

$$\psi(e, s) = -I \left(\frac{1}{2} + \sqrt{s - e + \frac{1}{4}}\right), \quad (e, s) \in \tilde{D}.$$ 

In Theorem 2, the formula is only semi-explicit because $x_1$ and $x_2$ depend on $e$ and $s$. Note that the formula depends only on $e$ and $s$. (To understand the dependence better, see the subsection uniqueness of the optimizer: geometric proof in the proof of Theorem 2)

Note that we have not found any interesting singular behavior of $\psi$, in contrast with the recent results of Kenyon et. al. [14] for the undirected version of the model. On the other hand, we are able to prove that our graphs are bipodal, whereas in [14] it was proved only that the graphs are multipodal (though simulation evidence from the paper suggests bipodal structure).

Our next main result concerns $\psi(e, \beta_2)$ and $\psi(\beta_1, s)$.

Theorem 3. (i) There is a $U$-shaped region

$$U_e = \{(e, \beta_2) : x_1 < e < x_2, \beta_2 > \beta_2^e\}$$

whose closure has lowest point

$$(e^c, \beta_2^c) = \left(\frac{p-1}{p}, \left(\frac{p-1}{p}\right)^p\right)$$

such that the limiting free energy density $\psi = \psi(e, \beta_2)$ is analytic outside $\partial U_e$. The limiting free energy density has the formula

$$\psi(e, \beta_2) = \begin{cases} 
\beta_2 e^p - I(e), & (e, \beta_2) \in U_e^c \\
\beta_2 [\frac{e-x_1}{x_2-x_1} x_1^p + \frac{e-x_2}{x_2-x_1} x_2^p] \\
- \left[\frac{e-x_1}{x_2-x_1} I(x_1) + \frac{e-x_2}{x_2-x_1} I(x_2)\right], & (e, \beta_2) \in U_e
\end{cases} \quad (3.3)$$
where $0 < x_1 < x_2 < 1$ are the global maximizers of $\ell$ at the point $(q^{-1}(\beta_2), \beta_2)$ on the phase transition curve. In particular, $\partial^2 \psi / \partial e^2$ has jump discontinuities across $\partial U_e$ away from $(e^c, \beta_2^c)$, and $\partial^4 \psi / \partial e^4$ is discontinuous at $(e^c, \beta_2^c)$.

(ii) There is a U-shaped region

$$U_s = \{(\beta_1, s) : x_1^p < s < x_2^p, \beta_1 < \beta_1^p \}$$

whose closure has rightmost point

$$\left(\beta_1^p, s^p\right) = \left(\log(p-1) - \frac{p}{p-1} \left(\frac{p-1}{p}\right)^p\right)$$

such that the limiting free energy density $\psi = \psi(\beta_1, s)$ is analytic outside $\partial U_s$. The limiting free energy density has the formula

$$\psi(\beta_1, s) = \begin{cases} 
\beta_1 s^p - I(s^p), & (\beta_1, s) \in U_s^c \\
\beta_1 \left[\frac{x_2^p-x_1^p}{x_2^p-x_1} x_1 + \frac{x_1^p-x_2^p}{x_2^p-x_1} x_2\right] - \left[\frac{x_2^p-x_1^p}{x_2^p-x_1} I(x_1) + \frac{x_1^p-x_2^p}{x_2^p-x_1} I(x_2)\right], & (\beta_1, s) \in U_s
\end{cases}$$

(3.4)

where $0 < x_1 < x_2 < 1$ are the global maximizers of $\ell$ at the point $(\beta_1, q(\beta_1))$ on the phase transition curve. In particular, $\partial^2 \psi / \partial s^2$ has jump discontinuities across $\partial U_s$ away from $(\beta_1^p, s^p)$, and $\partial^4 \psi / \partial s^4$ is discontinuous at $(\beta_1^p, s^p)$.

The sharp change in Theorem 3 is called a phase transition (because of the singularity in the derivatives of $\psi$). The phase transition corresponds to a sharp change from uniform to bipodal structure of the optimizers of the variational problem for (2.3); see the discussion below Theorem 6. The bipodal structure in the regions $U_e$ and $U_s$ is sometimes called a replica symmetry breaking phase.

In contrast with Theorem 2, the $x_1$ and $x_2$ in Theorem 3 are functions of $\beta_1$ or $\beta_2$ only and do not depend on $e$ or $s$. See Figure 1 for the region $D$ from Theorem 2 and Figure 2 for the U-shaped regions $U_e$ and $U_s$ in Theorem 3.
4. Large Deviations

We will need the following terminology before proceeding. A sequence \((Q_n)_{n \in \mathbb{N}}\) of probability measures on a topological space \(X\) is said to satisfy a large deviation principle with speed \(a_n\) and rate function \(J: X \to \mathbb{R}\) if \(J\) is non-negative and lower semicontinuous, and for any measurable set \(A\),

\[
\inf_{x \in A^o} J(x) \leq \liminf_{n \to \infty} \frac{1}{a_n} \log Q_n(A) \leq \limsup_{n \to \infty} \frac{1}{a_n} \log Q_n(A) \leq \inf_{x \in A} J(x).
\]

Here, \(A^o\) is the interior of \(A\) and \(A\) is its closure. See e.g. Dembo and Zeitouni [6] or Varadhan [32].

We will equip the set \(G\) of measurable functions \([0,1] \to [0,1]\) with the cut norm, written \(\|\cdot\|_{\Box}\) and defined by

\[
\|g\|_{\Box} = \sup \left| \int_A g(x) \, dx \right|,
\]

where the supremum is taken over measurable subsets \(A\) of \([0,1]\).

**Theorem 4.** The sequence of probability measures \(P_n (e(X) \in \cdot, s(X) \in \cdot)\) satisfies a large deviation principle on the space \([0,1]^2\) with speed \(n^2\) and rate function

\[
\inf_{g \in \mathcal{G}_{e,s}} \int_0^1 I(g(x)) \, dx,
\]

where \(\mathcal{G}_{e,s}\) is the set of measurable functions \(g: [0,1] \to [0,1]\) such that

\[
\int_0^1 g(x) \, dx = e, \quad \int_0^1 g(x)^p \, dx = s.
\]

By convention, \(I(x) = \infty\) if \(x \notin [0,1]\), and the infimum is \(\infty\) if \(\mathcal{G}_{e,s}\) is empty.
The following is an immediate consequence of Theorem 4.

**Theorem 5.** For any $e, s \in [0, 1]$,
\[
\psi(e, s) = \sup_{G_{e,s}} \left[ -\int_{0}^{1} I(g(x)) \, dx \right].
\]

The next theorem is an easy consequence of Theorem 4 and Varadhan’s lemma (see e.g. [6]).

**Theorem 6.** For any $e, s \in [0, 1]$ and $\beta_1, \beta_2 \in \mathbb{R}$,
\[
\psi(e, \beta_2) = \sup_{G_{e}} \left[ \beta_2 \int_{0}^{1} g(x)^p \, dx - \int_{0}^{1} I(g(x)) \, dx \right],
\]
\[
\psi(\beta_1, s) = \sup_{G_{s}} \left[ \beta_1 \int_{0}^{1} g(x) \, dx - \int_{0}^{1} I(g(x)) \, dx \right],
\]
where $G_{e,s}$ (resp. $G_{e,s}$) is the set of measurable functions $g : [0, 1] \to [0, 1]$ satisfying
\[
\int_{0}^{1} g(x) \, dx = e \quad (\text{resp.} \int_{0}^{1} g(x)^p \, dx = s).
\]

From Theorem 4, the proofs of Theorem 5 and Theorem 6 are standard, so we omit them.

Theorem 2 and Theorem 4 together imply that for large number of nodes, the graph has the following behavior. Approximately $n(x_2 - e)/(x_2 - x_1)$ of the nodes each have on average $nx_1$ outward pointing edges, while the other approximately $n(e - x_1)(x_2 - x_1)$ nodes each have on average $nx_2$ outward pointing edges. When $x_1 \neq x_2$ we call this structure bipodal; otherwise we call it uniform.

Chatterjee and Varadhan [4] established large deviations for undirected random graphs on the space of graphons (see also Lovasz [19]). Szemerédi’s lemma was needed in order to establish the compactness needed for large deviations. Since our model consists of directed graphs, the results in [4] do not apply directly. Theorem 4 avoids these technical difficulties: it is large deviations principle only on the space $[0, 1]^2$ of edge and star densities, instead of on the (quotient) function space of graphons. Our proof relies on the simplicity of our edge/directed $p$-star model; it cannot be easily extended to the case where edges and directed triangles (or other more complicated directed subgraphs) are constrained. We expect that these models can be handled by adapting the results of [4] to the directed case.

In Aristoff and Zhu [1], it was proved that
\[
\lim_{n \to \infty} \frac{1}{n^2} \log \mathbb{E} \left[ e^{n^2 \psi(e(X), s(X))} \right] = \sup_{0 \leq x \leq 1} (\beta_1 x + \beta_2 x^p - I(x)). \tag{4.2}
\]
Observe that the Gärtner-Ellis theorem cannot be used to obtain the large deviations principle in Theorem 4 above, due to the fact, first observed in Radin and Yin [23], that the right hand side of (4.2) is not differentiable. Instead, we used Mogulskii’s theorem and the contraction principle in the proof of Theorem 4.

On the other hand, once we have established the large deviations principle in Theorem 4, we can use Varadhan’s lemma to obtain an alternative expression for the limiting free energy,
\[
\lim_{n \to \infty} \frac{1}{n^2} \log \mathbb{E} \left[ e^{n^2 \psi(e(X), s(X))} \right] = \sup_{(e, s) \in [0, 1]^2} (\beta_1 e + \beta_2 s + \psi(e, s)).
\]
The limiting free energy in the directed and undirected models differ by only a constant factor of $1/2$ (see Chatterjee and Diaconis [3] and Radin and Yin [24] for the undirected model, and Aristoff and Zhu [1] for the directed model). On the other hand, the limiting entropy density $\psi(e, s)$ we obtain here differs nontrivially from the one recently obtained in Kenyon et al. [14] for undirected graphs.

5. Proofs

We start with the proof of the large deviations principle of Section 4. Then we turn to the proofs of our main results in Section 3.

Proof of Theorem 4. Observe that $(X_{ij})_{1 \leq i, j \leq n}$ are i.i.d. Bernoulli random variables that take the value 1 with probability $\frac{1}{2}$ and 0 with probability $\frac{1}{2}$. Therefore, the logarithm of the moment generating function of $X_{ij}$ is, for $\theta \in \mathbb{R}$,

$$\log \mathbb{E}[e^{\theta X_{ij}}] = \log \left( \frac{1}{2} e^{\theta} + \frac{1}{2} \right) = \log(e^{\theta} + 1) - \log 2.$$ 

Its Legendre transform is

$$\sup_{\theta \in \mathbb{R}} \{\theta x - \log \mathbb{E}[e^{\theta X_{ij}}]\} = x \log x + (1 - x) \log(1 - x) + \log 2 = I(x),$$

where by convention $I(x) = \infty$ for $x \notin [0, 1]$. Let $Y_i$ be the $i$th entry of the vector $(X_{11}, X_{12}, \ldots, X_{1n}, X_{21}, X_{22}, \ldots, X_{2n}, \ldots, X_{n1}, X_{n2}, \ldots, X_{nn})$. Then, $Y_i$ are i.i.d. Bernoulli random variables. Mogulskii theorem (see e.g. Dembo and Zeitouni [6]) shows that

$$\mathbb{P} \left( \frac{1}{n^2} \sum_{i=1}^{\lfloor nx \rfloor} Y_i \in \cdot, 0 \leq x \leq 1 \right)$$

satisfies a sample path large deviation principle on the space $L_\infty[0, 1]$ consisting of functions on $[0, 1]$ equipped with the supremum norm; the rate function is given by

$$I(G) = \begin{cases} \int_0^1 I(G'(x)) \, dx & \text{if } G \in \mathcal{AC}_0[0, 1] \\ +\infty & \text{otherwise} \end{cases},$$

where $\mathcal{AC}_0[0, 1]$ is the set of absolutely continuous functions defined on $[0, 1]$ such that $G(0) = 0$ and $0 \leq G'(x) \leq 1$. The restriction $0 \leq G'(x) \leq 1$ comes from the fact that $0 \leq Y_i \leq 1$. On the other hand, for any $\epsilon > 0$,

$$\limsup_{n \to \infty} \frac{1}{n^2} \log \mathbb{P} \left( \sup_{0 \leq x \leq 1} \left| \frac{1}{n^2} \sum_{i=1}^{\lfloor nx \rfloor} \sum_{j=1}^{n} X_{ij} - \frac{1}{n^2} \sum_{i=1}^{\lfloor nx \rfloor} Y_i \right| \geq \epsilon \right)$$

$$\leq \limsup_{n \to \infty} \frac{1}{n^2} \log \mathbb{P} \left( \sup_{0 \leq i \leq n^2 - n} \{Y_{i+1} + Y_{i+2} + \cdots Y_{i+n} \} \geq n^2 \epsilon \right)$$

$$= -\infty,$$

since

$$\sup_{0 \leq i \leq n^2 - n} \{Y_{i+1} + Y_{i+2} + \cdots Y_{i+n} \} \leq n.$$
Therefore,
\[ \mathbb{P} \left( \frac{1}{n^2} \sum_{i=1}^{\lfloor nx \rfloor} \sum_{j=1}^{n} X_{ij} \in \cdot, 0 \leq x \leq 1 \right) \]
satisfies a large deviation principle with the same space and rate function as
\[ \mathbb{P} \left( \frac{1}{n^2} \sum_{i=1}^{\lfloor nx \rfloor} Y_i \in \cdot, 0 \leq x \leq 1 \right). \]

To complete the proof, we need to use the contraction principle, see e.g. Dembo and Zeitouni [6] or Varadhan [32]. Given \( G \in \mathcal{AC}_0[0,1] \), we may write \( G(x) = \int_0^x g(y)dy \) for a measurable function \( g : [0,1] \to [0,1] \). It is easy to see that if \( G_n \in \mathcal{AC}_0[0,1] \) and \( G_n \to G \) in the supremum norm, then \( g_n \to g \) in the cut norm. Hence, if \( G_n \to G \) in the supremum norm, then
\[ \int_0^1 g_n(x)dx \to \int_0^1 g(x)dx. \]
Moreover, for any \( p \geq 2 \),
\[ \int_0^1 g_n(x)^p - g(x)^pdx = \left[ \int_{g_n \geq g} g_n(x)^p - g(x)^pdx \right] - \left[ \int_{g_n < g} g(x)^p - g_n(x)^pdx \right], \]
and since \( g_n \to g \) in the cut norm and \( 0 \leq g_n, g \leq 1 \), the mean value theorem shows that
\[ \int_{g_n \geq g} g_n^p(x) - g(x)^pdx \leq p \int_{g_n \geq g} g_n(x) - g(x)dx \to 0 \]
and
\[ \int_{g_n < g} g^p(x) - g_n(x)^pdx \leq p \int_{g_n < g} g(x) - g_n(x)dx \to 0. \]
Therefore, the maps
\[ G \mapsto \int_0^1 G'(x)dx, \quad G \mapsto \int_0^1 (G'(x))^pdx, \]
are continuous. The result follows from the contraction principle. \( \Box \)

The following proofs are for our main results in Section 3.

**Proof of Theorem 2.** By Theorem 5,
\[ \psi(e,s) = \sup_{g \in \mathcal{G}_{e,s}} - \int_0^1 I(g(x))dx \quad (5.1) \]
where we recall \( \mathcal{G}_{e,s} \) is the set of measurable functions \( g : [0,1] \to [0,1] \) satisfying
\[ \int_0^1 g(x)dx = e, \quad \int_0^1 g(x)^pdx = s. \quad (5.2) \]

**Domain of \( \psi(e,s) \).** By Jensen’s inequality,
\[ s = \int_0^1 g(x)^pdx \geq \left( \int_0^1 g(x)dx \right)^p = e^p. \]
On the other hand, since \( g \) takes values in \([0,1]\) and \( p > 1 \),
\[ s = \int_0^1 g(x)^pdx \leq \int_0^1 g(x)dx = e. \]
Hence by convention \(\psi(e, s)\) is infinite outside \(\bar{D}\). We will show later in the proof that \(\psi(e, s)\) is finite in \(\bar{D}\).

**Optimizing over a quotient space.** So that we can use standard variational techniques, we show that it suffices to optimize over a compact quotient space of \(G_{e, s}\). Recall that \(G\) is the set of measurable functions \([0, 1] \to [0, 1]\) endowed with the cut norm (4.1). Let \(\tilde{G}\) be the quotient space obtained by the following equivalence relation: \(g \sim h\) if and only if there is a measure-preserving bijection \(\sigma : [0, 1] \to [0, 1]\) such that \(g = h \circ \sigma\). Note that for any such \(\sigma\) we have \(\|g\|_{\square} = \|g \circ \sigma\|_{\square}\), and so

\[
\delta_{\square}(\tilde{g}, \tilde{h}) := \inf_{\sigma} \|g - h \circ \sigma\|_{\square}
\]
defines a metric on \(\tilde{G}\). With this metric \(\tilde{G}\) is compact [13]. Observe that

\[
\psi(e, s) = \sup_{g \in G_{e, s}} - \int_0^1 I(g(x)) \, dx = \sup_{\tilde{g} \in \tilde{G}_{e, s}} - \int_0^1 I(\tilde{g}(x)) \, dx
\]

where \(\tilde{G}_{e, s}\) is the projection of \(G_{e, s}\) in the quotient space, and on the right hand side \(g\) is any element of the equivalence class of \(\tilde{g}\). Next we check that the functionals

\[
\tilde{g} \mapsto - \int_0^1 I(\tilde{g}(x)) \, dx, \quad \tilde{g} \mapsto \int_0^1 g(x) \, dx, \quad \tilde{g} \mapsto \int_0^1 g(x)^p \, dx,
\]

(5.3) defined on \(\tilde{G}\), are all continuous. Let \(\tilde{g}_n\) be a sequence in \(\tilde{G}\) converging to \(\tilde{g}\). We will show that

\[
\left| \int_0^1 F(g(x)) \, dx - \int_0^1 F(g_n(x)) \, dx \right| \to 0 \text{ as } n \to \infty
\]

(5.4)

for any uniformly continuous function \(F\) defined on \([0, 1]\). For each \(n\), choose \(\sigma_n\) such that

\[
\|g - g_n \circ \sigma_n\|_{\square} \to 0 \text{ as } n \to \infty.
\]

For any \(\delta > 0\), define

\[
A_{n, \delta} = \{ x : |g(x) - g_n(\sigma_n(x))| \geq \delta \}.
\]

As the cut norm is equivalent to the \(L^1\) norm (this is true only in one dimension; see [13]), we have for any \(\delta > 0\),

\[
|A_{n, \delta}| \to 0 \text{ as } n \to \infty,
\]

(5.5)

where \(|A_{n, \delta}|\) is the Lebesgue measure of \(A_{n, \delta}\). Now, observe that

\[
\left| \int_0^1 F(g(x)) \, dx - \int_0^1 F(g_n(x)) \, dx \right|
\]

\[
= \left| \int_0^1 F(g(x)) \, dx - \int_0^1 F(g_n \circ \sigma_n(x)) \, dx \right|
\]

\[
\leq 2|A_{n, \delta}| \sup_{x \in [0, 1]} |F(x)| + \left| \int_{[0, 1]\setminus A_{n, \delta}} [F(g(x)) - F(g_n \circ \sigma_n(x))] \, dx \right|.
\]

(5.6)
Let $\epsilon > 0$. Using uniform continuity of $F$, let $\delta > 0$ be such that $|x - y| < \delta$ implies $|F(x) - F(y)| < \epsilon$. Then (5.6) shows that
\[
\left| \int_0^1 F(g(x)) \, dx - \int_0^1 F(g(x)) \, dx \right| \leq 2|A_{n,\delta}| \sup_{x \in [0,1]} |F(x)| + \epsilon.
\] (5.7)

Now (5.5) establishes (5.4), as desired. These arguments show that there exist (global) maximizers $g$ of
\[
\psi(e, s) = \sup_{g \in G_{e,s}} - \int_0^1 I(g(x)) \, dx.
\] (5.8)

**Bipodal structure of the optimizers.** If $(e, s) \in D^{up}$, then for any $g \in G_{e,s}$,
\[
|\{ x : g(x) \in [0,1] \}| = 1.
\]

Suppose then that $(e, s) \in \bar{D} \setminus D^{up}$. Since $I'(x) \to -\infty$ as $x \to 0$ and $I'(x) \to \infty$ as $x \to 1$, it is not hard to see that, given $(s, e) \in \bar{D} \setminus D^{up}$, there exists $\epsilon > 0$ such that any optimizers of (5.9) must be in the following set:
\[
G' := \{ g \in G : g(x) \in [e, 1 - \epsilon] \text{ for a.e. } x \in [0,1] \}.
\] (5.9)

To see this, note that if $g \in G_{e,s} \setminus G'$, then the values of $g$ can be adjusted to be $\epsilon$ distance away from 0 and 1 so that still $g \in G_{e,s}$ and $g$ attains a larger value for the integral in (5.8). Then, optimizing over $G'$, standard results in variational calculus (see [5], Theorem 9.1, pg. 178) show that optimizers $g$ satisfy, for all $\delta g \in G$,
\[
- \eta \int_0^1 I'(g(x)) \delta g(x) \, dx + \beta_1 \int_0^1 \delta g(x) \, dx + \beta_2 \int_0^1 pg(x)^{p-1} \delta g(x) \, dx = 0,
\] (5.10)

where $\eta \in \{0, 1\}$, $\beta_1, \beta_2 \in \mathbb{R}$ are Lagrange multipliers, and at least one of $\eta, \beta_1, \beta_2$ is nonzero. The integrals in (5.10) are the Fréchet derivatives of
\[
g \mapsto \int_0^1 I(g(x)) \, dx, \quad g \mapsto \int_0^1 g(x) \, dx, \quad g \mapsto \int_0^1 g(x)^p \, dx,
\]
evaluated at $\delta g \in G$; a simplified version of the arguments in (5.4) - (5.7) shows the Fréchet derivatives are continuous in $g \in G'$. (To apply the results mentioned in [5], we must switch to the uniform topology induced by the sup norm $|| \cdot ||_{\infty}$ on the Banach space of bounded measurable functions $[0,1] \to \mathbb{R}$. The statement about continuity of Fréchet derivatives then follows from the simple fact that $||g - h||_{\infty} < \epsilon$ implies $||g - h||_{1} < \epsilon$.)

When $\eta = 1$ (called the normal case), we see that for some $\beta_1, \beta_2$,
\[
\ell'(g(x)) = 0, \quad \text{for a.e. } x \in [0,1].
\]

When $\eta = 0$ (called the abnormal case), we find that $\beta_1 + p\beta_2 g(x)^{p-1} = 0$ for a.e. $x \in [0,1]$, so that $g$ is constant a.e. From (5.2) and Jensen’s inequality, this occurs precisely when $s = e^p$.

Let $g$ be a maximizer of (5.1). We have shown that:
(a) if $(e, s) \in D^{up}$, then $g(x) \in \{0,1\}$ for a.e. $x \in [0,1]$;
(b) if $(e, s) \in D$, then $\ell'(g(x)) = 0$ for a.e. $x \in [0,1]$; or
(c) if $s \in \bar{D} \setminus (D \cup D^{up})$, then $g$ is constant a.e.
Concerning case (b), Theorem 1 shows that, for each $(\beta_1, \beta_2)$, either $\ell'(y) = 0$ at a unique $y \in (0, 1)$ or $\ell'(y) = 0$ at exactly two points $0 < y_1 < y_2 < 1$. Thus, to maximize (5.11) it suffices to maximize

$$- \int_0^1 I(g(x)) \, dx$$

over the set of functions $g \in \mathcal{G}_{e,s}$ of the form

$$g(x) = \begin{cases} y_1, & x \in A \\ y_2, & x \notin A \end{cases}$$

(5.11)

where $|A| = \lambda \in [0, 1]$ and $0 \leq y_1 \leq y_2 \leq 1$. Observe that for such $g$,

$$- \int_0^1 I(g(x)) \, dx = -\lambda I(y_1) - (1 - \lambda)I(y_2),$$

$$\int_0^1 g(x) \, dx = \lambda y_1 + (1 - \lambda)y_2,$$

$$\int_0^1 g(x)^p \, dx = \lambda y_1^p + (1 - \lambda)y_2^p.$$  

It is therefore enough to maximize

$$- \lambda I(y_1) - (1 - \lambda)I(y_2)$$

subject to the constraints

$$\lambda y_1 + (1 - \lambda)y_2 = e,$$

$$\lambda y_1^p + (1 - \lambda)y_2^p = s.$$  

(5.13)

In case (a), we must have $y_1 = 0$, $y_2 = 1$ and $1 - \lambda = e = s$. In case (c), we may take $y_1 = y_2 = e$. It remains to consider (b). In this case we have seen that $0 < y_1 \leq y_2 < 1$. Moreover if $y_1 = y_2$ or $\lambda \in \{0, 1\}$ then (5.13) cannot be satisfied, so $y_1 < y_2$ and $\lambda \in (0, 1)$. Introducing Lagrange multipliers $\beta_1, \beta_2$, we see that

$$-\lambda \beta_1' + \lambda \beta_1 + \lambda p\beta_2 y_1^{p-1} = 0,$$

$$(1 - \lambda)\beta_2' + (1 - \lambda)\beta_1 + (1 - \lambda)p\beta_2 y_2^{p-1} = 0,$$

$$[I(y_1) - I(y_2)] + \beta_1(y_1 - y_2) + \beta_2(y_1^p - y_2^p) = 0.$$  

Thus,

$$\ell'(y_1) = \ell'(y_2) = 0, \quad \ell(y_1) = \ell(y_2).$$

This means that $y_1 = x_1 < x_2 = y_2$ are global maximizers of $\ell$ on the phase transition curve, away from the critical point.

**Uniqueness of the optimizer (geometric proof).** We must prove uniqueness for $(e, s) \in D$. Consider the class of lines

$$\lambda(x_1, x_1^p) + (1 - \lambda)(x_2, x_2^p), \quad 0 < \lambda < 1,$$

(5.14)

where $0 < x_1 < x_2 < 1$ are global maximizers of $\ell$ on the phase transition curve, away from the critical point. Since $x_1$ (resp. $x_2$) is strictly increasing (resp. strictly decreasing) in $\beta_1$ with $x_1 \leq x_2$, no two distinct lines of this class can intersect. Continuity of $x_1, x_2$ in $\beta_1$ along with (5.1) show that the union of all the lines equals $D$. Thus, given $(e, s) \in D$, there is a unique optimizer $g$ of the form (5.11), obtained by locating the unique line from (5.14) which contains the point $(e, s)$.
and choosing \( \lambda \) satisfying the constraint (5.13). Note that we have now established formula (3.2).

**Uniqueness of the optimizer (algebraic proof).** Fix \((e, s) \in D\). From (5.13),

\[
\lambda = \frac{e - x_2}{x_2 - x_1} = \frac{s - x_2^p}{x_2^p - x_1^p}
\]

and so

\[
e - x_2 = -q'(\beta_1)(s - x_2^p). \tag{5.15}
\]

We must show that (5.15) has a unique solution. Define

\[
F(\beta_1) := e - x_2 + q'(\beta_1)(s - x_2^p).
\]

Note that

\[
\lim_{\beta_1 \to -\infty} F(\beta_1) = e - 1 - (s - 1) = e - s \geq 0,
\]

and

\[
\lim_{\beta_1 \to \beta_1^*} F(\beta_1) = e - \left(\frac{p - 1}{p}\right)^2 - s \frac{p^{p-2}}{(p-1)^{p-1}} \leq e - \left(\frac{p - 1}{p}\right)^2 - \frac{p^{p-2}}{(p-1)^{p-1}}.
\]

Also define

\[
G(x) := x - \left(\frac{p - 1}{p}\right)^2 - x^p \frac{p^{p-2}}{(p-1)^{p-1}}, \quad 0 \leq x \leq 1.
\]

Then \(G(0) < 0\) and \(G(1) < 0\). Moreover,

\[
G'(x) = 1 - x^{p-1} \left(\frac{p}{p-1}\right)^{p-1}
\]

is positive if \(0 < x < \frac{p-1}{p}\) and it is negative if \(\frac{p-1}{p} < x < 1\). Finally,

\[
G \left(\frac{p - 1}{p}\right) = \frac{p - 1}{p} - \frac{(p - 1)^2}{p^2} - \frac{p - 1}{p}^p = 0.
\]

Therefore,

\[
\lim_{\beta_1 \to \beta_1^*} F(\beta_1) \leq e - \left(\frac{p - 1}{p}\right)^2 - e^p \frac{p^{p-2}}{(p-1)^{p-1}} \leq 0.
\]

Now by the Intermediate Value Theorem, there exists \(\beta_1^* \leq \beta_1^c\) such that \(F(\beta_1^*) = 0\).

Next we prove \(\beta_1^*\) is unique. Observe that

\[
F'(\beta_1) = -\left[1 + q'(\beta_1)x_2^{p-1}\right] \frac{\partial x_2}{\partial \beta_1} + q''(\beta_1)(s - x_2^p).
\]

Since \(0 \leq \lambda \leq 1\), we have \(s - x_2^p \leq 0\). We also know that \(q''(\beta_1) \geq 0\) and \(\partial x_2 / \partial \beta_1 > 0\). Moreover, since \(q'(\beta_1) = -\frac{x_1 - x_2}{x_1^{p-1} - x_2^{p-1}} < 0\)
and $0 < x_1 < \frac{e-1}{p} < x_2 < 1$, we have
\[ 1 + q'(\beta_1)px_2^{p-1} = 1 - \frac{x_1 - x_2}{x_1 - x_2} px_2^{p-1} < 0. \]
Hence, we conclude that $\partial F/\partial \beta_1 < 0$ for $\beta_1 < \beta_2^*$ and therefore $\beta_1^*$ is unique.

Regularity of $\psi(e,s)$. We turn now to the claimed regularity of $\psi(e,s)$, starting with analyticity.
Fix $e \in (0, 1)$. Then each $s \in (e^p, e)$ satisfies, for some $x_1 < x_2$,
\[ \frac{x_2 - e}{x_2 - x_1} x_1 + \frac{e - x_1}{x_2 - x_1} x_2^p = s. \]
(5.16)
We claim that (5.16) defines $\beta_1$ implicitly as an analytic function of $s$ for $s \in (e^p, e)$. By differentiating the left hand side of (5.16) with respect to $\beta_1$, we find the expression
\[ \left( \frac{x_1 - e}{x_2 - x_1} \frac{\partial x_2}{\partial \beta_1} + \frac{e - x_2}{x_2 - x_1} \frac{\partial x_1}{\partial \beta_1} \right) \frac{x_2^p - x_1^p}{x_2 - x_1} - \frac{x_1 - e}{x_2 - x_1} \frac{\partial x_2}{\partial \beta_1} p x_2^{p-1} - \frac{e - x_2}{x_2 - x_1} \frac{\partial x_1}{\partial \beta_1} p x_1^{p-1}. \]
By the mean value theorem, there is $x_1 < y < x_2$ such that this expression becomes
\[ \left[ \frac{x_1 - e}{x_2 - x_1} \frac{\partial x_2}{\partial \beta_1} (py - 1 - px_2^{p-1}) \right] + \left[ \frac{e - x_2}{x_2 - x_1} \frac{\partial x_1}{\partial \beta_1} (py - 1 - px_1^{p-1}) \right]. \]
Since $\partial x_1/\partial \beta_1 > 0$ and $\partial x_2/\partial \beta_1 < 0$, each of the terms in brackets is negative, so this expression is nonzero. By the analytic implicit function theorem [16], we conclude that $\beta_1$ is an analytic function of $s$ inside $D$. Similar arguments show that $\beta_1$ is an analytic function of $e$ inside $D$. (By Theorem 1, this means $\beta_2$ must also be an analytic function of $e$ and $s$ inside $D$.) Since $x_1$ and $x_2$ are analytic functions of $\beta_1$, we see that $x_1$ and $x_2$ are analytic functions of $e$ and $s$ inside $D$.
Inspecting (3.2), we conclude that $\psi = \psi(e,s)$ is analytic in $D$.

Next we show that $\psi$ is continuous on $D$. We have already shown that $\psi$ is analytic, hence continuous, in $D$. It is easy to check that $\psi$ is continuous along each line
\[ \lambda(x_1, x_2^p) + (1 - \lambda)(x_2, x_2^p), \quad 0 \leq \lambda \leq 1, \]
and that the restriction of $\psi$ to the lower boundary \{(e, s) : s = e, 0 < e < 1\} is continuous. This is enough to conclude that $\psi$ is continuous on $\overline{D \setminus D_{op}}$. Finally for $(e_0, e_0) \in D_{op}$, we have
\[ \lim_{(e,s) \to (e_0,e_0)} \psi(e,s) = \lim_{x_1 \to 0, x_2 \to 1} - \frac{x_2 - e}{x_2 - x_1} I(x_1) - \frac{e - x_1}{x_2 - x_1} I(x_2) = - \log 2 = \psi(e_0, e_0). \]

Next we prove continuity of the first order derivatives on $\overline{D \setminus D_{op}}$. It suffices to show that: (i) the first order partial derivatives of $\psi$ are continuous in $D$; and (ii) the limits of the first order partial derivatives of $\psi$ at the lower boundary \{(e, s) : s = e^p, 0 < e < 1\} exist. With
\[ \lambda = \frac{x_2 - e}{x_2 - x_1} \]
and using (3.2), we see that for $(e,s) \in D$,
\[ \frac{\partial \psi}{\partial s} = \frac{\partial \lambda}{\partial s} (I(x_1) - I(x_2)) + \lambda I'(x_1) \frac{\partial x_1}{\partial s} + (1 - \lambda) I'(x_2) \frac{\partial x_2}{\partial s}. \]
(5.17)
Using the fact that $I(x) = \beta_1 x + \beta_2 x^p - \ell(x) + \log 2$,
\[
\frac{\partial \psi}{\partial s} = \frac{\partial \lambda}{\partial s}(\beta_1 x_1 + \beta_2 x_2^p - \beta_1 x_1 - \beta_2 x_2^p) + \lambda \frac{\partial x_1}{\partial s} \left( \beta_1 + p \beta_2 x_1^{p-1} \right) + (1 - \lambda) \frac{\partial x_2}{\partial s} \left( \beta_1 + p \beta_2 x_2^{p-1} \right).
\]
It is straightforward to compute that
\[
\frac{\partial \lambda}{\partial s} = \lambda \frac{\partial x_1}{\partial s} \frac{1}{x_2 - x_1} + (1 - \lambda) \frac{\partial x_2}{\partial s} \frac{1}{x_2 - x_1}.
\]
(5.18)
Thus,
\[
\frac{\partial \psi}{\partial s} = - \left( \lambda \frac{\partial x_1}{\partial s} + (1 - \lambda) \frac{\partial x_2}{\partial s} \right) \left( \beta_1 + \beta_2 \frac{x_2^p - x_1^p}{x_2 - x_1} \right) + \lambda \frac{\partial x_1}{\partial s} \left( \beta_1 + p \beta_2 x_1^{p-1} \right) + (1 - \lambda) \frac{\partial x_2}{\partial s} \left( \beta_1 + p \beta_2 x_2^{p-1} \right)
\]
\[= \beta_2 \left[ \lambda \frac{\partial x_1}{\partial s} \left( px_1^{p-1} - \frac{x_2^p - x_1^p}{x_2 - x_1} \right) + (1 - \lambda) \frac{\partial x_2}{\partial s} \left( px_2^{p-1} - \frac{x_2^p - x_1^p}{x_2 - x_1} \right) \right].\]
Differentiating $\lambda x_2^p + (1 - \lambda) x_1^p = s$ with respect to $s$ and using (5.18), we find that
\[1 = \lambda \frac{\partial x_1}{\partial s} \left( px_1^{p-1} - \frac{x_2^p - x_1^p}{x_2 - x_1} \right) + (1 - \lambda) \frac{\partial x_2}{\partial s} \left( px_2^{p-1} - \frac{x_2^p - x_1^p}{x_2 - x_1} \right),\]
and so
\[\frac{\partial \psi}{\partial s} = \beta_2.\]
We have already seen that $\beta_2$ is an analytic, hence continuous, function of $(e, s)$ inside $D$. Since
\[q^{-1}(\beta_2) + p \beta_2 x_i^{p-1} - I'(x_i) = 0, \quad i = 1, 2,\]
we see that for $e_0 \in (0, 1),$
\[\lim_{(e, s) \to (e_0, e_0)} \beta_2 = \lim_{x_i \to e_0} \frac{I'(x_i) - q^{-1}(\beta_2)}{px_i^{p-1}} = \frac{I'(e_0) - \beta_1^*}{p e_0^{p-1}}\]
where $i = 1$ if $e_0 \in (0, (p-1)/p)$ and otherwise $i = 2$. Also, for any $e_0 \in [0, 1],$
\[\lim_{(e, s) \to (e_0, e_0)} \beta_2 = \lim_{x_1 \to 0} \beta_2 = \infty.\]
Proofs of regularity for $\partial \psi/\partial e$ are similar so we omit them.

*Explicit formula when $p = 2.* When $p = 2$, we can explicitly solve
\[\lambda x_1 + (1 - \lambda) x_2 = e\]
\[\lambda x_1^2 + (1 - \lambda) x_2^2 = s\]
to obtain
\[x_1 = \frac{1 - \sqrt{1 - 4(e - s)}}{2} \quad x_2 = \frac{1 + \sqrt{1 - 4(e - s)}}{2}\]
and
\[ \lambda = \frac{x_2 - e}{x_2 - x_1} = \frac{\sqrt{1 - 4(e - s) + 1 - 2e}}{2\sqrt{1 - 4(e - s)}}. \]

This yields
\[
\psi(e, s) = -\lambda I(x_1) - (1 - \lambda)I(x_2)
\]
\[
= -\left( \frac{1}{2} + \frac{1 - 2e}{2\sqrt{1 - 4(e - s)}} \right) I\left( \frac{1}{2} - \frac{1}{2}\sqrt{1 - 4(e - s)} \right)
\]
\[
- \left( \frac{1}{2} - \frac{1 - 2e}{2\sqrt{1 - 4(e - s)}} \right) I\left( \frac{1}{2} + \frac{1}{2}\sqrt{1 - 4(e - s)} \right)
\]
\[
= -I\left( \frac{1}{2} + \frac{1}{2}\sqrt{1 - 4(e - s)} \right),
\]

where the last line uses the fact that \( I \) is symmetric around 1/2.
\[ \square \]

Proof of theorem 3

Proof of part (i). By Theorem 6,
\[
G \text{ exist and have the form }
\]
Arguments similar to those in the proof of Theorem 2 show that optimizers of (5.19)
\[
where \int_0^1 g(x)e\,dx = e.
\]

(5.20)

(5.21)

(5.22)

(5.23)

If \( \lambda \in \{0, 1\} \) or \( e \in \{0, 1\} \), then (5.23) shows that \( g(x) \equiv e \). So assume that
\( e, \lambda \in (0, 1) \). It is easy to see in this case that \( 0 < y_1 < y_2 < 1 \). Moreover if \( y_1 = y_2 \)
then again \( g(x) \equiv e \), so assume \( y_1 < y_2 \). Introducing the Lagrange multiplier \( \beta_1 \),
we find that
\[
-\lambda I'(y_1) + \lambda \beta_1 + \lambda p\beta_2 y_1^{p-1} = 0,
\]
\[
- (1 - \lambda)I'(y_2) + (1 - \lambda)\beta_1 + (1 - \lambda)p\beta_2 y_2^{p-1} = 0,
\]
\[
- [I(y_1) - I(y_2)] + \beta_1(y_1 - y_2) + \beta_2 y_1^p - y_2^p = 0,
\]

\[ \blacksquare \]
and so
\[ \ell'(y_1) = \ell'(y_2) = 0, \quad \ell(y_1) = \ell(y_2). \quad (5.24) \]

If \( \beta_2 \leq \beta'_2 \), then there are no solutions to (5.24), while if \( \beta_2 > \beta'_2 \), solutions occur precisely when \( y_1 = x_1 < x_2 = y_2 \) are the global maximizers of \( \ell \) at the point \( (q^{-1}(\beta_2), \beta_2) \) along \( q \). In the latter case, (5.23) implies
\[ x_1 < e \leq x_2. \]

If \( e = x_1 \) or \( e = x_2 \), then \( q(x) \equiv e \). Since for \( (e, \beta_2) \in U^c_e \) we have (by definition) \( e \notin (x_1, x_2) \), we have established that (3.3) is valid in \( U^c_e \).

Next, for \( (e, \beta_2) \in U_e \) define
\[ \lambda = \frac{x_2 - e}{x_2 - x_1} \]

and
\[ H(e) = \beta_2 e^p - I(e) - (\beta_2 [\lambda x_1^p + (1 - \lambda) x_2^p] - [\lambda I(x_1) + (1 - \lambda) I(x_2)]). \]

To establish that (3.3) is valid in \( U_e \), it suffices to show that \( H(e) < 0 \) for all \( e \in (x_1, x_2) \). It is easy to check that \( H(x_1) = H(x_2) = 0 \) and
\[ H'(e) = p \beta_2 e^{p-1} - I'(e) - \frac{1}{x_2 - x_1} \left( \beta_2 (x_2^p - x_1^p) - (I(x_2) - I(x_1)) \right) \]
\[ = \ell'(e) - \beta_1 - \frac{1}{x_2 - x_1} \left( \ell(x_2) - \ell(x_1) + \beta_1 (x_2 - x_1) \right) \]
\[ = \ell'(e). \]

Thus, \( H'(x_1) = H'(x_2) = 0 \). Finally,
\[ H''(e) = p(p - 1) \beta_2 e^{p-2} - I''(e) = \ell''(e). \]

From the proof of Proposition 11 in [1], we know \( \ell''(x_1) < 0, \ell''(x_2) < 0 \), and moreover there exists \( x_1 < u_1 < u_2 < x_2 \) such that \( \ell''(e) < 0 \) for \( e \in (x_1, u_1) \cup (u_2, x_2) \) while \( \ell''(e) > 0 \) for \( e \in (u_1, u_2) \). The result follows.

We note that the star density can be computed easily as
\[ s(e, \beta_2) := \frac{\partial}{\partial \beta_2} \psi(e, \beta_2) = \begin{cases} e^p, & (e, \beta_2) \in U^c_e, \\ \frac{e - x_2}{x_1 - x_2} x_1^p + \frac{x_1 - e}{x_1 - x_2} x_2^p, & (e, \beta_2) \in U_e. \end{cases} \]

It is clear that the star density \( s(e, \beta_2) \) is continuous everywhere.

Regularity of \( \psi(e, \beta_2) \). From the formula it is easy to see that \( \psi(e, \beta_2) \) is analytic away from \( \partial U_e \). Write \( \psi = \psi(e, \beta_2) \) and fix \( \beta_2 > \beta'_2 \). In the interior of \( U^c_e \),
\[ \frac{\partial \psi}{\partial e} = p \beta_2 e^{p-1} - I'(e), \]
while the interior of \( U_e \),
\[ \frac{\partial \psi}{\partial e} = \frac{\beta_2 x_1^p}{x_1 - x_2} - \frac{\beta_2 x_2^p}{x_1 - x_2} - \frac{I(x_1)}{x_1 - x_2} + \frac{I(x_2)}{x_1 - x_2} \]
\[ = \frac{\ell(x_1) - \ell(x_2)}{x_1 - x_2} - \beta_1 = -\beta_1. \]

Observe that
\[ \lim_{(e, \beta_2) \in U^c_e, e \to x_1} \frac{\partial \psi}{\partial e} = p \beta_2 x_1^{p-1} - I'(x_1) = \ell'(x_1) - \beta_1 = -\beta_1. \]
So \( \partial \psi / \partial e \) is continuous across \( \partial U_e \) when \( e < e^c \). Note that
\[
\frac{\partial^j \psi}{\partial e^j} = 0, \quad (e, \beta_2) \in U_e, \quad j \geq 2. \tag{5.25}
\]

Proposition 11 of [1] gives
\[
\lim_{(e, \beta_2) \in U^c_e, e \to x_1} \frac{\partial^2 \psi(e, \beta_2)}{\partial e^2} = \ell''(x_1) < 0.
\]
Thus, \( \partial^2 \psi(e, \beta_2) / \partial e^2 \) has a jump discontinuity across \( \partial U_e \) when \( e < e^c \). Analogous statements hold true for \( e > e^c \). Now consider the situation at the point \((e^c, \beta_2^c)\). Proposition 11 of [1] gives
\[
\lim_{(e, \beta_2) \in U^c_e, e \to e^c} \frac{\partial^4 \psi}{\partial e^4} = \ell^{(4)}(e^c) < 0.
\]

From (5.25) we see that \( \partial^4 \phi / \partial e^4 \) is discontinuous at \((e^c, \beta_2^c)\).

Proof of part (ii). By Theorem 6,
\[
\psi(\beta_1, s) = \sup_{G_{x_1}} \left[ \beta_1 \int_0^1 g(x) \, dx - \int_0^1 I(g(x)) \, dx \right] \tag{5.26}
\]
where we recall \( G_{x_1} \) is the set of measurable functions \( g : [0, 1] \to [0, 1] \) satisfying
\[
\int_0^1 g(x)^p \, dx = s. \tag{5.27}
\]

Arguments analogous to those in the proof of part (i) show that \( \psi(\beta_1, s) \) has the formula \([3.4]\).

We note that the limiting edge density has the formula
\[
e(\beta_1, s) := \frac{\partial}{\partial \beta_1} \psi(\beta_1, s) = \begin{cases} \frac{s^p}{x_1^p - x_2^p} x_1 + \frac{x_1^p - s}{x_1^p - x_2^p} x_2 & (\beta_1, s) \in U^c_e, \\ x_1^p - x_2^p & (\beta_1, s) \in U_s. \end{cases}
\]

It is easy to see that \( e(\beta_1, s) \) is continuous everywhere.

**Regularity of \( \psi(\beta_1, s) \).** From the formula it is easy to see that \( \psi(\beta_1, s) \) is analytic away from \( \partial U_s \). Write \( \psi = \psi(\beta_1, s) \) and fix \( \beta_1 < \beta_1^c \). In the interior of \( U^c_s \),
\[
\frac{\partial \psi}{\partial s} = \frac{1}{p} \beta_1 s^{\frac{1}{p} - 1} - \frac{1}{p} s^{\frac{1}{p} - 1} I'(s^{\frac{1}{p}}),
\]
and in the interior of \( U_s \),
\[
\frac{\partial \psi}{\partial s} = \frac{\beta_1 x_1}{x_1^p - x_2^p} - \frac{\beta_1 x_2}{x_1^p - x_2^p} = \frac{I(x_1) - I(x_2)}{x_1^p - x_2^p}.
\]

Note that
\[
\lim_{(\beta_1, s) \in U^c_s, s \to x_1^p} \frac{\partial \psi}{\partial s} = \frac{1}{p} \beta_1 x_1^{1-p} - \frac{1}{p} x_1^{1-p} I'(x_1) = \frac{x_1^{1-p}}{p} \left( \ell'(x_1) - p \beta_2 x_1^{p-1} \right) = -\beta_2.
\]
So \( \partial \psi / \partial s \) is continuous across \( \partial U_s \) when \( s < s^c \). Note that
\[
\frac{\partial^j \psi}{\partial s^j} = 0, \quad (\beta_1, s) \in U_s, \quad j \geq 2. \tag{5.28}
\]
In the computations below, let \((\beta_1, s) \in U_e^c\) and \(t = s^\frac{1}{p}\). Note that

\[
\frac{\partial \psi}{\partial s} = [\beta_1 - I'(t)] \frac{\partial t}{\partial s} = [\ell'(t) - \beta_2 pt^{p-1}] \frac{\partial t}{\partial s},
\]

and

\[
\frac{\partial^2 \psi}{\partial s^2} = \left[\ell'(t) - \beta_2 pt^{p-1}\right] \frac{\partial^2 t}{\partial s^2} + \left[\ell''(t) - \beta_2 p(p-1)t^{p-2}\right] \left(\frac{\partial t}{\partial s}\right)^2
\]

\[
= \ell'(t) \frac{\partial^2 t}{\partial s^2} + \ell''(t) \left(\frac{\partial t}{\partial s}\right)^2.
\]  (5.29)

Using (5.29) and Proposition 11 of \(\Pi\), we get

\[
\lim_{(\beta_1, s) \in U_e^c, s \to s^c} \frac{\partial^2 \psi}{\partial s^2} = \ell''(x_1) \left(\frac{1}{p}x_1\right)^2 < 0.
\]

Comparing with (5.28), we see that \(\frac{\partial^2 \psi}{\partial s^2}\) has a jump discontinuity across \(\partial U_e\) for \(s < s^c\). Analogous results hold for \(s > s^c\). Now consider the situation at the point \((\beta_1^c, s^c)\). From (5.29),

\[
\frac{\partial^3 \psi}{\partial s^3} = \ell'(t) \frac{\partial^3 t}{\partial s^3} + \ell'''(t) \left(\frac{\partial t}{\partial s}\right)^3 + 3\ell''(t) \frac{\partial t}{\partial s} \frac{\partial^2 t}{\partial s^2},
\]

and

\[
\frac{\partial^4 \psi}{\partial s^4} = 4\ell''(t) \frac{\partial t}{\partial s} \frac{\partial^3 t}{\partial s^3} + \ell'(t) \frac{\partial^4 t}{\partial s^4} + \ell''(t) \left(\frac{\partial t}{\partial s}\right)^4
\]

\[
+ 6\ell'''(t) \left(\frac{\partial t}{\partial s}\right)^2 \frac{\partial^2 t}{\partial s^2} + 3\ell''(t) \left(\frac{\partial^2 t}{\partial s^2}\right)^2.
\]

As \(s \to s^c\), \(t \to e^c\) and since \(\ell'(e^c) = \ell''(e^c) = \ell'''(e^c) = 0\), \(\ell''(e^c) < 0\), we have

\[
\lim_{s \to s^c} \frac{\partial^2 \psi}{\partial s^2} = \lim_{s \to s^c} \frac{\partial^3 \psi}{\partial s^3} = 0,
\]

while Proposition 11 of \(\Pi\) gives

\[
\lim_{s \to s^c} \frac{\partial^4 \psi}{\partial s^4} = \lim_{s \to s^c} \ell''(t) \left(\frac{\partial t}{\partial s}\right)^4 = \ell''(e^c) \left(\frac{(e^c)^{1-p}}{p}\right)^4 < 0.
\]

The next result concerns the curve \(\beta_2 = q(\beta_1)\) and the shapes of \(U_e\) and \(U_s\).

**Proposition 7.** (i) The curve \(\beta_2 = q(\beta_1)\) is analytic in \(\beta_1 < \beta_1^c\).
(ii) For any \(\beta_1 < \beta_1^c\), \(\frac{\partial x_1}{\partial \beta_1} > 0\) and \(\frac{\partial x_2}{\partial \beta_1} < 0\). Moreover,

\[
\lim_{\beta_1 \to \beta_1^c} \frac{\partial x_1}{\partial \beta_1} = +\infty, \quad \lim_{\beta_1 \to -\infty} \frac{\partial x_1}{\partial \beta_1} = 0,
\]

\[
\lim_{\beta_1 \to \beta_1^c} \frac{\partial x_2}{\partial \beta_1} = -\infty, \quad \lim_{\beta_1 \to -\infty} \frac{\partial x_2}{\partial \beta_1} = 0.
\]
For any $\beta_2 > \beta_2$, $\frac{\partial x_1}{\partial y_2} < 0$ and $\frac{\partial x_2}{\partial y_2} > 0$. Moreover,

$$\lim_{\beta_2 \to \beta_2} \frac{\partial x_1}{\partial \beta_2} = -\infty, \quad \lim_{\beta_2 \to +\infty} \frac{\partial x_1}{\partial \beta_2} = 0,$$

$$\lim_{\beta_2 \to \beta_2} \frac{\partial x_2}{\partial \beta_2} = +\infty, \quad \lim_{\beta_2 \to +\infty} \frac{\partial x_2}{\partial \beta_2} = 0.$$

Proof. First we show that $q$ is analytic. There is an open V-shaped set containing the phase transition curve $\beta_2 = q(\beta_1)$ except the critical point $(\beta_1^*, \beta_2^*)$, inside which $\ell$ has exactly two local maximizers, $y_1 < y_2$. (See [23] and [1].) It can be seen from the proof of Proposition 11 of [1] that $\ell'(y_1) < 0$ and $\ell'(y_2) < 0$ inside the V-shaped region. The analytic implicit function theorem [16] then shows that $y_1$ and $y_2$ are analytic functions of $\beta_1$ and $\beta_2$ inside this region. Note that $q$ is defined implicitly by the equation

$$\beta_1 y_1 + \beta_2 y_1^p - I(y_1) - (\beta_1 y_2 + \beta_2 y_2^p - I(y_2)) = 0.$$

Differentiating the left hand side of this equation w.r.t. $\beta_2$ gives

$$\beta_1 \frac{\partial y_1}{\partial \beta_2} + y_1^p + \left( p \beta_2 y_1^{p-1} - I'(y_1) \right) \frac{\partial y_1}{\partial \beta_2} - \left[ \beta_1 \frac{\partial y_2}{\partial \beta_2} + y_2^p + \left( p \beta_2 y_2^{p-1} - I'(y_2) \right) \frac{\partial y_2}{\partial \beta_2} \right] = y_1^p - y_2^p < 0.$$

Another application of the analytic implicit function theorem implies $\beta_2 = q(\beta_1)$ is analytic for $\beta_1 < \beta_0$.

Now we turn to the statements involving $x_1$ and $x_2$. Along $\beta_2 = q(\beta_1)$, we have

$$\beta_1 + pq(\beta_1) x_1^{p-1} - \log \left( \frac{x_1}{1 - x_1} \right) = 0.$$

Differentiating with respect to $\beta_1$, we get

$$1 + pq'(\beta_1) x_1^{p-1} + \left[ p(p - 1)q(\beta_1) x_1^{p-2} - \frac{1}{x_1(1 - x_1)} \right] \frac{\partial x_1}{\partial \beta_1} = 0.$$

Therefore,

$$\frac{\partial x_1}{\partial \beta_1} = \frac{1 + pq'(\beta_1) x_1^{p-1}}{\frac{1}{x_1(1 - x_1)} - p(p - 1)q(\beta_1) x_1^{p-2}} = \frac{1 - \frac{x_1 - x_2}{z_1 - z_2} px_1^{p-1}}{-\ell''(x_1)} > 0.$$

Since $\lim_{\beta_1 \to \beta_1^*} \left\{ 1 + pq'(\beta_1) x_1^{p-1} \right\} = \lim_{\beta_1 \to \beta_1^*} \left\{ -\ell''(x_1) \right\} = 0$, by L'Hôpital's rule,

$$\lim_{\beta_1 \to \beta_1^*} \frac{\partial x_1}{\partial \beta_1} = \lim_{\beta_1 \to \beta_1^*} \frac{pq''(\beta_1) x_1^{p-1} + p(p - 1)q'(\beta_1) x_1^{p-2} \frac{\partial x_1}{\partial \beta_1}}{-p(p - 1)q'(\beta_1) x_1^{p-2} - \ell''(x_1) \frac{\partial x_1}{\partial \beta_1}},$$

which implies that

$$\lim_{\beta_1 \to \beta_1^*} \frac{\partial x_1}{\partial \beta_1} = +\infty.$$

Since $x_1 \to 0$ as $\beta_1 \to \beta_1^*$, it is easy to see that

$$\lim_{\beta_1 \to -\infty} \frac{\partial x_1}{\partial \beta_1} = 0.$$
The results for $x_2$ can be proved using the similar methods. Finally, notice that

$$\frac{\partial x_i}{\partial \beta_2} = \frac{\partial x_i}{\partial \beta_1} \frac{\partial q^{-1}(\beta_2)}{\partial \beta_2} = \frac{\partial x_i}{\partial \beta_1} \frac{1}{q'(\beta_1)}, \quad i = 1, 2.$$ 

Therefore the results involving $\beta_2$ also hold. \hfill \Box

Acknowledgements

David Aristoff was supported in part by AFOSR Award FA9550-12-1-0187. Lingjiong Zhu is grateful to his colleague Tzu-Wei Yang for helpful discussions. The authors are grateful for useful comments from the anonymous referees and associate editor.

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