

EMERGENCE IN GRAPHS WITH NEAR-EXTREME CONSTRAINTS

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ABSTRACT. We consider optimal graphons associated with extreme and near-extreme constraints on the densities of edges and triangles. We prove that the optimizers for near-extreme constraints are unique and multipodal and are perturbations of the previously known unique optimizers for extreme constraints. This proves the existence of infinitely many phases. We determine the podal structures in these phases and prove the existence of phase transitions between them.

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1. RESULTS AND SETTING

1.1. **New results.** We investigate the large scale structures called *podes* which emerge as node number increases in simple graphs with given edge and triangle densities (e, t) . In particular we focus on *phase transitions* which appear as discontinuities in the podes structure as (e, t) is varied.

The boundary curves in Figure 1 show the extreme accessible values of pairs (e, t) of those densities. Using graphons, the Large Deviation Principle (LDP) of $\mathbb{G}(n, p)$ graphs, and a Boltzmann entropy taken from statistical mechanics [37], one can associate [37] with each extreme-density pair (e, t) a *unique* optimal graphon, i.e. a graphon with the given densities which optimizes the LDP rate function.

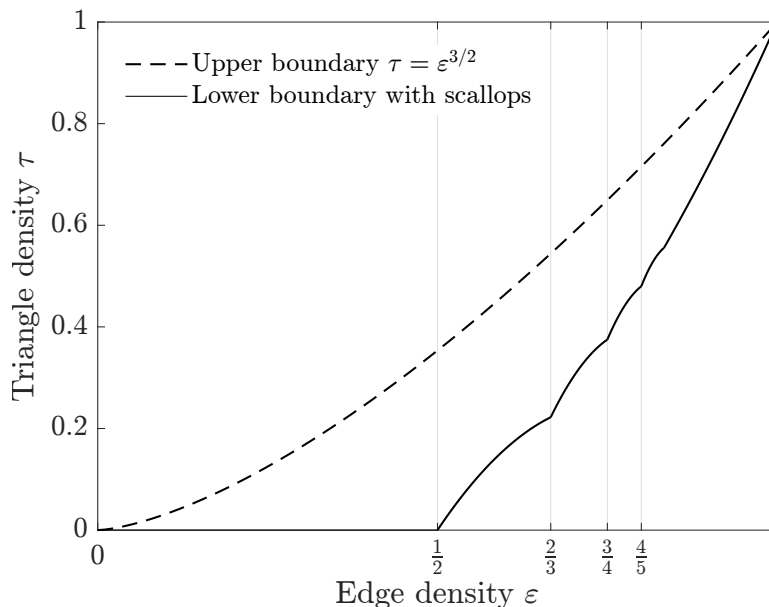


FIGURE 1. The Razborov triangle, made from curves displaying the extreme values of pairs of accessible edge and triangle densities. The curvature of the “scallop” on the lower right is exaggerated for visibility.

In this paper we prove that the unique optimal graphons at the extreme densities extend smoothly into unique optimal graphons in the nearby interior of the triangle, and we fully determine their podes structure. An important technical result of the paper is a new technique for proving the existence of these near-extreme phases, in particular distinct phases emanating from each of the infinitely many scallops at the bottom of Figure 1.

1.2. **The background.** To prove sharp transitions in large simple graphs we depend heavily on the graph-limit or graphon formalism of Lovász et al [7, 8, 26, 27, 28] (following the work

of Aldous [1], Hoover [18] and Kellenberg [20]; see [4, 16] for background). Graphons are an *infinite-node idealization* of graphs. They do not have edges, but they do have well-defined *densities* of finite graphs, including edges. Emergence contrasts a large scale with a small scale in finite simple graphs. The smallest scale is that of individual edges, and the large scale is that of dense graphs with many edges on many nodes. Our proofs use graphons in place of large finite graphs, but we justify the distinction. We prove the existence of arbitrarily sharp transitions in asymptotically large finite graphs, based on a dependency between edges produced by triangles. In 2010 Chatterjee and Varadhan proved [13] their LDP for $\mathbb{G}(n, p)$, built on top of the graphon formalism. We introduced in [37] the Boltzmann entropy $\mathbb{B}(e, t)$ as the exponential rate of growth of the number of graphs with densities (e, t) . Using the rate function $I(g)$ of the LDP, we proved [37] the representation of $\mathbb{B}(e, t)$ as the *maximum* of $S(g) = -I(g)$ over all graphons g with edge-triangle constraints $(\varepsilon(g), \tau(g)) = (e, t)$. The LDP then implied that if this constrained optimization has a unique graphon solution $g_{e,t}$ (an important proviso!), then all but an exponentially small fraction of large but finite graphs with edge and triangle densities close to (e, t) are well-approximated by $g_{e,t}$ [38]. The latter implies that any true singularities proven at the infinite-node graphon scale represent the approximate phenomenon for exponentially-most large finite constrained graphs.

Completion of Figure 1 in 2012 [35] was a significant achievement by Pikhurko and Razborov. This paper is part of a series based on analyzing phase transitions which emerge at various places in the Razborov triangle. In the initial papers we developed methods to determine a few phases *far in the interior* of the Razborov triangle, near the curve $t = e^3$ associated with graphs with independent edges. We defined a phase as a connected open set in the (e, t) plane in which the unique optimal graphons, and therefore \mathbb{B} , vary smoothly with (e, t) , so that phase transitions would be seen as singularities separating phases. This assumed that smoothness prevailed over most of Figure 1 so one could concentrate on the transitions. Although this turned out to be the case, the proof took several years.

Our project thus amounted to showing that, apart from rare (codimension-1) values of (e, t) , the $S(g)$ -maximizing graphon with densities (e, t) is unique and varies smoothly with (e, t) , implying that $\mathbb{B}(e, t)$ is smooth at (e, t) . From computer simulations we were led in 2017 to conjecture [21] that this is the case except across the curves shown in Figure 2. Consequently, all unconstrained subgraph densities associated with exponentially-most graphs should be piecewise-smooth functions of (e, t) , with singularities at phase boundaries. This conjecture gave the project a more concrete goal.

Progress was slow until now. We first proved that the picture in Figure 2 was correct just above the Erdős-Rényi curve, $t = e^3$, (the $F(1, 1)$ phase in the figure) [22], then just below the Erdős-Rényi curve when $e > 1/2$ (the $B(1, 1)$ phase) [32], and then a neighborhood of the $e = 1/2$ line for $t < e^3$ (part of the $A(2, 0)$ phase) [39, 33].

1.3. Connections with other optimization problems. By far the most highly developed mathematical formalism concerned with emergence is equilibrium statistical mechanics. In

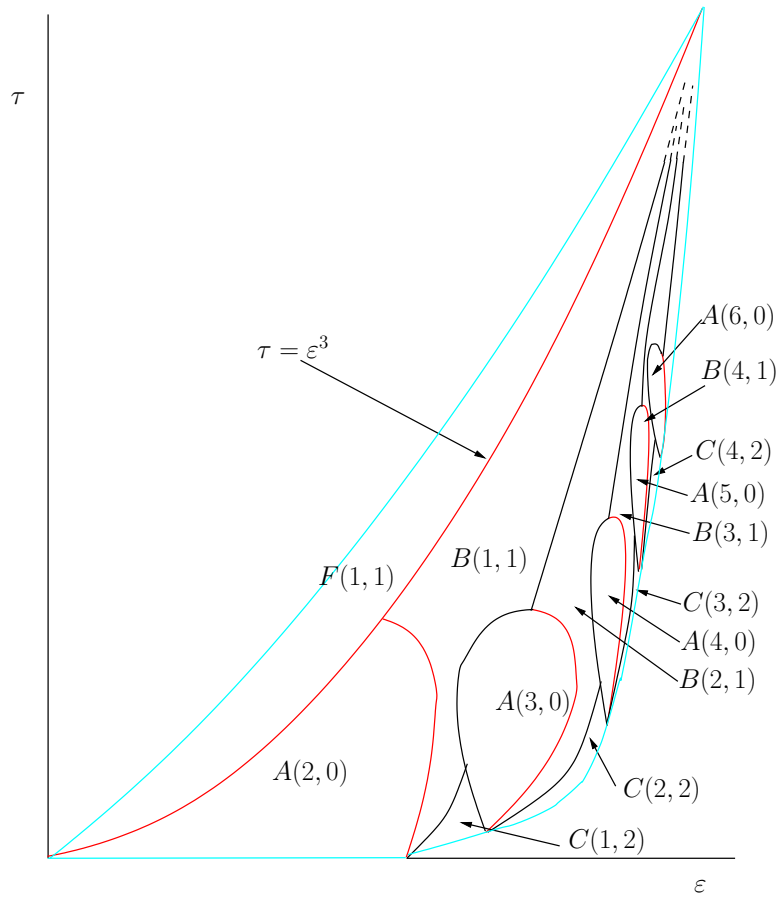


FIGURE 2. Schematic drawing of a conjecture from 2017 [21], based on computer simulations of optimal graphons associated with the phases of large graphs with edge and triangle constraints.

our project we have sought to create an analogous formalism for simple constrained graphs, motivated by the Razborov triangle, Figure 1. One of our goals is to better understand constrained graphs, to extend the classic study of extremal graphs. Another is to provide an example for other optimization problems facing similar obstacles. For this reason we give a brief sketch of emergence in statistical mechanics [41, 47, 46], emphasizing the significance of *convexity*.

A common feature of edge-triangle graphs and statistical mechanics is constrained optimization. There are several ways to view equilibrium statistical mechanics as a constrained optimization problem [19, 17, 40, 23], all of which involve the global optimization of any of a range of free energy functionals, or the entropy. The entropy in statistical mechanics is a measure of the number of possible particle configurations with given constraints. It is a fundamental quantity. It is no exaggeration to view statistical mechanics as built on the

convexity of this entropy (see the lectures of Lanford in [23] and the introduction by Wightman in [19]). The convexity of the entropy allows one to analyze the system without loss of information by the use of a variety of free energies [46], such as the Gibbs free energy $G(p, T)$, which is more familiar than the entropy.

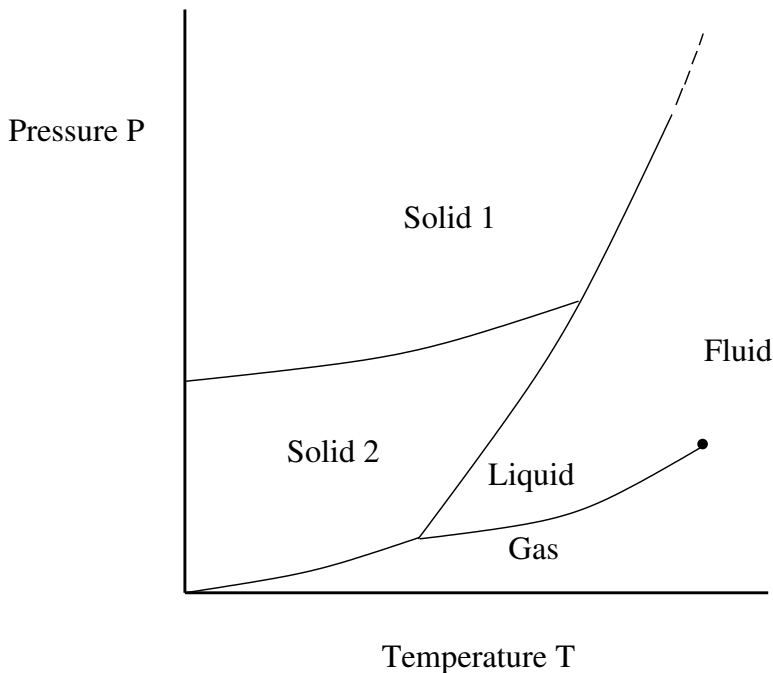


FIGURE 3. This is a crude sketch of the phases of bulk matter, separated by transition curves. There are more than 20 known different solid phases of water, different crystalline structures.

Figure 3 shows a primitive thermodynamic phase diagram, illustrating the pattern of solid and fluid phases in a physical bulk material (i.e. the large scale in the emergent picture), as functions of constraint parameters pressure p and temperature T [36]. The experimentally measurable Gibbs free energy $G(p, T)$ [47, 42] is found to vary smoothly within each region, but shows singular behavior when constraints cross some lower dimension curves (see [40] and section VI in [19]), where bulk material properties such as mass density and heat capacity can change abruptly.

In the analogy between constrained graphs and statistical mechanics, discussed for instance in [34], [44] and [12], edges play the role of individual particles and the energy of a graph is the number of copies of some subgraph H , such as triangles. A key to understanding phases in both statistical mechanics and constrained graphs is defining an *order parameter* [3], which is a function that is identically zero in one phase but nonzero in another. We show its use in Section 4.6.

Unfortunately, with graphs there is no analog of equivalent free energies. This is analyzed in Section 6. This was the starting point of our project in 2013 [37]. (The “inequivalence of ensembles” in constrained graphs was rediscovered and analyzed later; see [15].) This inequivalence presents a serious obstacle. In statistical mechanics free energies provide considerable technical advantages. In their absence we had to develop replacement tools. One such tool, which we introduce in this paper, is the “worth” $W(C)$ that we associate to each column C of a graphon. Developing our variational arguments at the level of columns of graphons is a significant advance in our understanding of optimal graphons and therefore phase transitions in constrained graphs.

We note that some important optimization problems suffer from nonconvexity complications. For instance, the form of optimal transport theory developed by Kantorovich and Brenier was based on convex analysis. It required significant developments over several years to allow the original *nonconvex* Monge problem to access that convex analysis. (For an introduction to optimal transport see the preface in [45] or chapter 1 in [29]).

The emergence of structure in large but finite physical materials is dramatic, particularly the diversity of solid phases, such as the graphite and diamond phases of carbon. All the richness displayed by the phases of all materials, not just the pure elements but also the huge number of compounds like water and alcohol, is created by the electromagnetic interaction within and between molecules. All of inorganic chemistry comes down to the 100 or so different (integer) electric charges of atomic nuclei.

Emergence gives rise to the complicated structure of “water” in Figure 3 and in the edge-triangle model in Figure 2. The study of the emergence of such diversity from the interaction of invisibly small components of a small number of types has led to a great deal of interesting mathematics in the past twenty years. It is this promising history which was the motivation to bring the richness of statistical mechanics, which is built on the *convexity* of its entropy, into the *nonconvex* setting of the Boltzmann entropy \mathbb{B} of constrained graphs.

1.4. Definitions. In order to state our results more precisely, we need a series of definitions. For an in-depth presentation of graphons see [25]. For an introduction to Large Deviation Principles (and also a compact introduction to graphons) see [9].

Here are a few of the basic definitions. A *graphon* is a measurable function $g : [0, 1]^2 \rightarrow [0, 1]$, with $g(y, x) = g(x, y)$ for every ordered pair (x, y) . Two graphons g_1 and g_2 are said to be *equivalent* if there is a measure-preserving transformation $\sigma : [0, 1] \rightarrow [0, 1]$ such that $g_2(x, y) = g_1(\sigma(x), \sigma(y))$ for almost every (x, y) . The equivalence classes of graphons are called *reduced graphons*. The *Shannon entropy*, *edge density* and *triangle density* of a graphon are given by the functionals

$$(1) \quad S(g) = \iint H(g(x, y)) dx dy,$$

$$(2) \quad \varepsilon(g) = \iint g(x, y) dx dy,$$

$$(3) \quad \tau(g) = \iiint g(x, y)g(y, z)g(z, x) dx dy dz,$$

where

$$(4) \quad H(u) = -[u \ln(u) + (1 - u) \ln(1 - u)]$$

is the usual entropy of independent coin flips with probability u of getting heads. Note that if g_1 and g_2 are equivalent graphons, then $S(g_1) = S(g_2)$, $\varepsilon(g_1) = \varepsilon(g_2)$ and $\tau(g_1) = \tau(g_2)$. These quantities should really be viewed as functionals on the space of reduced graphons. $S(g)$ is the negative of the LDP rate function $I(g)$.

The following definitions are less standard.

If the graphon g maximizes $S(g)$ subject to constraints on the densities on edges and another graph, we say that g is an *optimal graphon* at those densities. When we speak of an optimal graphon being unique, we mean that the *reduced* graphon is unique. In other words, that the optimal graphon is unique up to equivalence.

A graphon is said to be *k-podal* if we can partition the interval $[0, 1]$ into measurable sets I_1, \dots, I_k such that $g(x, y)$ is constant on each “rectangle” $I_i \times I_j$. By picking an appropriate representative of the equivalence class of g , we can assume that each I_i is an interval. We refer to the sets I_i as *podes*. If g is k -podal for some integer k , we say that g is *multipodal*. We often use the words *bipodal* and *tripodal* to mean 2-podal and 3-podal. We say that an $(n + m)$ -podal graphon has (n, m) *symmetry* if g is invariant under permutation of the first n podes and is also invariant under permutation of the remaining m podes. The space of such (n, m) -symmetric graphons is only 6-dimensional (or less if n or m is less than 2), with parameters specifying the relative size of the two kinds of podes and the value of $g(x, y)$ on the five (or fewer) equivalence classes of rectangles $I_i \times I_j$. A graphon with $(2, 0)$ symmetry is said to be *symmetric bipodal*.

In a model with constraints on the densities ε, η of edges and another graph H , the *phase diagram* is the set of all achievable values (e, t) of (ε, η) . A *phase* is a connected open set in the phase diagram where the optimal graphon is unique and is a real analytic function of (e, t) . More precisely, for each finite graph K (such as a square or tetrahedron or pentagon), there is a function $\kappa(g)$, similar to $\varepsilon(g)$ and $\tau(g)$, that gives the density of K 's in g . Within a phase, each such functional applied to the optimal graphon is required to yield an analytic function of (e, t) . In practice, analytic dependence of the optimal graphon g on (e, t) is usually proven by describing g (and thus the density of every subgraph K) via a finite set of

parameters and then showing that these parameters are analytic functions of (e, t) . A *phase transition* occurs where the density of some K is not analytic or is not even defined, such as when the optimal graphon is not unique. Phase transitions have only been shown to occur on boundaries of phases.

1.5. Detailed results. The following theorems give a simple description of what happens near almost all points along the boundary of the Razborov triangle. We prove that the unique optimal graphons in the phases near the boundary are multipodal. The cited theorems in the text include additional estimates on how the podes of the optimal graphons scale as the constraints approach the boundary.

Theorem 1 (Theorem 6). *For each fixed $e < 1/2$ and all t sufficiently small, the optimal graphon with edge/triangle densities (e, t) is unique and is symmetric bipodal, with parameters that vary analytically with (e, t) .*

Theorem 2 (Theorem 7). *Let $n \geq 1$ be an integer. For every $e \in (\frac{n}{n+1}, \frac{n+1}{n+2})$, with corresponding minimal triangle density t_0 (depending on e), and for all Δt sufficiently small, the optimal graphon with edge/triangle densities $(e, t_0 + \Delta t)$ is unique and $n + 2$ -podal, with $(n, 2)$ symmetry and with parameters that vary analytically with (e, t) .*

Note that these theorems do not make any claims about what happens exactly over the cusps, i.e. when $e = \frac{n}{n+1}$. When $e = 1/2$ ($n = 1$), the optimal graphon has long been known to have a symmetric bipodal structure. When n is larger, the optimal graphon is believed to have $(n + 1, 0)$ symmetry. However, a small neighborhood of each cusp is believed to intersect four(!) different phases, making a precise characterization difficult.

Theorem 3 (Theorem 8). *All of the phases above the scallops proven in Theorems 1 and 2 have unique optimal graphons with distinct symmetries and cannot be analytically continued to one another.*

In the notation of Figure 2, Theorem 1 proves that the region just above the flat part of the bottom boundary is part of the $A(2, 0)$ phase. Theorem 2 proves the existence of all of the $C(n, 2)$ phases, and Theorem 3 shows that these phases are all different.

Theorem 4 (Theorem 9). *For each fixed $e \in (0, 1)$ and all t sufficiently close to (but below) $e^{3/2}$, the optimal graphon with edge/triangle densities (e, t) is unique and bipodal, with parameters that vary analytically with (e, t) .*

That is, the region just below the upper boundary is part of a bipodal phase. There is every reason to believe that this is part of the same bipodal $F(1, 1)$ phase that is found just above the ER curve, but this has not yet been proved.

All of these theorems can be viewed as extensions of extremal graph theory. Pikhurko and Razborov's results [35] determine unique optimal graphons on the boundary of Figure

1 [37]. Theorems 1–4 describe their unique extensions nearby. This is in contrast to our earlier results that relied on perturbing Erdős-Rényi graphs, or on perturbing known results on the $e = 1/2$ line for $t < e^3$, all well within the interior of the Razborov triangle.

2. THE SEMI-LOCAL “WORTH” FUNCTIONAL

In this section we develop the concept of “worth”. This is a quantity associated with columns of a graphon. We will see that all columns of an optimal graphon must maximize worth. Working with columns, rather than just with the value $g(x, y)$ of the graphon at each point separately, gives us the analytic control needed to prove our main theorems.

We recall the basic theory of Lagrange multipliers. Let g be a graphon that maximizes the Shannon entropy $S(g)$ for particular values (e, t) of $(\varepsilon(g), \tau(g))$. We call an infinitesimal change to the graphon *reversible* if it is possible to make the opposite change, for which the infinitesimal changes dS , $d\varepsilon$, and $d\tau$ are minus those associated with the original change. For instance, increasing the value of a graphon in a portion of $[0, 1]^2$ from 0.5 to slightly above 0.5 is reversible, since we could just as well lower the value slightly below 0.5. Likewise, expanding the area of the region where $g(x, y) = 0.5$ (at the expense of a region where $g(x, y)$ takes on a different value) is reversible, since we could just as well shrink the region. However, increasing the value of a graphon from 0 to a positive number, or increasing the area of a region from 0 to a positive number, are *irreversible* changes.

Note that the terms *reversible* and *irreversible* do not refer to changes in time, as we are not working with any notion of dynamics. Rather, we can visualize infinitesimal changes as tangent vectors to the space of possible graphons. In this heuristic picture, irreversible changes correspond to inward-pointing vectors at the boundary of the space, while reversible changes either refer to points in the interior or are tangent to the boundary.

When considering reversible changes to an optimal graphon, the infinitesimal changes dS , $d\varepsilon$ and $d\tau$ to the entropy, edge density and triangle density cannot be linearly independent at g . If they were, we could find a reversible change that increased S while leaving ε and τ fixed, contradicting the optimality of g . There must therefore exist constants α and β (depending on g) such that, for any reversible infinitesimal change to g ,

$$(5) \quad dS = \alpha d\varepsilon + \frac{\beta}{3} d\tau.$$

Equation (5) applies not only at points where $d\varepsilon$ and $d\tau$ are linearly independent, but also on the Erdős-Rényi curve, where $d\varepsilon$ and $d\tau$ are collinear. However, at such points the constants (α, β) are not uniquely defined. Rather, each Erdős-Rényi graphon is associated with infinitely many possible values of (α, β) .

For irreversible changes, the equality is replaced by an inequality: $dS \leq \alpha d\varepsilon + \frac{\beta}{3} d\tau$. There is no problem with such moves costing us entropy relative to the prevailing exchange rate for ε and τ , since the opposite move is not possible, but they cannot gain entropy.

This principle is sometimes described in terms of a functional

$$(6) \quad F(g) = S(g) - \alpha\varepsilon(g) - \frac{\beta}{3}\tau(g).$$

To first order, reversible changes to g cannot change F , while irreversible changes can decrease F but cannot increase F .

The functionals S and ε are local, in that there is a contribution from each point $(x, y) \in [0, 1]^2$ and we integrate the local contributions to get the global quantity. If the triangle density were also local, then F would be the integral of a local density and our variational equations would come from setting the derivative of this density with respect to $g(x, y)$ equal to zero. That is the typical situation when doing calculus of variations, especially in classical and quantum field theory, with the global action being the integral of a local Lagrangian density [5].

However, the triangle density

$$(7) \quad \tau(g) = \iiint g(x, y)g(y, z)g(z, x) dx dy dz$$

is *not* local. Rather, it involves interactions between the values of g at three different points. To accommodate this complication, we consider (reversible and irreversible) changes to entire columns of g and not just to isolated points. We work up to that in stages, first considering infinitesimal changes to g near a single point, then considering macroscopic changes to g near that point, and finally considering macroscopic changes on an entire column.

If we vary slightly the value of $g(x, y)$ in a neighborhood of a point, then standard methods apply. The functional derivatives of S , ε and τ with respect to $g(x, y)$ are $H'(g(x, y))$, 1 and $3G(x, y)$, respectively, where

$$(8) \quad G(x, y) = \int_0^1 g(x, z)g(y, z) dz.$$

We conclude that

$$(9) \quad H'(g(x, y)) = \alpha + \beta G(x, y)$$

at every point where $g(x, y)$ is continuous. As for points of discontinuity, equation (9) must be understood in a weak sense. If we multiply $H'(g(x, y))$ and $\alpha + \beta G(x, y)$ by an arbitrary test function and integrate, the two integrals must be the same.

We can also consider changing the value of $g(x, y)$ by a larger amount, albeit on an infinitesimally small region R . Note that this is still an infinitesimal change, in that the resulting (infinitesimal) changes in ε and τ can be turned into changes in S by making infinitesimal changes to g elsewhere. The change in F is proportional to the area of R times the change in

$$(10) \quad V(x, y) = H(g(x, y)) - \alpha g(x, y) - \beta G(x, y)g(x, y).$$

The derivative of $V(x, y)$ with respect to $g(x, y)$ is precisely

$$(11) \quad H'(g(x, y)) - \alpha - \beta G(x, y),$$

so maxima of V are automatically solutions to (9). Furthermore, the second derivative of V with respect to $g(x, y)$ is always negative, so solutions to (9) always maximize V .

An optimal graphon must maximize V at each point, but that local optimization is not sufficient. To account for the non-locality of the τ function, we define the *worth* of a function $C : [0, 1] \rightarrow [0, 1]$ to be

$$(12) \quad W(C) = \int_0^1 H(C(y)) - \alpha C(y) dy - \frac{\beta}{2} \iint C(y)C(z)g(y, z) dy dz.$$

Theorem 5. *If a graphon g maximizes the Shannon entropy $S(g)$ for given values of edge and triangle density, then every column of g maximizes W , using the values of α and β determined by equation (5) (for instance via equation (9)). In particular, all columns of g must have the same worth.*

Proof. Suppose that the column g_x has a worth lower than that of a competitor C . Imagine changing the columns near x (say on an infinitesimal interval I of width $|I|$) to C , and also changing the corresponding rows. To first order in $|I|$, we would change the entropy by $2|I| \int_0^1 H(C(y)) - H(g_x(y)) dy$, the edge density by $2|I| \int_0^1 C(y) - g_x(y) dy$ and the triangle density by $3|I| \int g(y, z)(C(y)C(z) - g_x(y)g_x(z)) dy dz$. To first order in $|I|$, the change in F is then $2|I|(W(C) - W(g_x)) > 0$, which contradicts the optimality of g . \square

Using Theorem 5, we can now prove Theorems 1, 2 and 4.

3. PROOF OF THEOREM 1

We will prove a slightly more quantitative version of Theorem 1:

Theorem 6. *For each fixed $e < 1/2$ and all t sufficiently small, the optimal graphon with edge/triangle densities (e, t) is unique and is symmetric bipodal, with parameters that vary analytically with (e, t) . As $t \rightarrow 0$, the increase $\Delta\mathbb{B} = \mathbb{B}(e, t) - \mathbb{B}(e, 0)$ in the Boltzmann entropy scales as $t \ln(1/t)$ and the Lagrange multiplier β scales as $\ln(1/t)$.*

3.1. Strategy. The proofs of Theorems 6, 7 and 9 all follow the same general outline. We will present the proof of Theorem 6 in full detail. The subsequent proofs of Theorems 7 and 9 will be somewhat abbreviated, concentrating on what is different in those cases.

Using the fact that the unique entropy maximizing graphon g_0 at $(e, 0)$ is symmetric bipodal, we show that the optimizing graphons at points near the boundary have the same general structure away from a small exceptional set. Specifically, we partition the unit interval into subsets I_1 , I_2 and I_3 such that the columns g_x of the optimal graphon are L^2 -close to the columns of the first pode of g_0 when $x \in I_1$ and are L^2 -close to the columns of the second pode of g_0 when $x \in I_2$, and where I_3 has small measure. At this stage, we do not have any control over g_x when $x \in I_3$.

Knowing the columns g_x when $x \in I_1 \cup I_2$ (to within a small error in L^2) gives us pointwise control of the function $G(x, y)$ on $(I_1 \cup I_2) \times (I_1 \cup I_2)$. The Euler-Lagrange equations (9) then give us pointwise estimates of $g(x, y)$ in each of the four main rectangles.

We then study the worth functional $W(C)$. The dependence of this functional on the graphon g comes via the integral $\iint C(y)C(z)g(y, z) dy dz$. Since C is bounded, and since we know $g(y, z)$ away from a set of small measure, we have good control over $W(C)$. We determine that a worth-maximizing column can only take one of two approximate forms, namely those exhibited by g_x for $x \in I_1$ and for $x \in I_2$. We then reassign each point $x \in I_3$ to I_1 or I_2 , depending on which worth-maximizing form g_x takes. The result is then a graphon with two (approximate) podes.

Using the pointwise equations (9), we bound the maximum fluctuation of $g(x, y)$ in each rectangle $I_i \times I_j$ by a multiple of the maximum fluctuation in a neighboring rectangle. Combining these results, the maximum fluctuation in each rectangle is bounded by a small multiple of itself, and so must be zero. That is, our optimal graphon must be exactly bipodal.

The space of bipodal graphons with given values of (e, t) is only 2-dimensional. Using ordinary calculus, we determine that the entropy is maximized when the graphon is symmetric.

3.2. Defining approximate podes. There is a unique entropy maximizer g_0 at $(e, 0)$ on the bottom boundary of the Razborov triangle (up to measure-preserving transformations of the unit interval, as usual). This graphon is symmetric bipodal, taking values 0 on the

diagonal blocks and $2e$ on the off-diagonal blocks. As we approach the bottom boundary of the Razborov triangle, we claim that any sequence $\{g_i\}$ of entropy maximizers must converge (after appropriate measure-preserving transformations) to g_0 in L^2 .

To see this, we invoke the compactness of the space of reduced graphons in the cut metric. A subsequence must converge to a limit g_∞ in the cut metric. By the semicontinuity of the entropy and the fact that the limit of the entropies of the entropy maximizers is at least $S(g_0)$, we must have $S(g_\infty) \geq S(g_0)$. But g_0 is the unique entropy maximizer at $(e, 0)$, so $g_\infty = g_0$.

The entire sequence $\{g_i\}$, and not just a subsequence, must converge to g_0 . If it did not, we could find a subsequence where all points were bounded away from g_0 in the cut metric. Applying the previous argument to this subsequence would then yield a contradiction.

The entropy $S(g)$ is continuous in L^2 but only semicontinuous in the cut metric. Limits in the cut metric that are not limits in L^2 are associated with jumps in the entropy. Since $S(g_0) = \lim S(g_i)$, the convergence of g_i to g_0 must occur in L^2 as well as in the cut metric. That is, for every $\epsilon > 0$ there is a $\delta > 0$ such that, for all $t < \delta$ and all optimal graphons g at (e, t) , $\|g - g_0\|_{L^2} < \epsilon$. (Note that we have not assumed that the optimal graphon g is unique. That will be proven in due course.)

Let g be such an optimal graphon for a particular value of (e, t) . Then

$$(13) \quad \epsilon^2 \geq \int_0^1 dx \int_0^1 dy (g(x, y) - g_0(x, y))^2,$$

so

$$(14) \quad \int_0^1 (g(x, y) - g_0(x, y))^2 dy < \epsilon,$$

except on a set of x 's of measure ϵ or less. Call that exceptional set I_3 . Let I_1 and I_2 be the intersection of I_3^c with $[0, 1/2]$ and $[1/2, 1]$, respectively. That is, we have broken the unit interval into three pieces I_1, I_2, I_3 , such that:

- For all $x \in I_1$, $\|g_x - C_1\| < \sqrt{\epsilon}$.
- For all $x \in I_2$, $\|g_x - C_2\| < \sqrt{\epsilon}$.
- When $x \in I_3$ we do not yet have any estimates on g_x .

Here C_1 and C_2 are the columns of g_0 on the two poles, namely $2e$ times the indicator functions of $[1/2, 1]$ and $[0, 1/2]$, respectively. We will refer to the sets I_1, I_2 and I_3 as poles, even though we are **not** assuming that the graphon g is exactly tripodal.

3.3. Variational equations. We examine the terms in our variational equations (9). The first two derivatives of the function H are

$$(15) \quad H'(u) = \ln(1 - u) - \ln(u), \quad H''(u) = -\left(\frac{1}{u} + \frac{1}{1 - u}\right).$$

The quantity $G(x, y)$ is the L^2 -inner product of g_x and g_y , which we denote $\langle g_x | g_y \rangle$. That is,

$$(16) \quad G(x, y) = \langle g_x | g_y \rangle = \int_0^1 g(x, z)g(y, z)dz.$$

If x and y are both in I_1 , or both in I_2 , then $G(x, y) = 2e^2 + O(\sqrt{\epsilon})$. If one is in I_1 and the other is in I_2 , then $G(x, y) = O(\sqrt{\epsilon})$. If either or both are in I_3 , then our estimates do not apply.

For $(x, y) \in I_1 \times I_1$ or $I_2 \times I_2$, we have

$$(17) \quad H'(g(x, y)) = \alpha + 2\beta e^2(1 + O(\sqrt{\epsilon})) = 2\beta e^2(1 + O(\sqrt{\epsilon})),$$

so

$$(18) \quad g(x, y) = \exp(-2e^2\beta(1 + O(\sqrt{\epsilon}))).$$

(Since β is divergent as $t \rightarrow 0$ but α is not, we can absorb α into the $O(\beta\sqrt{\epsilon})$ error.) This means that the contribution of $g(x, y)$ in $I_1 \times I_1$ or $I_2 \times I_2$ to βG goes as β times a negative exponential in β , and thus has an extremely small effect on the value of $g(x, y)$ in $I_1 \times I_2$ or $I_2 \times I_1$.

However, we cannot yet precisely estimate $g(x, y)$ in those regions because $G(x, y) = \langle g_x | g_y \rangle$ also gets a contribution, potentially of order ϵ , from $z \in I_3$.

3.4. Maximizing worth and eliminating I_3 . Let $C : [0, 1] \rightarrow [0, 1]$ be a function whose worth we wish to estimate. Let

$$(19) \quad a = 2 \int_0^{1/2} C(y) dy, \quad b = 2 \int_{1/2}^1 C(y) dy.$$

That is, a and b are the average values of C on $[0, 1/2]$ and $[1/2, 1]$.

We now consider the three expressions that contribute to $W(C)$:

- The entropy term $\int_0^1 H(C(y)) dy$ is bounded above by $\frac{1}{2}(H(a) + H(b))$, thanks to H'' being everywhere negative.
- The term $-\alpha \int_0^1 C(y) dy$ is exactly $-\frac{\alpha}{2}(a + b)$.
- The term $-\frac{\beta}{2} \iint C(y)C(z)g(y, z) dy dz$ is approximately $-\frac{e\beta}{2}ab$.

Up to small deviations due to the differences between g and g_0 , maximizing $W(C)$ amounts to taking $C(y)$ to be constant on $[0, 1/2]$ and constant on $[1/2, 1]$ and choosing a and b to maximize

$$(20) \quad H(a) + H(b) - \alpha(a + b) - e\beta ab.$$

Setting the derivatives of (20) to zero gives the equations

$$(21) \quad H'(a) = \alpha + \beta eb, \quad H'(b) = \alpha + \beta ea.$$

Since there is a worth-maximizer with a close to 0 and b close to $2e$ (namely any column with $x \in I_1$), and another worth-maximizer with a close to $2e$ and b close to 0, α must be close to $H'(2e)$, while β is large and positive.

If a is substantially nonzero (say, bigger than $1/\sqrt{\beta}$), then $e\beta a$ is gigantic and b is extremely close to zero, being $O(\exp(-\sqrt{\beta}))$. This makes $e\beta b$ tiny so $H'(a) \approx \alpha \approx H'(2e)$ and $a \approx 2e$. Similarly, if b is substantially nonzero then a is tiny and $b \approx 2e$. In both those cases, $W(C) \approx \frac{1}{2}H(2e) - eH'(2e) = -\frac{1}{2}\ln(1-2e)$. The third possibility is that a and b are both tiny, but in that case $W(C) \approx 0$, which is strictly less than $-\frac{1}{2}\ln(1-2e)$.

The upshot is that there are three stationary points of (20) but only two maxima, one that resembles g_x for $x \in I_1$ and one that resembles g_x for $x \in I_2$. Since every column g_x with $x \in I_3$ must be a worth-maximizer, and since every worth-maximizer must come close to maximizing (20), every column g_x with $x \in I_3$ resembles g_x for $x \in I_1$ or I_2 . We can then reassign the points of I_3 to I_1 or I_2 depending on the nature of g_x .

3.5. Exact bipodality. Our next step is to upgrade our L^2 estimates on the forms of the different columns into pointwise estimates. Thanks to each column of g being L^2 -close to a column of g_0 , the function $G(x, y) = \langle g_x | g_y \rangle$ is close to $2e^2$ on $I_1 \times I_1$ and on $I_2 \times I_2$. By (9), this forces $g(x, y)$ to be exponentially small (in β) in these quadrants. This in turn makes $G(x, y)$ exponentially small on $I_1 \times I_2$ and $I_2 \times I_1$, which means that $H'(g)$ is exponentially close to α in these quadrants, and therefore that $g(x, y)$ is pointwise close to constant in these rectangles.

We next show that the optimal graphon g is *exactly* constant on each of those rectangles. Let A, B , and D be the average values of $g(x, y)$ on $I_1 \times I_1, I_2 \times I_2$ and $I_1 \times I_2$, respectively. Let Δ_A, Δ_B and Δ_D be the difference between the maximum and minimum values of $g(x, y)$ on those rectangles. Let c be the width of I_1 .

On $I_1 \times I_1$, the quantity $G(x, y)$ is bounded below by

$$(22) \quad c(A - \Delta_A)^2 + (1 - c)(D - \Delta_D)^2$$

and bounded above by

$$(23) \quad c(A + \Delta_A)^2 + (1 - c)(D + \Delta_D)^2.$$

The difference between these two expressions is $4cA\Delta_A + 4(1 - c)D\Delta_D$.

All points satisfy the variational equations

$$(24) \quad H'(g(x, y)) = \alpha + \beta G(x, y).$$

Subtracting this equation at the smallest value of $G(x, y)$ from that at the largest value, applying the mean value theorem to the left hand side, and applying our bounds on the variation in $G(x, y)$, we obtain

$$(25) \quad -H''(A_0)\Delta_A \leq 4Ac\beta\Delta_A + 4D(1 - c)\beta\Delta_D,$$

where A_0 is some number between $A + \Delta_A$ and $A - \Delta_A$. A little algebra then shows that

$$(26) \quad \Delta_A \leq \frac{4D(1-c)\beta}{-H''(A_0) - 4Ac\beta} \Delta_D \leq \frac{3D\beta}{-H''(A)} \Delta_D,$$

where we have used the difference between 3 and $4(1-c) \approx 2$ to cover for simplifying the denominator and replacing A_0 with A . A similar analysis on $I_2 \times I_2$ shows that

$$(27) \quad \Delta_B \leq \frac{3D\beta}{-H''(B)} \Delta_D.$$

Meanwhile, on $I_1 \times I_2$, $G(x, y)$ is bounded above and below by

$$(28) \quad c(A \pm \Delta_A)(D \pm \Delta_D) + (1-c)(B \pm \Delta_B)(D \pm \Delta_D),$$

where the plus signs give an upper bound and the minus signs give a lower bound. The difference between the upper and lower bounds is

$$(29) \quad 2\beta[(cA + (1-c)B)\Delta_D + (c\Delta_A + (1-c)\Delta_B)D].$$

This implies that

$$(30) \quad -H''(D_0)\Delta D \leq 2\beta(cA + (1-c)B)\Delta_D + 2\beta D(c\Delta_A + (1-c)\Delta_B).$$

A little algebra then gives

$$(31) \quad \begin{aligned} \Delta_D &\leq \frac{2\beta D(C\Delta A + (1-c)\Delta B)}{-H''(D_0) - 2\beta(cA + (1-c)B)} \\ &\leq \frac{3\beta D(\Delta_A + \Delta_B)}{-2H''(D)} \\ &\leq \frac{9\beta^2 D^2}{-2H''(D)} \left(\frac{-1}{H''(A)} + \frac{-1}{H''(B)} \right) \Delta_D. \end{aligned}$$

Now recall that A and B are exponentially small in β and that

$$(32) \quad \frac{-1}{H''(A)} = A(1-A) < A \quad \text{and} \quad \frac{-1}{H''(B)} = B(1-B) < B.$$

The coefficient of Δ_D on the right hand side of the last line goes to zero roughly as $\beta^2 \exp(-2e^2\beta)$ as $t \rightarrow 0$ and $\beta \rightarrow \infty$. Once the coefficient is less than one, the only solution is $\Delta_D = 0$, which then implies that $\Delta_A = 0$ and $\Delta_B = 0$. In other words, our optimal graphon is exactly bipodal.

3.6. Symmetric bipodality. All that remains is showing that the best bipodal graphon is symmetric, with pole sizes $\frac{1}{2}$ and $\frac{1}{2}$ and with $A = B$. This requires extensive calculations but no sophisticated analysis. Ultimately, it is just a (grungy) problem in multivariable calculus.

For each triple (e, t, c) we consider the bipodal graphon that maximizes the entropy, subject to the constraints that the edge and triangle densities are (e, t) and that the first pole has

width c . Let $S(e, t, c)$ be the entropy of this optimal graphon. We must show that this entropy is maximized at $c = 1/2$. Note that this function is analytic in c for fixed (e, t) , insofar as the parameters are determined by analytic Euler-Lagrange equations, and is even in $\Delta c := c - \frac{1}{2}$.

When $t = 0$, the function is easy to compute. The graphon must be zero on $I_1 \times I_1$ and $I_2 \times I_2$ and take on the constant value $\frac{e}{2c(1-c)} = \frac{2e}{1-4\Delta c^2}$ on $I_1 \times I_2$. The entropy is then

$$\begin{aligned} S(e, 0, c) &= \frac{1}{2}(1 - 4\Delta c^2)H\left(\frac{2e}{1 - 4\Delta c^2}\right) \\ (33) \qquad &= S(e, 0, 1/2) + 2\ln(1 - 2e)\Delta c^2 + O(\Delta c^4). \end{aligned}$$

That is, there is an entropy cost proportional to Δc^2 associated with having $\Delta c \neq 0$.

Now consider the effect of having t nonzero. Having the graphon nonzero on $I_1 \times I_1$ and $I_2 \times I_2$ provides additional entropy of order $t \ln(1/t)$. Shifting the value of the graphon on $I_1 \times I_2$ by an $O(t)$ amount changes the entropy by an additional $O(t)$, but since this is small compared to $t \ln(1/t)$, $S(e, t, c) - S(e, 0, c)$ is still $O(t \ln(1/t))$. In order to overcome the $-2\ln(1 - 2e)\Delta c^2$ cost, we must have $\Delta c = O(\sqrt{t \ln(1/t)})$. Since $t \sim \exp(-2e^2\beta)$, this means that Δc must be exponentially small in β and in particular that $\beta\Delta c$ is a small parameter.

We now compute the quantity $G(x, y)$ in each rectangle and look at the Euler-Lagrange equations for a particular value of β :

$$\begin{aligned} H'(A) &= \alpha + \frac{\beta}{2}(A^2 + D^2) - \beta\Delta c(D^2 - A^2) \\ &\approx \alpha + \frac{\beta}{2}D^2 - \beta\Delta cD^2, \\ H'(B) &= \alpha + \frac{\beta}{2}(B^2 + D^2) + \beta\Delta c(D^2 - B^2) \\ &\approx \alpha + \frac{\beta}{2}D^2 + \beta\Delta cD^2, \\ H'(D) &= \alpha + \frac{\beta D}{2}(A + B + 2\Delta c(A - B)) \\ (34) \qquad &\approx \alpha, \end{aligned}$$

where in our approximations we use the fact that A and B are exponentially small in β . Since $D \approx 2e$, this makes $\alpha \approx H'(2e)$. The terms proportional to Δc serve to multiply A by a factor of $\exp(-4e^2\beta\Delta c) \approx 1 - 4e^2\beta\Delta c$ and to multiply B by a factor of $\exp(4e^2\beta\Delta c) \approx 1 + 4e^2\beta\Delta c$. These changes in the values of A and B (relative to their values when $\Delta c = 0$) slightly change the triangle density for a given value of β , but only by a fraction $O(\beta\Delta c^2)$. Likewise, the contribution to the entropy of the $I_1 \times I_1$ and $I_2 \times I_2$ squares changes by a fraction $O(\beta\Delta c^2)$. However, that entropy is only $O(t \ln(1/t))$, so we are dealing with an expression that is

$$(35) \qquad O(\beta t \ln(1/t)\Delta c^2) = O(t(\ln(1/t)^2)\Delta c^2),$$

since $\beta = O(\ln(1/t))$. This possible entropy gain from having $\Delta c \neq 0$ is much smaller than the $-2 \ln(1 - 2e)\Delta c^2$ cost, so the optimal value of Δc is exactly zero. That is, we must have $c = 1/2$.

When $c = 1/2$, two of the Euler-Lagrange equations read:

$$(36) \quad \begin{aligned} H'(A) &= \alpha + \beta(A^2 + D^2)/2, \\ H'(B) &= \alpha + \beta(B^2 + D^2)/2. \end{aligned}$$

If $A > B$, then the right hand side of the first equation is greater than that of the second, so $H'(A) > H'(B)$. But that is a contradiction, since $H'(u) = \ln(1 - u) - \ln(u)$ is a decreasing function of u . Likewise, we cannot have $A < B$. So A and B must be equal, making our optimal graphon symmetric bipodal.

The parameters of a symmetric bipodal graphon are uniquely (and analytically) determined by (e, t) .

We also consider how various quantities scale as $t \rightarrow 0$. After setting $c = 1/2$ and $B = A$, a direct calculation shows that

$$(37) \quad t = \frac{3}{4}AD^2 + \frac{1}{4}A^3,$$

so

$$(38) \quad A = \frac{4t}{3D^2} + O(t^3) = \frac{t}{3e^2} + O(t^2),$$

where we have used the fact that $D = 2e - A$. Since A was exponentially small in β , β must scale as $\ln(1/t)$. The entropy is

$$(39) \quad \frac{1}{2}(H(A) + H(2e - A)) = \frac{1}{2}H(2e) - \frac{1}{2}A \ln(A) + O(A),$$

so $S(g) - \frac{1}{2}H(2e)$ scales as $t \ln(1/t)$.

The Boltzmann entropy $\mathbb{B}(e, t)$ is equal to the Shannon entropy $S(g)$ of the optimal graphon at (e, t) , so $\Delta \mathbb{B} := \mathbb{B}(e, t) - \mathbb{B}(e, 0) = S(g) - \frac{1}{2}H(2e)$. Since $A \approx (t/3e^2)$ and $A \approx \exp(-2e^2\beta)$, $\beta \approx \frac{-1}{2e^2} \ln(t/3e^2) \sim \ln(1/t)$. \square

4. PROOF OF THEOREM 2

As in the last section, we will prove a slightly extended version of Theorem 2:

Theorem 7. *Let $n \geq 1$ be an integer. For every $e \in (\frac{n}{n+1}, \frac{n+1}{n+2})$, with corresponding minimal triangle density t_0 (depending on e), and for all Δt sufficiently small, the optimal graphon with edge/triangle densities $(e, t_0 + \Delta t)$ is unique and $n + 2$ -podal, with $(n, 2)$ symmetry. Asymptotically, $\Delta \mathbb{B} = \mathbb{B}(e, t) - \mathbb{B}(e, t_0)$ scales as $\sqrt{\Delta t}$. and the Lagrange multiplier β scales as $1/\sqrt{\Delta t}$. In the optimal graphon, the diagonal entries are all $\exp(-\Theta(\beta))$ and, except for the $(n + 1, n + 2)$ and $(n + 2, n + 1)$ entries, the off-diagonal entries are all $1 - \exp(-\Theta(\beta))$.*

Proof. The proof of Theorem 7 (and therefore Theorem 2) follows the same script as the proof of Theorem 6, namely

- (1) Using the proximity of an entropy-maximizing graphon g at (e, t) to the unique entropy-maximizing graphon g_0 at (e, t_0) to define approximate podes I_1, \dots, I_{n+3} where the columns with $x \in I_j$ with $j \leq n + 2$ are L^2 -close to the corresponding columns of g_0 , and where the exceptional set I_{n+3} is small.
- (2) Using the Euler-Lagrange equations to show that all of the graphon values are exponentially close to 0 or 1, except on $I_{n+1} \times I_{n+2}$, $I_{n+2} \times I_{n+1}$, or when one of the coordinates is in I_{n+3} .
- (3) Showing that the only possible worth-maximizing columns are small perturbations of the columns of g_0 , thus allowing us to reassign the points of I_{n+3} to the other podes.
- (4) Bounding the variation in $g(x, y)$ in each rectangle $I_i \times I_j$ by a small multiple of the variation in other rectangles. Combining estimates, this shows that the variation in each rectangle is bounded by a small multiple of itself, and must therefore be zero.
- (5) Analyzing the finite-dimensional space of $(n + 2)$ -podal graphons near g_0 and determining that the best one has $(n, 2)$ symmetry. We then determine how S , β , and various entries of the optimal graphon scale with Δt .

There is one important difference between the situation of Theorem 6 and that of Theorem 7. The additional podes that appear on the scallops provide an additional, and more efficient, means of generating entropy at the expense of added triangles. As a result, $\Delta \mathbb{B}$ scales as $\sqrt{\Delta t}$ rather than $\Delta t \ln(1/\Delta t)$. Before getting into the details of the proof, we explain how this works, starting near the first scallop, with $e \in (\frac{1}{2}, \frac{2}{3})$.

Consider tripodal graphons of the form shown in Figure 4. The total edge density is

$$(40) \quad e = 2c(1 - c) + \frac{1}{2}p(1 - c)^2,$$

so we must have

$$(41) \quad p = \frac{2(e - 2c(1 - c))}{(1 - c)^2}.$$

The triangle density is

$$(42) \quad t = \frac{3}{2}pc(1-c)^2 = 3c(e - 2c(1-c)) = 3ec - 6c^2 + 6c^3.$$

Taking derivatives, we see that

$$(43) \quad \frac{dt}{dc} = 3(6c^2 - 4c + e) \text{ and } \frac{d^2t}{dc^2} = 36c - 12.$$

The first derivative is zero when

$$(44) \quad c = \frac{1}{3} \left(1 + \sqrt{1 - \frac{3e}{2}} \right).$$

Since d^2t/dc^2 is always positive, this gives the minimum triangle density among graphons of this kind. In fact, it minimizes t among all possible graphons [35] and is the unique optimal graphon with densities (e, t_0) [37].

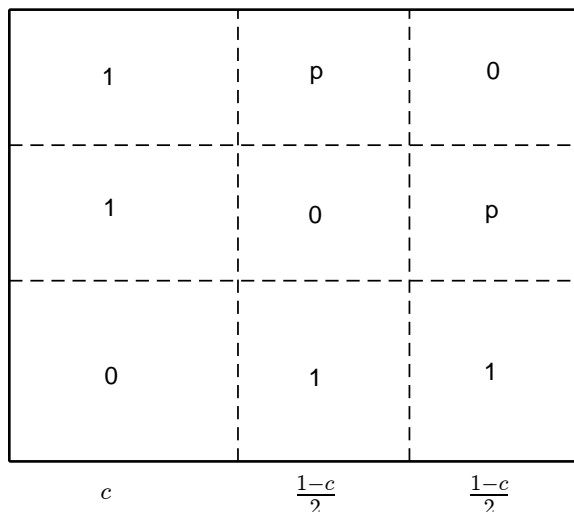


FIGURE 4. A tripodal graphon of the form seen on the first scallop

Now imagine varying c and p while preserving the structure of Figure 4. The entropy of the graphon displayed in Figure 4 is

$$(45) \quad S = \frac{1}{2}(1-c)^2 H(p),$$

where p is given by equation (41). A little algebra then gives

$$(46) \quad p = 4 - 4(1-c)^{-1} + 2e(1-c)^{-2},$$

so

$$(47) \quad \frac{dp}{dc} = 4e(1-c)^{-3} - 4(1-c)^{-2} = \frac{4(e - (1-c))}{(1-c)^3}.$$

We then compute

$$\begin{aligned}
\frac{dS}{dc} &= -(1-c)H(p) + \frac{1}{2}(1-c)^2 H'(p) \frac{dp}{dc} \\
&= -(1-c)H(p) + \frac{2H'(p)(e+c-1)}{1-c} \\
&= -(1-c)H(p) + \frac{H'(p)}{1-c}(p(1-c)^2 + 6c - 4c^2 - 2) \\
&= (1-c)(pH'(p) - H(p)) + (4c-2)H'(p) \\
&= (1-c)\ln(1-p) + 4c-2(\ln(1-p) - \ln(p)) \\
(48) \quad &= (3c-1)\ln(1-p) + 2(1-2c)\ln(p).
\end{aligned}$$

Since c is between $\frac{1}{2}$ and $\frac{2}{3}$, the coefficients of $\ln(1-p)$ and $\ln(p)$ are both positive, making $\frac{dS}{dc}$ negative. We can increase the entropy to first order by decreasing c . That only increases the triangle count to second order in Δc , so we have achieved an entropy increase that scales as the square root of Δt .

The situation is similar near the other scallops. There is a family of graphons parametrized by the size c of each of the n identical podos, as in Figure 5 for $n = 3$. There is a value c_0 that minimizes the triangle density, but dS/dc is not zero at $c = c_0$. Instead, the calculation shown in the next paragraph shows that dS/dc is negative for all relevant values of c . As a result, we can increase S to first order in Δc by decreasing c while only increasing t to second order, so $\Delta S \sim \sqrt{\Delta t}$.

For a general value of n , the graphon on the n -th scallop is 1 everywhere except on the diagonal blocks and on the two off-diagonal blocks in the upper right corner. The edge density is

$$(49) \quad e = 1 - nc^2 - (1 - nc)^2 + \frac{(1 - nc)^2}{2}p.$$

This means that

$$\begin{aligned}
p &= \frac{2}{(1 - nc)^2} (e + nc^2 - 1 + (1 - nc)^2) \\
(50) \quad &= 2 \left(e - \frac{n-1}{n} \right) (1 - nc)^{-2} - \frac{4}{n}(1 - nc)^{-1} + \frac{2(n+1)}{n}.
\end{aligned}$$

Taking a derivative with respect to c is then easy:

$$(51) \quad \frac{dp}{dc} = \frac{4n}{(1 - nc)^3}(e + c - 1).$$

The entropy is $S = \frac{(1-nc)^2}{2}H(p)$ and derivative of S with respect to c is

$$\begin{aligned}
\frac{dS}{dc} &= -n(1 - nc)H(p) + \frac{1}{2}(1 - nc)^2 H'(p) \frac{dp}{dc} \\
&= -n(1 - nc)H(p) + \frac{2nH'(p)(e + c - 1)}{1 - nc}
\end{aligned}$$

1	1	1	p	0
1	1	1	0	p
1	1	0	1	1
1	0	1	1	1
0	1	1	1	1
c	\dots	c	$\frac{1-nc}{2}$	$\frac{1-nc}{2}$

FIGURE 5. A multipodal graphon of the form seen on the scallops, in this case with $n = 3$

$$\begin{aligned}
&= -n(1-nc)H(p) + nH'(p)((n+1)c - 1 + p) \\
&= n(1-nc)(pH'(p) - H(p)) + 2n((n+1)c - 1)H'(p) \\
(52) \quad &= -n(1-nc)\ln(1-p) + 2n((n+1)c - 1)(\ln(1-p) - \ln(p)) \\
&= n((n+2)c - 1)\ln(1-p) + 2n(1 - (n+1)c)\ln(p).
\end{aligned}$$

Since c is between $\frac{1}{n+2}$ and $\frac{1}{n+1}$, the coefficients of $\ln(p)$ and $\ln(1-p)$ are both positive, making each term negative, so $\frac{ds}{dc} < 0$, as claimed.

4.1. Defining approximate podes. We now turn to the details of the proof. As usual, let g_0 be the unique entropy maximizer g_0 at (e, t_0) . This graphon takes the form shown in Figure 5, with

$$(53) \quad c = c_0 = \frac{1 + \sqrt{1 - \frac{n+2}{n+1}e}}{n+2},$$

which is the value of c that minimizes

$$(54) \quad t = n(n+1)(n+2)c^3 - 3n(n+1)c^2 + 3nec.$$

As we approach the scallop, any sequence of entropy maximizers must converge to g_0 in L^2 by exactly the same argument as in the proof of Theorem 6.

As before, we pick a sufficiently small value of ϵ and consider values of t small enough that $\|g - g_0\|_{L^2} < \epsilon$ for each optimal graphon g . Let I_1, I_2, \dots, I_{n+2} be the subsets of the podes of g_0 for which g_x lies within $\sqrt{\epsilon}$ in L^2 of the corresponding column of g_0 and let I_{n+3} be the exceptional set where g_x is not close to the corresponding column of g_0 . Note that I_{n+3} may contain points x where g_x is close to a different column of g_0 . Those points will soon be reassigned.

4.2. Variational equations. Next we need to compute $G(x, y)$ in different cases. Let $G_{i,j}$ denote a typical value of $G(x, y)$ when $x \in I_i$ and $y \in I_j$. We can estimate these quantities to within $O(\sqrt{\epsilon})$ using the columns of g_0 . Thanks to our $(n, 2)$ symmetry, there are only five different numbers to compute, namely $G_{1,1}$, $G_{1,2}$, $G_{1,n+1}$, $G_{n+1,n+1}$ and $G_{n+1,n+2}$. The results are

$$\begin{aligned}
 G_{1,1} &\approx 1 - c, \\
 G_{1,2} &\approx 1 - 2c, \\
 G_{1,n+1} &\approx (n-1)c + \frac{1-nc}{2}p, \\
 G_{n+1,n+1} &\approx nc + \frac{1-nc}{2}p^2, \\
 G_{n+1,n+2} &\approx nc,
 \end{aligned}
 \tag{55}$$

where “ \approx ” means “equal to within $O(\sqrt{\epsilon})$ ”. Note that $G_{1,1}$ and $G_{n+1,n+1}$ are greater than $G_{n+1,n+2}$ by amounts that are $\Omega(1)$ as $t \rightarrow 0$ while $G_{1,2}$, and $G_{1,n+1}$ are less than $G_{n+1,n+2}$ by amounts that are $\Omega(1)$. Multiplying by β and adding α , and using the fact that

$$H'(p) = \alpha + \beta G_{n+1,n+2} = (\alpha + nc) + O(\beta\sqrt{\alpha}).
 \tag{56}$$

we get that $H'(g(x, y))$ is $\Omega(\beta)$ on the diagonal rectangles that do not involve I_{n+3} and is $-\Omega(\beta)$ on the off-diagonal blocks that do not involve I_{n+3} , with the exception of $I_{n+1} \times I_{n+2}$ and $I_{n+2} \times I_{n+1}$. This implies that $g(x, y)$ is exponentially small on the diagonal blocks, exponentially close to 1 on all but two of the off-diagonal blocks, and of course is close to p on $I_{n+1} \times I_{n+2}$ and $I_{n+2} \times I_{n+1}$.

4.3. Maximizing worth. Let $C : [0, 1] \rightarrow [0, 1]$ be a function whose worth we aim to maximize. For each $i = 1, 2, \dots, n+2$, let a_{n+2} be the average values of $C(y)$ for $y \in I_i$. Of the terms contributing to $W(C)$, the entropy term is bounded above by $c \sum_{i=1}^n H(a_i) + \frac{1-nc}{2}(H(a_{n+1}) + H(a_{n+2}))$, since fluctuations in C within each podes can only decrease the entropy. The edge density term is $-\alpha(c \sum_{i=1}^n a_i + \frac{1-nc}{2}(a_{n+1} + a_{n+2}))$.

The most important term comes from triangles. To within the accuracy of our approximation that $g(y, z)$ is constant on each rectangle, it is the quadratic function

$$-\frac{\beta}{2} \sum_{i,j=1}^{n+2} M_{ij} a_i a_j,
 \tag{57}$$

where M_{ij} is the integral of $g(y, z)$ over $I_i \times I_j$.

If we are at a maximum of W , then the gradient of W must be zero and the Hessian must be negative semi-definite. The Hessian of W with respect to the variables $\{a_i\}$ is precisely $-\beta M$ plus diagonal terms proportional to $H''(a_i)$. The matrix M is (nearly) zero on the diagonal, with all of the off-diagonal terms being close to 1 or p , and so has eigenvalues of both signs. The only way for the Hessian to be negative semi-definite is for all but one of entries $H''(a_i)$ to be at least of order β . In other words, all columns that maximize W must have every entry but one (or every entry) approximately equal to 0 or 1. In terms of G , for y in any podé but one, $|G(x, y) - nc|$ must exceed $\Theta(1/\beta)$.

We now examine the possibilities.

- If $G(x, y) \approx nc$ for $y \in I_1$, then $c \sum_{i=2}^n a_i + \frac{1-nc}{2}(a_{n+1} + a + n + 2) \approx nc$. But that is impossible if each a_i (other than a_1) is equal to 0 or 1. Contradiction. Likewise, it is not possible to have $G(x, y) \approx nc$ for $y \in I_2, \dots, I_n$. The first n variables a_i are all either pegged to 0 or to 1.
- If two or more of the variables a_1, \dots, a_n are pegged to 0, then $G(x, y) < nc$ for all y , so $g(x, y) \approx 1$ for all y , which is a contradiction. Thus either one or none of the first n a_i 's is pegged to 0 and the rest are pegged to 1.
- If exactly one of these variables is pegged to 0, then for $y \in I_{n+1}$ or $y \in I_{n+2}$ we have $G(x, y) \leq p \frac{1-c}{2} + (n-1)c < nc$, so a_{n+1} and a_{n+2} are pegged to 1. In other words, our column is just like the columns when x is in one of the first n podés.
- If all of the variables a_1, \dots, a_n are pegged to 1, then we examine a_{n+1} and a_{n+2} . Neither one is pegged to 1, since $G(x, y)$ is at least nc for y in either I_{n+1} or I_{n+2} . They cannot both be pegged to 0, since that would make $G(x, y) = nc$ in both podés, meaning that the values are *not* pegged and the Hessian is not negative-definite. Thus one value must be pegged to 0 while the other is intermediate between 0 and 1. The closeness of all but one a_i to 0 or 1 gives us the same equation for the remaining a_i as satisfied by the actual columns of I_{n+1} or I_{n+2} , implying that the final a_i must be close to p . That is, C is close to the actual columns when $x \in I_{n+1}$ or I_{n+2} .

The upshot is that all worth-maximizers are already L^2 -close to columns of g_0 . Since each column is a worth-maximizer, we can reassign all of the points of I_{n+3} to other podés. Note that this reassignment can result in the podés of g having sizes that are slightly different from those of the corresponding podés of g_0 .

Controlling the columns to within a small L^2 error gives us pointwise control over $G(x, y) = \langle g_x | g_y \rangle$. On all rectangles except for $I_{n+1} \times I_{n+2}$ and $I_{n+2} \times I_{n+1}$, this forces $g(x, y)$ to be exponentially close to 0 or 1. This makes $G(x, y)$ exponentially close to constant on $I_{n+1} \times I_{n+2}$ and $I_{n+2} \times I_{n+1}$ and so makes $g(x, y)$ exponentially close to a constant (that is close to p , but not necessarily exponentially close) on these rectangles.

4.4. Exact multipodality. So far we have shown that an optimal graphon has to be approximately multipodal. There are n podes I_1, \dots, I_n of width close to

$$(58) \quad c = \frac{1 + \sqrt{1 - \frac{n+2}{n+1}e}}{n+2}$$

and two podes of width close to $\frac{1-nc}{2}$. The graphon is exponentially close to 0 on the diagonal blocks, exponentially close to 1 on all of the off-diagonal blocks but two, and close to p on $I_{n+1} \times I_{n+2}$ and $I_{n+2} \times I_{n+1}$. We next show that the graphon is exactly constant on each rectangle. The proof is essentially a rerun of the analogous step in the proof of Theorem 6, only with more terms.

Let g_{ij} be the average value of the graphon on the rectangle $I_i \times I_j$ and let Δg_{ij} be the difference between the greatest and lowest value of the graphon in that rectangle. Let c_i be the width of I_i . We have already determined that all g_{ij} 's except for $g_{n+1,n+2}$ and $g_{n+2,n+1}$ are exponentially close (in β) to 0 or 1, and hence that $1/H''(g_{ij})$ is exponentially small.

If $x \in I_i$ and $y \in I_j$, then the maximum and minimum possible values of $G(x, y)$, and their difference, are

$$(59) \quad \begin{aligned} \max &= \sum_{k=1}^{n+2} c_k (g_{ik} + \Delta g_{ik})(g_{jk} + \Delta g_{jk}), \\ \min &= \sum_{k=1}^{n+2} c_k (g_{ik} - \Delta g_{ik})(g_{jk} - \Delta g_{jk}), \\ \text{difference} &= \sum_{k=1}^{n+2} 2c_k (g_{ik} \Delta g_{jk} + g_{jk} \Delta g_{ik}). \end{aligned}$$

Applying the mean value theorem to the Euler-Lagrange equations, and noting that $H''(u)$ is always negative, we have

$$(60) \quad -H''(g_{ij,0}) \Delta g_{ij} \leq 2\beta \sum_{k=1}^{n+2} c_k (g_{ik} \Delta g_{jk} + g_{jk} \Delta g_{ik}),$$

where $g_{ij,0}$ is some number between the values of g corresponding to the maximum and minimum possible values of $G(x, y)$.

The sum on the right contains terms proportional to Δg_{ij} itself, coming from $k = i$ or $k = j$. We bring those terms to the left hand side, noting that coefficients of those terms are much smaller than $H''(g_{ij,0})$. When $\{i, j\} \neq \{n+1, n+2\}$, this is because $g_{ij,0}$ is exponentially close to 0 or 1, so $H''(g_{ij,0})$ is exponentially large, while the coefficients on the right hand side are $O(\beta)$. When $\{i, j\} = \{n+1, n+2\}$, this is because the coefficients of $\Delta g_{n+1,n+2}$ on the right hand side are proportional to $\beta g_{n+1,n+1}$ or $\beta g_{n+2,n+2}$, both of which are exponentially small. By changing the factor of 2 on the right hand side to a 3, we can absorb these small

corrections to the coefficient of Δg_{ij} and also replace $H''(g_{ij,0})$ with just $H''(g_{ij})$. We also bound g_{ik} and g_{jk} by 1. The upshot is that

$$(61) \quad \begin{aligned} \Delta g_{ij} &\leq \frac{3\beta}{-H''(g_{ij})} \sum_k c_k (\Delta g_{jk} + \Delta g_{ik}) \\ &\leq \frac{6\beta}{-H''(g_{ij})} \max(\Delta g_{ik} \text{ or } \Delta g_{jk}), \end{aligned}$$

where the sum on the first line and the maximum on the second line skips terms involving Δg_{ij} itself.

Whenever $\{i, j\} \neq \{n+1, n+2\}$, $\frac{6\beta}{-H''(g_{ij})}$ is exponentially small, so Δg_{ij} is bounded by a tiny multiple of a sum of similar errors. In particular, the largest Δg_{ij} of this sort is bounded by a sum of contributions much smaller than itself, possibly plus a contribution from $\Delta g_{n+1, n+2}$. The conclusion is that all Δg_{ij} 's other than $\Delta g_{n+1, n+2}$ are bounded by $\beta \exp(-\Omega(\beta)) \Delta g_{n+1, n+2}$.

Now consider the equation for $\Delta g_{n+1, n+2}$. This equation indicates that $\Delta g_{n+1, n+2}$ is bounded by an $O(1)$ multiple of β times the largest of the remaining Δg_{ij} 's, and so is bounded by a constant times $\beta^2 \exp(-\Omega(\beta)) \Delta g_{n+1, n+2}$. When β is large, $\Delta g_{n+1, n+2}$ is thus bounded by a constant (less than one) times itself, and so must be zero. But then all of the other Δg_{ij} 's must also be zero, so our graphon is multipodal.

4.5. Graphons with $(n, 2)$ symmetry. Finally, we show that the optimal graphon is symmetric in the first n nodes and symmetric in the last two. Let c_1, \dots, c_{n+2} be the sizes of the various nodes, let \bar{c} be the average size of the first n nodes, and let Δc_i be $c_i - \bar{c}$ or $c_i - \frac{1-n\bar{c}}{2}$, depending on whether we are talking about the first n nodes or the last two. Let W_i be the worth of columns in the i -th node. There are five kinds of rectangles, namely $I_i \times I_j$ with $i = j \leq n$, with $i < j \leq n$ or $j < i \leq n$, with $i \leq n < j$ or $j \leq n < i$, with $i = j > n$, and finally with $\{i, j\} = \{n+1, n+2\}$. In each class, let \bar{g}_{ij} be the average value of the graphon and let $\Delta g_{ij} = g_{ij} - \bar{g}_{ij}$. We also refer to $g_{n+1, n+2}$ as p .

A key fact is that all of the entries in the first n columns are exponentially close to 0 or 1. Meanwhile, the Euler-Lagrange equations for $g_{n+1, n+2}$ say that

$$(62) \quad \begin{aligned} H'(p) &\approx \alpha + \beta \sum_{i=1}^n c_i, \\ \alpha &\approx H'(p) - \beta \sum_{i=1}^n c_i, \end{aligned}$$

where “ \approx ” means “equal up to exponentially small corrections”.

Now suppose that i and j are indices less than or equal to n . Since all of the entries g_{ik} and g_{jk} are exponentially close to 0 or 1, the entropy contribution to W_i or W_j is exponentially

small. The coefficient of α is $\sum_{k \neq i} c_k = 1 - c_i$, while the coefficient of $\beta/2$ is the integral of the graphon over everything that doesn't involve the i -th node. The upshot is that

$$(63) \quad \begin{aligned} W_i &\approx -\alpha(1 - c_i) - \frac{\beta}{2}(e - 2c_i(1 - c_i)) \\ &= -\left(\alpha + \frac{\beta e}{2}\right) + c_i(\alpha + \beta) - c_i^2\beta, \end{aligned}$$

with a similar result for W_j . Taking the difference gives

$$(64) \quad \begin{aligned} 0 &= W_i - W_j \\ &\approx (c_i - c_j)(\alpha + \beta - \beta(c_i + c_j)) \\ &\approx (c_i - c_j)(H'(p) + \beta(c_{n+1} + c_{n+2} - c_i - c_j)), \end{aligned}$$

where we have used the fact that $\sum_{i=1}^n c_i = 1 - c_{n+1} - c_{n+2}$. However, c_{n+1} and c_{n+2} are close to $\frac{1-n\bar{c}}{2}$, while c_i and c_j are close to \bar{c} , so the coefficient of β is bounded away from zero. We conclude that $c_i - c_j$ must be exponentially small. More precisely, $c_i - c_j$ must be exponentially smaller than the largest $|\Delta g_{ik}|$ or $|\Delta g_{jk}|$. A similar argument shows that $c_{n+1} - c_{n+2}$ is also exponentially smaller than the largest $|\Delta g|$.

We now look at the Euler-Lagrange equations for $g_{i\ell}$ and $g_{j\ell}$, where ℓ is different from i or j . The difference between $G(x, y)$ in $I_i \times I_\ell$ and $I_j \times I_\ell$ is

$$(65) \quad \begin{aligned} \sum_{k=1}^{n+2} c_k g_{\ell k} (g_{ik} - g_{jk}) &= \sum_{k=1}^{n+2} c_k g_{\ell k} (\Delta g_{ik} - \Delta g_{jk}) \\ &\quad + (c_i g_{\ell i} - c_j g_{\ell j})(\bar{g}_{ii} - \bar{g}_{ij}). \end{aligned}$$

The first line is of the order of the largest Δg . The second line has a similar contribution from the difference of $\Delta g_{\ell i}$ and $\Delta g_{\ell j}$, plus a contribution of order $c_i - c_j$. But then

$$(66) \quad H'(g_{i\ell}) - H'(g_{j\ell}) = \beta(G_{i\ell} - G_{j\ell}),$$

which is β times a linear combination of Δg 's and $c_i - c_j$. Since H'' is enormous on the interval from $g_{i\ell}$ to $g_{j\ell}$ (both of which are exponentially close to 1), $\Delta g_{i\ell} - \Delta g_{j\ell}$ is bounded by a tiny combination of other Δg 's and Δc 's.

Repeating this argument for $g_{ii} - g_{jj}$ and for $g_{n+1, n+1} - g_{n+2, n+2}$, we get that

- The biggest Δc_i is bounded by a tiny constant times the biggest Δg .
- The biggest Δg is bounded by a tiny constant times the biggest Δc .

We conclude that all of the Δc 's and Δg 's are zero.

We have determined the form of the optimal graphon g at (e, t) . Noting that the Boltzmann entropy $\mathbb{B}(e, t)$ equals the Shannon entropy $S(g)$ of the optimal graphon g , all statements about S are easily converted into statements about \mathbb{B} .

Finally, we must show that the values of g on each rectangle, and the sizes of the different nodes, are analytic functions of (e, t) . This follows from a general principle in algebraic

geometry, which in turn is essentially just the implicit function theorem. Within the product of the Razborov triangle and the finite-dimensional space of graphons with $(n, 2)$ symmetry, the set of optimal graphons is a 2-dimensional analytic variety, cut out by the analytic Euler-Lagrange equations. As long as the tangent space does not degenerate, we can write all but two of the variables as analytic functions of the last two, which we can choose to be (e, t) .

□

4.6. Distinct phases and rank.

Theorem 8. *Each of the phases above the scallops proven in Theorems 6 and 7 have unique optimal graphons with distinct symmetries and cannot be analytically continued to one another.*

Proof. The optimal graphons described by Theorem 6 have rank 2, while the optimal graphons above the n -th scallop described by Theorem 7 have rank $n+2$. We will construct a sequence of “order parameters,” each a polynomial in finitely many subgraph densities, to distinguish between graphons of different rank. Specifically, the k th order parameter is identically zero whenever the rank of the optimal graphon is $k-1$ or less, and is never zero when the rank of the graphon is k . Since an analytic function on a connected set that is zero on an open subset is zero everywhere, there cannot be an analytic path connecting the $(k-2)$ -nd scallop (where the graphon has rank k and the order parameter is nonzero) to the previous scallops or to the $A(2, 0)$ phase, where the order parameter is zero. In other words, the phases above the different scallops are all distinct.

Newton’s identities relate the determinant of a $k \times k$ matrix A to the traces of A^j for $j = 1, 2, \dots, k$. For instance, if we let $t_j = \text{Tr}(A^j)$, then the determinants of small matrices are given by the formulas

$$(67) \quad \det(A) = \begin{cases} (t_1^2 - t_2)/2 & k = 2, \\ (t_1^3 - 3t_1t_2 + 2t_3)/6 & k = 3, \\ (t_1^4 - 6t_1^2t_2 + 8t_1t_3 - 3t_4)/24 & k = 4. \end{cases}$$

Let $p_k(A)$ be the polynomial in the variables $\{t_j\}$ that gives the determinant of a $k \times k$ matrix A .

The same ideas work for arbitrary diagonalizable linear operators, for which the rank equals the number of nonzero eigenvalues, counted with multiplicity. If we evaluate p_k on any diagonalizable trace-class operator, we get zero if the rank of the operator is less than k and the product of the nonzero eigenvalues (counted with multiplicity) if the rank is equal to k . The key algebraic fact is that, for operators of rank k or less, we have

$$(68) \quad t_j = \lambda_1^j + \dots + \lambda_k^j,$$

where some of the eigenvalues λ_i ’s may be zero, and p_k computes $\lambda_1 \cdots \lambda_k$, which is nonzero precisely when there are k nonzero eigenvalues (counted with multiplicity).

In particular, we can apply these formulas to graphons. (Graphons are always diagonalizable, being symmetric and trace class.) For instance, the expression $(t_1^4 - 6t_1^2t_2 + 8t_1t_3 - 3t_4)/24$, where now $t_j = \text{Tr}(g^j)$, gives zero if the rank of the graphon g is less than 4 and gives a nonzero number if the rank is equal to 4.

When $j > 2$, t_j is the density of j -gons. The problem is that we cannot realize t_1 and t_2 as subgraph densities, so we cannot assume *a priori* that t_1 and t_2 are analytic functions of (e, t) in each phase. To get around this problem, we define our k th order parameter to be $p_k(g^3)$. This is still a polynomial in $\{t_j\}$, only now j ranges from 3 to $3k$ in steps of 3. In particular, t_j is the density of j -gons for each applicable j .

The k -th order parameter is then zero if g^3 has rank less than k and is nonzero if g^3 has rank k . But g^3 has the same rank as g , so we are actually testing the rank of g .

In summary: the k th order parameter is an analytic function of (e, t) in each phase, being built from subgraph densities. It is identically zero on the regions above the 0th, 1st, \dots , $(k-3)$ rd scallops but is never zero on the region above the $(k-2)$ nd scallop. Thus the region above the $(k-2)$ nd scallop is in a different phase from the regions above all the previous scallops. Each scallop has its own unique phase.

□

5. PROOF OF THEOREM 4

Once again we prove a slightly stronger version of the theorem stated in the introduction.

Theorem 9. *For each fixed $e \in (0, 1)$ and all t sufficiently close to (but below) $e^{3/2}$, the optimal graphon with edge/triangle densities (e, t) is unique and bipodal. Asymptotically, the Boltzmann entropy scales as $-(e^{3/2} - t) \ln(e^{3/2} - t)$ and the Lagrange multiplier β scales as $\ln(e^{3/2} - t)$.*

Proof. We follow the same overall roadmap as the proofs of Theorems 6 and 7. Specifically,

- (1) Using the proximity to the upper boundary, we break $[0, 1]$ into two large podes I_1 and I_2 and a small exceptional set I_3 such that g_x is L^2 -close to the indicator function of I_1 when $x \in I_1$ and is L^2 -close to zero when $x \in I_2$.
- (2) Equating the worths of g_x when $x \in I_1$ to those of g_x when $x \in I_2$, we determine that $\beta/\alpha \approx -2/e$. The multiplier β is large and negative, while α is large and positive.
- (3) Maximizing $W(C)$ for an arbitrary $C : [0, 1] \rightarrow [0, 1]$, we show that every column is close to a typical column in the first or second pode. After reassigning points, I_3 is then empty. The control this gives us on $G(x, y)$ shows that $g(x, y)$ is everywhere exponentially close to 0 or 1.
- (4) Bounding the fluctuations in each rectangle by multiples of the fluctuations in other rectangles to show that all fluctuations are in fact zero. In other words, our optimal graphon is exactly bipodal with values that are exponentially close to 0 or 1.

Step 1 is identical to what we have done before. There is a unique graphon at $(e, e^{3/2})$, namely a graphon g_0 that is 1 on $I_1 \times I_1$ and zero elsewhere, where I_1 is a pode of size \sqrt{e} . Every graphon with t close to $e^{3/2}$, and in particular any entropy-maximizing graphon, must be L^2 close to g_0 . This means that for all x 's outside of a set of small measure, g_x is L^2 -close to the corresponding column of g_0 . This also implies that $G(x, y)$ is close to \sqrt{e} when x and y are both in I_1 and is close to zero when either is in I_2 .

The worth of a column that is nearly zero is of course nearly zero. The worth of a column that is nearly 1 on I_1 and nearly zero elsewhere is approximately

$$(69) \quad -\alpha\sqrt{e} - \frac{\beta e^{3/2}}{2}.$$

Since all columns must have the same worth, we must have $\beta/\alpha \approx -2/e$. The Lagrange multipliers α and β diverge at the same rate as we approach the boundary, with $\alpha \rightarrow \infty$ and $\beta \rightarrow -\infty$.

Now consider an arbitrary function $C : [0, 1] \rightarrow [0, 1]$. Let a be the average of $C(y)$ on I_1 and let b be the average on I_2 . Using the approximation that G is L^2 -close to \sqrt{e} times the

indicator function of $I_1 \times I_1$, we get that

$$(70) \quad W(C) \leq \sqrt{e}H(a) + (1 - \sqrt{e})H(b) - \alpha\sqrt{e}a - \alpha(1 - \sqrt{e})b - \frac{\beta}{2}e^{3/2}a^2,$$

with equality if C is constant on I_1 and constant on I_2 . Since α is large and positive, we must have b exponentially close to 0. Setting $b \approx 0$, our worth is then approximately

$$(71) \quad \alpha\sqrt{e}(a^2 - a).$$

This is of course maximized at the endpoints $a = 1$ and $a = 0$, being negative when $a \in (0, 1)$. In other words, any worth-maximizing column must either have $a \approx 1$ and $b \approx 0$, and so must be close to the columns in I_1 , or $a \approx 0$ and $b \approx 0$, and so must be close to the columns in I_2 . Reassigning the points of I_3 to I_1 or I_2 accordingly, we obtain a situation where I_3 is empty.

To constrain the fluctuations in $g(x, y)$ in each rectangle, we recall the variational equations

$$(72) \quad H'(g(x, y)) = \alpha + \beta G(x, y).$$

Since $G(x, y) \approx 0$ or \sqrt{e} , depending on which quadrant we are in, this implies that $g(x, y)$ is exponentially close to 1 on $I_1 \times I_1$ and exponentially close to 0 on $I_1 \times I_2$ and $I_2 \times I_2$. In particular, $H''(g)$, which scales as the larger of $1/g$ and $1/(1-g)$, is much larger than $|\beta|$. Looking at the change in the left hand side and right hand side of this equation within a single quadrant, we see that $H''(g)$ times the maximum fluctuation within any quadrant is of the same order as $|\beta|$ times the maximum fluctuation within any quadrant. But that means that the maximum fluctuation is bounded by a small multiple of itself, and so must be zero. Our graphon is exactly bipodal.

Finally, we do some calculations in the space of bipodal graphons. Let g_{11} , g_{12} and g_{22} be the values of the optimal graphon on $I_1 \times I_1$, $I_1 \times I_2$ and $I_2 \times I_2$, respectively. We treat g_{11} , g_{12} and g_{22} as free variables and adjust the width of I_1 to keep the edge density fixed. To leading order, $e^{3/2} - t$ is a linear function of $(1 - g_{11}, g_{12}, g_{22})$. However, $1 - g_{11}$, g_{12} and g_{22} all scale as exponents of β , so β must scale as $\ln(e^{3/2} - t)$. The entropy goes as $-(1 - g_{11}) \ln(1 - g_{11}) - g_{12} \ln(g_{12}) - g_{22} \ln(g_{22})$, which then scales as $-(e^{3/2} - t) \ln(e^{3/2} - t)$.

The analyticity of g as a function of (e, t) follows from the same argument as in the proof of Theorem 7, only with the space of $(n, 2)$ symmetric graphons replaced by the space of bipodal graphons.

□

6. INEQUIVALENCE OF ENSEMBLES

Using Lagrange multipliers is superficially similar to studying an exponential random graph model (ERGM; see Section 6 in [10], or [14], or [12] for a relevant introduction), where one starts with values α and β and defines a free energy

$$(73) \quad \Psi(\alpha, \beta) = \max_g \left(S(g) - \alpha\varepsilon(g) - \frac{\beta}{3}\tau(g) \right).$$

(In the literature, ERGMs are usually described in terms of parameters $\beta_1 = -\alpha$ and $\beta_2 = -\beta/3$, but that linear rescaling is not important.) The function $\Psi(\alpha, \beta)$ is the Legendre transform of the Boltzmann entropy $\mathbb{B}(e, t)$:

$$(74) \quad \Psi(\alpha, \beta) = \max_{e,t} \left(\mathbb{B}(e, t) - \alpha e - \frac{\beta}{3}t \right).$$

An LDP relates the graphon that maximizes the right hand side of (73), in other words that maximizes F for the given values of α and β , to typical large graphs in a certain ensemble. In that alternate ensemble, all graphs on n vertices are allowed, only with probability proportional to $\exp(-n^2(\alpha\varepsilon + \frac{\beta}{3}\tau))$, where ε and τ are the edge and triangle densities of the graph in question.

If the Boltzmann entropy function were convex and the Razborov triangle were convex, then the Legendre transform (74) would be invertible within each phase [46]. If that were true, we could tune α and β within each phase to get whatever values of (e, t) we wanted, much as we can tune the temperature and pressure of a physical material to get whatever energy density and particle density that we want. In statistical mechanics, this ability to switch back and forth between fundamental variables and conjugate variables is called *equivalence of ensembles*. (Note that the equivalence of ensembles only involves invertibility in the interior of phases, not on the boundaries. The same temperature and pressure can describe a variety of water/ice mixtures with a range of energies.)

With graphs, the Boltzmann entropy function is not convex and neither is the Razborov triangle. There is no equivalence of ensembles; the Legendre transform (74) is not invertible. Specifically, there are many values of (e, t) for which there do not exist **any** values of (α, β) whose F -maximizing graphons have edge/triangle densities (e, t) . We call such points (e, t) *ERGM-invisible*. We can still understand $\Psi(\alpha, \beta)$ and the phases of an ERGM by studying $\mathbb{B}(e, t)$, since Ψ is still the Legendre transform of \mathbb{B} . However, we cannot understand $\mathbb{B}(e, t)$, or graphs with general densities (e, t) , by studying $\Psi(\alpha, \beta)$.

It has long been known that all points with t greater than e^3 , and even moderately less than e^3 , are ERGM-invisible [12]. The only points off the Erdős-Rényi curve that *might* be ERGM-visible lie close to the lower boundary of the triangle. We now show that, because of the nonconvexity of the Razborov triangle, most of those are also ERGM-invisible.

Theorem 10. *If n is a positive integer and $\frac{n}{n+1} < e < \frac{n+1}{n+2}$, and if t is sufficiently close to the minimum triangle density t_0 , then (e, t) is ERGM-invisible.*

Proof. Fix a value of e strictly between $\frac{n}{n+1}$ and $\frac{n+1}{n+2}$. The points with edge density e and triangle density just above the minimum must have large values of the Lagrange multipliers α and β . However, the scallop itself is concave down, so for positive values of β , the linear function $\alpha e + \beta t$ is greater at one or both of the neighboring cusps (at edge density $\frac{n}{n+1}$ and $\frac{n+1}{n+2}$) than near the interior of the scallop. For large positive values of β (and correspondingly large negative values of α), this difference is greater than the bounded difference in Shannon entropy between the graphons described by Theorem 7 and the zero-entropy graphons at the cusps. Since large values of β correspond to small values of Δt , we conclude that, for all sufficiently small values of Δt , the point $(e, t_0 + \Delta t)$ is ERGM-invisible. \square

A similar result applies at the top of the Razborov triangle.

Theorem 11. *For each $e \in (0, 1)$ and for all t sufficiently close to (and less than) $e^{3/2}$, (e, t) is ERGM-invisible.*

Proof. Near the top boundary, α is large and positive while β is large and negative. However, the boundary curve $t = e^{3/2}$ is concave up, so we can decrease $\alpha e + \beta t/3$ by moving to one endpoint $(0, 0)$ or the other $(1, 1)$. Whenever α and β are big enough in magnitude, in other words whenever we are close enough to the top boundary, these gains swamp any changes in $S(g)$. Either the constant graphon $g = 0$ or the constant graphon $g = 1$ yields a larger value of F than the optimal graphon at (e, t) . \square

The statement of Theorem 11 is not new; see Theorem 6.2 in [12]. However, the simplicity of the proof gets to the heart of why points in this region are ERGM-invisible.

Considering the Razborov triangle as a whole, only a few pieces are ERGM-visible. The Erdős-Rényi curve $t = e^3$ is ERGM-visible. Since $d\varepsilon$ and $d\tau$ are collinear at constant graphons, each point on the Erdős-Rényi curve actually corresponds to an infinite set of (α, β) values. A neighborhood of each cusp is ERGM-visible; that's what you get when β is large and positive. As far as we can tell, a neighborhood of the flat part of the lower boundary is also ERGM-visible. But that's all. It appears that ERGMs can be used to study Erdős-Rényi graphs and parts of the $A(n, 0)$ phases, but not the $F(1, 1)$, $B(n, 1)$ or $C(n, 2)$ phases of Figure 2.

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