

## Phases in large combinatorial systems

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**Abstract.** This is a status report on a companion subject to extremal combinatorics, obtained by replacing extremality properties with emergent structure, ‘phases’. We discuss phases, and phase transitions, in large graphs and large permutations, motivating and using the asymptotic formalisms of graphons for graphs and permutons for permutations. Phase structure is shown to emerge using entropy and large deviation techniques.

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### 1. Introduction

Consider the structure of these two families of problems, both fundamental to extremal combinatorics [1]:

- (1) determine those simple graphs with a given density of subgraphs  $A$  (say triangles) and with the highest possible density of subgraphs  $B$  (say edges);
- (2) determine those permutations with a given density of patterns  $A$  (say 123) and with the highest possible density of patterns  $B$  (say 321).

For subgraphs, density refers to the fraction of them in a graph compared to the number in the complete graph, while for a permutation in  $S_n$  a pattern is an element in  $S_k$ ,  $k \leq n$ , and the density of the pattern in the permutation is the fraction of them compared to  $\binom{n}{k}$ . We are only interested in asymptotic behavior, as  $n \rightarrow \infty$ , where for instance  $n$  is the number of nodes, for graphs, or the number of objects  $\{1, 2, \dots, n\}$  being permuted, for permutations. For each such extremum problem we define the phase space  $\Gamma \subseteq [0, 1]^2$  as the closure of the set of simultaneously achievable pairs  $(d_A, d_B)$  of densities of  $A$  and  $B$ , asymptotically in  $n$ . See Figure 1 for an example of  $\Gamma$  for graphs, and Figure 8 for an example for permutations. (These and some other figures are exaggerated to emphasize features.)

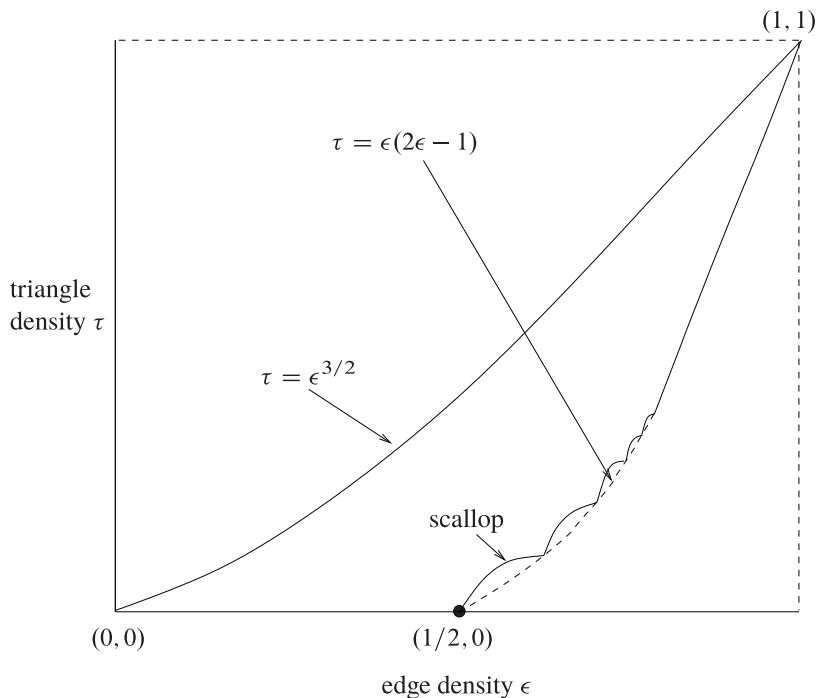


Figure 1. Phase space for subgraph constraints edges and triangles.

In this notation the above extremum problems 1 and 2 consist of determining those graphs or permutations with density pairs on the boundary of  $\Gamma$ . For some history of extremal graphs see [5]; for pattern avoidance in permutations see [21]. In contrast to these extremum problems, in this report we will be concerned with the *interior* of  $\Gamma$ , rather than its boundary, and not with determining those graphs or permutations with such density constraints, a hopeless and uninteresting problem, but with determining what a *typical one is like* for each achievable set of constraints. (This is made precise in Section 2.1.) The phenomenon on which we focus is that well-defined phases emerge in  $\Gamma$  as  $n \rightarrow \infty$ , regions in  $\Gamma$  in which typical behavior varies smoothly with constraint values, separated however by sharp regional boundaries where smoothness is lost (phase transitions), as indicated by dashed curves in Figure 2.

Analysis of such phases is greatly simplified by an asymptotic formalism, associated with the term graphons for graphs (see [22] for a comprehensive introduction) and permutons for permutations (developed in [14, 15]), and by large deviation theorems in those asymptotic settings, as discussed in Section 3. The study of phases is more advanced for graphs than permutations so this status

report will mostly be about graphs, and permutations are discussed in an appendix. There are very interesting extremum results in other parts of combinatorics too, for instance partially ordered sets, but we do not know of work on emergent phases in those fields (see however [26] and references therein).

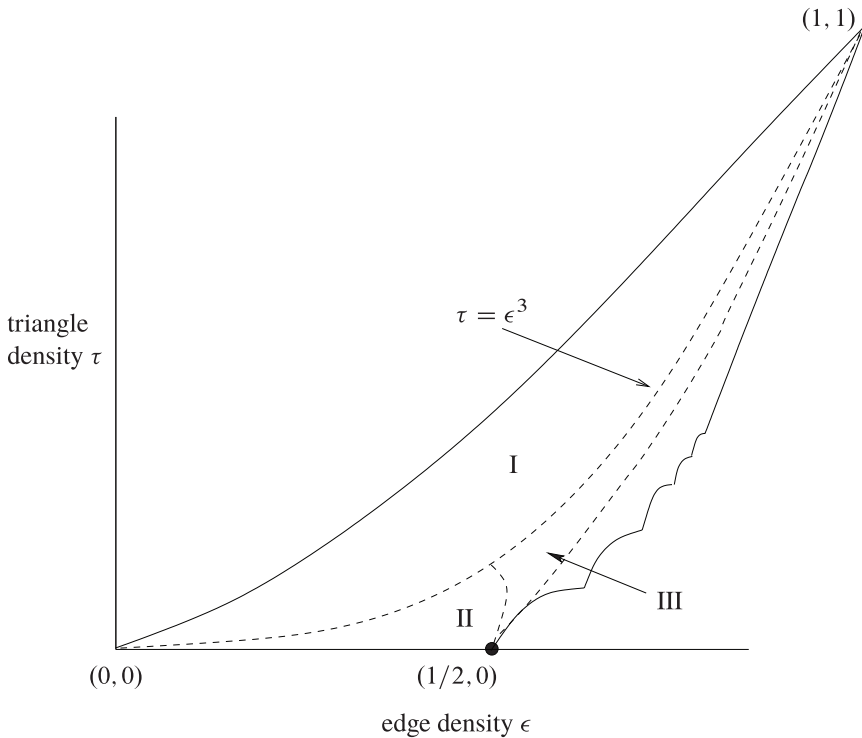


Figure 2. Three phases for edge/triangle constraints.

## 2. Introduction to phases in large constrained graphs

**2.1. Background.** Before we wade in, here is some background. The formalism of phases which we discuss in Section 3 mirrors that used in statistical mechanics models, in which one analyzes configurations of  $n$  particles in Euclidean space, with a specified potential energy function whose gradient gives the interaction forces defining the model. (For background in statistical mechanics see [39]; there is a short outline in [30].) There is a long history studying configurations of particles *minimizing* the energy density for given mass density (energy ground states) [27], or *maximizing* the mass density for given energy density (densest

packing) [12, 4]. Solid and fluid phases emerge when the achievable (energy density, mass density) pairs move away from the phase space boundary studied in these extremum problems, and this is the phenomenon we are mirroring in combinatorial systems. The physics models are much more complicated than the combinatorial ones due to the geometric dependence of the potential energy function, and indeed it is still an important open problem [7, 43, 40] to prove the existence of a fluid/solid phase transition in any reasonably satisfactory model (see however [6]). As we will see, progress has been quicker in the simpler combinatorial settings.

Our goal is to analyze ‘typical’ large combinatorial systems with variable constraints, for instance a typical large graph with edge/triangle densities  $(\epsilon, \tau)$  in the phase space of Figure 1. Our densities are real numbers, limits of densities which are attainable in large finite systems, so we begin by softening the constraints, considering graphs with  $n \gg 1$  nodes and with edge/triangle densities  $(\epsilon', \tau')$  satisfying  $\epsilon - \delta < \epsilon' < \epsilon + \delta$  and  $\tau - \delta < \tau' < \tau + \delta$  for some small  $\delta$  (which will eventually disappear.) It is easy to show that the number of such constrained graphs is of the form  $\exp(sn^2)$ , for some  $s = s(\epsilon, \tau, \delta) > 0$  and by a typical graph we mean one chosen from the uniform probability distribution  $\mu_{n,\delta}^{\epsilon,\tau}$  on the constrained set.

**Goal.** *We wish to analyze such families of constrained, uniform distributions of large combinatorial systems, in particular their dependence on the constraints.*

**2.2. Main results for graphs.** Specializing to graphs, we present here an overview of the main qualitative results on the asymptotics of constrained systems. Proofs are scattered throughout [31, 32, 33, 18, 19, 34, 20, 35], under various hypotheses. The phenomena have also been verified to hold under weaker restrictions by careful simulations. One goal of this paper is to make precise the degree of validation for each of the many results in those papers. By necessity the results must be considered separately, so these details are presented in Section 4, after we discuss the mathematical formalism.

- (1) For fixed constraint values, and asymptotically in  $n$ , the nodes fall into a finite number of equivalence classes. More specifically, in a typical large constrained graph the set of nodes can be partitioned into a finite (*usually small*) number of subsets, with well-defined fractions of edges connecting nodes within, and between, such subsets. Thus there are a small number of parameters describing our target distributions, and they are functions of the constraints. For instance using edge and triangle constraints,  $\epsilon$  and  $\tau$ ,

for most values of  $(\epsilon, \tau)$  and asymptotically in  $n$ , the uniform distribution has four parameters  $a, b, c, d$ : the node set is partitioned into two subsets of relative size  $c$ , with edges between a fraction  $a$  of node pairs in one set,  $b$  for the other set, and fraction  $d$  of node pairs split between the sets, and these are functions of  $(\epsilon, \tau)$ .

- (2) The phase space  $\Gamma$  of achievable constraint values can be partitioned into regions called phases, within which the parameters of the distribution are unique and smooth functions of the constraints, separated by lower dimensional boundaries on which parameter values may or may not be unique, but at which they lose their smoothness (phase transitions). Figure 2 exhibits three of the phases in the system with edge/triangle constraints. Phase II exhibits an unusual level of symmetry, between *classes* of nodes, rather than merely within classes.

Together these show how the phase structure is exhibited by typical graphs, through the development of levels of equivalence among nodes.

### 3. The basic tools: entropy and graphons

**3.1. Graphons.** The mathematics of asymptotically large graphs uses graphons, which we now review [22]. The set of graphs, on  $n$  nodes labelled  $\{1, \dots, n\}$ , will be denoted  $G_n$ . (Graphs are assumed simple, i.e. undirected and without multiple edges or loops. Given  $G$  in  $G_n$  we use its adjacency matrix to represent  $G$  by the function  $q_G$  on the unit square  $[0, 1]^2$  with constant value 0 or 1 in each of the subsquares of area  $1/n^2$  centered at the points  $([j - 1/2]/n, [k - 1/2]/n)$ . More generally, a graphon  $q \in \mathcal{G}$  is an arbitrary symmetric measurable function  $[0, 1]^2$  with values in  $[0, 1]$ . Informally,  $q(x, y)$  is the probability of an edge between nodes  $x$  and  $y$ , and so two graphons are called equivalent if they agree up to a ‘node rearrangement’ (see [22] for details). Taking representatives, we define the cut metric on the quotient space  $\tilde{\mathcal{G}}$  of ‘reduced graphons’ by

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

$\tilde{\mathcal{G}}$  is compact in this topology [22]. (We will define an equivalent metric on  $\tilde{\mathcal{G}}$  in (5).) The distance  $d(\tilde{f}, \tilde{g})$  between  $\tilde{f}$  and  $\tilde{g}$  is obtained by maximizing the difference of the integrals, over ‘boxes’  $S \times T \subset [0, 1]^2$ , of representatives  $f \in \tilde{f}, g \in \tilde{g}$ , and then minimizing over the  $f, g$ . There is a subtle difference between this and more common metrics defined with the absolute value signs *inside* the integral; for a history and analysis see Chapter 10 in [22].

We now consider ‘blowing up’ a graph  $G$  by replacing each node with a cluster of  $K$  nodes, for some fixed  $K = 2, 3, \dots$ , with edges inherited as follows: there is an edge between a node in cluster  $V$  (which replaced the node  $v$  of  $G$ ) and a node in cluster  $W$  (which replaced node  $w$  of  $G$ ) if and only if there is an edge between  $v$  and  $w$  in  $G$ . (The resultant graph is multipartite.) Note that the blowups of a graph are all represented by the same reduced graphon, and  $q_G$  can therefore be considered a graph on arbitrarily many – even infinitely many – nodes, which we exploit next.

The features of a graph  $G$  on which we have focused are the densities with which various subgraphs  $H$  sit in  $G$ . Assume for instance that  $H$  is a quadrilateral. We could represent the density of  $H$  in  $G$  in terms of the adjacency matrix  $A_G$  by

$$\frac{1}{\binom{n}{4}} \sum_{w,x,y,z} A_G(w,x)A_G(x,y)A_G(y,z)A_G(z,w), \quad (2)$$

where the sum is over distinct nodes  $\{w, x, y, z\}$  of  $G$ . For large  $n$  this can be approximated, within  $O(1/n)$ , as:

$$\int_{[0,1]^4} q_G(w,x)q_G(x,y)q_G(y,z)q_G(z,w) dw dx dy dz. \quad (3)$$

It is therefore useful to define the density  $t_H(q)$  of this  $H$  in a graphon  $q$  by

$$\int_{[0,1]^4} q(w,x)q(x,y)q(y,z)q(z,w) dw dx dy dz, \quad (4)$$

and use such densities for this  $H$ , and analogs for other subgraphs, in analyzing constrained distributions. We note that  $t_H(q)$  is a continuous function of  $q$  if we use the cut metric on reduced graphons. This set of functions is also separating: any two reduced graphons with the same values for all densities  $t_H$  are the same [22].

Next we give a different view of graphons. Let  $\mathcal{M}$  be the set of multipodal graphons, i.e. those for which there is a partition of  $[0, 1]$  into finitely many subsets  $F_j$  and the graphon is constant on each product  $F_j \times F_k$ , and let  $\mathcal{M}'$  be the subset of those functions of the form  $q_G$  for some graph  $G$ . Consider the metric  $\bar{d}$  on reduced graphons defined by

$$\bar{d}(\tilde{f}, \tilde{g}) = \sum_{j \geq 1} |t_{H_j}(\tilde{f}) - t_{H_j}(\tilde{g})|/2^j, \quad (5)$$

where  $\{H_j\}$  is any ordering of the countable set of finite simple connected graphs. This metric is equivalent on  $\tilde{\mathcal{G}}$  to the cut metric defined earlier [22]. We can thus realize  $\tilde{\mathcal{G}}$  in an obvious way as a space of sequences, with coordinates in  $[0, 1]$ , and metric  $\bar{d}$ , and note that the image  $\tilde{\mathcal{G}}'$  of  $\mathcal{M}'$  is dense in  $\tilde{\mathcal{G}}$ , see [22].

**3.2. Entropy and the variational principle for graphs.** Getting back to our goal of analyzing constrained uniform distributions,  $\mu_{n,\delta}^\alpha$ , a related step is to determine the cardinality of the set of graphs on  $n$  vertices subject to constraints. Our constraints are expressed in terms of a vector  $\alpha$  of values of a set  $C$  of densities, and a softening agent  $\delta$ . Denoting the cardinality by  $Z_n(\alpha, \delta)$ , it was proven in [31, 32] that  $\lim_{\delta \rightarrow 0} \lim_{n \rightarrow \infty} (1/n^2) \ln[Z_n(\alpha, \delta)]$  exists; it is called the constrained entropy  $s_\alpha$ . From thermodynamics it is known that much can be learned simply from knowing this function of the values  $\alpha$  of the constraints. In statistical mechanics one focuses differently, using probabilistic notions to analyze the asymptotic constrained uniform distributions, again as a function of the constraint values, and this is what we discuss for these combinatorial settings in this report.

There are  $2^{\binom{n}{2}} \approx e^{kn^2}$  graphs in  $G_n$ . There are at most  $n! \approx \exp^{n \ln(n) - n}$  graphs equivalent to any particular element of  $G_n$ , which for large  $n$  is negligible compared to  $e^{kn^2}$  and this fact will be relevant below.

Suppose we are interested in analyzing those  $G \in G_n$  with edge density approximately  $e_0 \in (0, 0.5]$  and the largest possible triangle density, which is  $(e_0)^{3/2}$  [22]. To attain this one must use  $m$  nodes to form a clique (all possible edges), where  $m$  is determined by  $2^{\binom{m}{2}} = 2^{\binom{n}{3}} e_0^{3/2}$ , and leave the remaining nodes as spectators (no connections). There are many ways to do this, but they are all represented by the same reduced graphon in  $\tilde{\mathcal{G}}'$ .

Alternatively, suppose we wanted the  $G$ 's to have edge density  $e_0 \in (0, 0.5]$  but with minimal possible triangle density, which is 0. To achieve this one can select two subsets  $A, B$  of the nodes, and choose  $ne_0$  edges but only between nodes in different sets. There are many inequivalent bipartite graphs of this type (except for  $e_0 = 0.5$ ), so a more productive goal might be to get a useful handle on the distribution of solutions  $G$ .

Finally, there is an enormous number of ways to attain edge density  $e_0 \in (0.5]$  and triangle density fixed between the maximum and minimum just discussed. For these intermediate cases we change the problem as suggested in the previous paragraph; we no longer try to identify the appropriate graphs, but it turns out we can often identify what a typical such graph is like, i.e. determine the (uniform) distribution on such constrained graphs. For instance for triangle density  $\tau \in [0, e_0^3]$  the constrained distribution is obtained by partitioning the node set into two equal sets  $A$  and  $B$ , and choosing edges between node pairs independently by the following two rules: for any two nodes in the same set the probability of an edge is  $[e_0 - (e_0^3 - \tau)^{1/3}]$ , and for any two nodes in different sets the probability is  $[e_0 + (e_0^3 - \tau)^{1/3}]$ . For  $\tau = e_0^3$  this reduces to the situation in which each pair of

nodes is connected with probability  $e_0$ , while for  $\tau = 0$  it reduces to the extreme case discussed above.

This is the point where the mathematics changes flavor. This is not due merely to our focus on asymptotics; as noted in Section 1, the extremal combinatorics associated with the boundary of the phase space already involves asymptotics, and for instance led to the beautiful flag algebra formalism of Razborov [36]. The difference here is that at points in the interior of  $\Gamma$ , where we want to understand not individual graphs but the constrained uniform distribution on graphs, our problem is naturally reformulated within the *calculus of variations*, since a key tool is the constrained entropy  $s_\alpha$  which can be represented as follows.

**Theorem 1.** (*The variational principle for constrained graphs [31, 32]*) For any vector  $H$  of subgraphs  $H_j$  and vector  $\alpha$  of numbers  $\alpha_j$ ,

$$s_\alpha = \max_{t_H(q)=\alpha} S(q), \quad (6)$$

where  $S$  is the Shannon entropy of graphons:

$$S(q) = - \int_{[0,1]^2} \frac{1}{2} \{q(x, y) \ln[q(x, y)] + [1 - q(x, y)] \ln[1 - q(x, y)]\} dx dy. \quad (7)$$

Our goal is to understand families of constrained uniform distributions,  $\mu_{n,\delta}^\alpha$ , on graphs on  $n$  nodes and constraints  $\alpha, \delta$ , with  $n$  large and  $\delta$  small. It can be tricky to ‘compare’ distributions for different  $n$ ; we overcome this using graph blowup as in Section 3.1 to work with graphons, giving us a uniform framework independent of  $n$ . We then get our approximation to  $\mu_{n,\delta}^\alpha$  using the optimal graphons  $\tilde{g}^\alpha$  of Theorem 1. Any reduced graphon  $\tilde{g}$  is a sequence of densities  $t_{H_j}$ , and we use the fact that the average values of these densities, with respect to the sequence  $\mu_{n,\delta}^\alpha$ , converge to those of  $\tilde{g}^\alpha$  (assuming  $\tilde{g}^\alpha$  is a unique optimizer) [31]. These limiting averages are computable from  $\tilde{g}^\alpha$  as in (4), and are our main use of the distributions  $\mu_{n,\delta}^\alpha$ . (They would also allow us to directly estimate the mass functions of the  $\mu_{n,\delta}^\alpha$  if desired.) We can therefore interpret the averages as the densities of a ‘typical’ large, constrained graph.

Variational principles such as Theorem 1 are well known in statistical mechanics [37, 38, 39], and for their simpler (discrete) models can be obtained from general large deviations results [11]. This was also the case for Theorem 1, for which the proof used the large deviation theory from [10]. (See [8] for a good review of large deviations in random graphs.) One aspect of the applicability of such variational principles in this context is not well understood. In all known graph examples the optimizers in the variational principle are unique in  $\tilde{\mathcal{G}}$  except occasionally



on a lower dimensional set of constraints where there is a phase transition. But we do not yet have a theoretical understanding of this fundamental issue, sometimes called the Gibbs phase rule in physics; see [38, 16] for weak versions in physics. Given such uniqueness however, the rest of the path is clear: the optimizer for (6) gives us the limiting constrained uniform distribution which we want to analyze! (Without uniqueness it is harder to obtain useful information.)

#### 4. Examples of constrained graph systems

We now give some details, including references, concerning the qualitative results claimed in Section 2.2. As noted there, our understanding of the range of validity of what is proven in our theorems is significantly enhanced by careful simulations, in a range of examples (models). To preserve continuity of argument we will clarify some statements with references to the Notes at the end of the text.

**4.1. Edge/triangle model.** Consider the edge/triangle model, using edge/triangle densities  $(\epsilon, \tau)$  as constraints, studied in [31, 32, 33, 18, 19, 34, 20]. The entropy optimizer is unique<sup>1</sup> in  $\tilde{\mathcal{G}}$  for every pair  $(\epsilon, \tau)$ . Also, the optimizer is multipodal, i.e. there is a partition of  $[0, 1]$  into finitely many subsets  $F_j$  and the graphon is constant on each product  $F_j \times F_k$ . This gives a distribution with finitely many parameters, which vary smoothly with  $(\epsilon, \tau)$  except on certain curves, separating phases.<sup>2</sup> Specifically, for over 95% of the area of  $\Gamma$ , corresponding to constraints in the phases I, II and III in Figure 2, it is bipodal – the partition of the nodes is into just two subsets – so there are only four parameters in the asymptotic distribution, each a function of the constraints. In particular, in phase II there is a very interesting symmetry: the two *sets* of nodes are in all ways interchangeable. This means, in terms of the parameters defined earlier, that  $a = b$  and  $c = 1$ , so there are only two independent variables,  $a$  and  $d$ , in this phase. One can then solve for  $a$  and  $b$  in terms of the constraints  $\epsilon$  and  $\tau$ , getting the graphon in Figure 3 (using convenient node labelling).

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<sup>1</sup> This has been proven in a thin region above the Erdős–Rényi curve [19] and on the line  $\{(\epsilon, \tau) \mid \epsilon = 0.5, 0 \leq \tau \leq 1/8\}$  [31], and seen in all the extensive simulations of the model noted in [33].

<sup>2</sup> Bipodality is proven in a thin region above the Erdős–Rényi curve [19] and on the line segment  $\{(\epsilon, \tau) \mid \epsilon = 0.5, 0 \leq \tau \leq 1/8\}$  [31]. Bipodality and tripodality has been seen in all other regions simulated in [33]. There are expected to be regions of  $m$ -podality with increasing  $m$  near the corners of the scallops along the boundary of the phase space [31, 32]. The rest of the claims about entropy optimizers in this paragraph are only known from the simulations referenced.

It is natural to study the boundaries of phases, to see how the system changes there. Consider the approach to the phase boundary  $\tau = \epsilon^3$ , from each side. Fixing  $\epsilon \leq 0.5$  and increasing  $\tau$  from 0, we see from Figure 3 that the large typical graph starts as perfectly symmetric bipartite, and steadily loses the distinction between the two sets.<sup>3</sup> At  $\tau = \epsilon^3$  the nodes are all equivalent; these are the Erdős–Rényi graphs, with iid edges, and since the constrained entropy peaks at the curve  $\tau = \epsilon^3$  when varying either  $\epsilon$  or  $\tau$  separately, these graphs are important in part because of their overwhelming number. They also play the same intuitive role for us as the ideal gas in statistical mechanics.

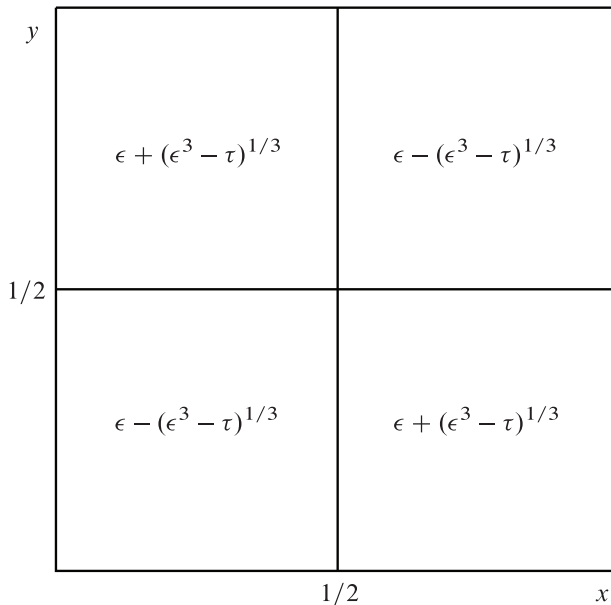


Figure 3. The (piecewise constant) edge/triangle graphon in phase II.

The approach to the Erdős–Rényi curve from phase I is quite different. Except at  $\epsilon = 0.5$  (the maximum of the unconstrained entropy), as one increases  $\tau$  from  $\epsilon^3$  the optimal graphon immediately becomes bipodal but now by the emergence of an infinitesimal set of nodes:  $c = O(\tau - \epsilon^3)$ . The asymptotic form of  $a$ ,  $b$  and  $d$  are proven in [19]. The behavior of phase I near its upper boundary,  $\tau = \epsilon^{3/2}$  has not been analyzed. But on the upper boundary itself the optimal graphon consists of spectator nodes, fully unconnected, and a cluster of fully interconnected nodes

<sup>3</sup> The bipodal graphon in Figure 3 is only proven along the line segment  $\{(\epsilon, \tau) \mid \epsilon = 0.5, 0 \leq \tau \leq 1/8\}$  [31], but has been thoroughly investigated by simulation [33] in the region described as phase II.

(a clique), of size needed to produce edge density  $\epsilon$ . It is not yet understood how these graphs connect to the ones emerging from the lower boundary of phase I, though extensive simulation data has been gathered [33]. And finally, perturbation about the boundary between phases III and II is particularly interesting because of the breaking of symmetry; see [34]. New features appear in other models, which we now discuss.

**4.2.  $k$ -star graph models.** A  $k$ -star is a graph with  $k$  edges with a node in common, and the  $k$ -star model is the one in which the constraints are the density  $\epsilon$  of edges and the density  $\tau_k$  of  $k$ -stars. The phase space  $\Gamma$  of the 2-star model is typical of them, and shown in Figure 4, see [18].<sup>4</sup> For any  $k$ -star model the lower boundary of  $\Gamma$  is the curve,  $\tau_k = \epsilon^k$ , represented by Erdős–Rényi (constant) graphons, and the upper boundary is the upper envelop of two intersecting smooth curves [18]. There is a unique bipodal graphon representing all but one point on the upper boundary, the intersection point just noted, where the two one-sided graphon limits differ [18]. We know for  $k$ -star models that in the interior of  $\Gamma$  there is a unique entropy-optimizing bipodal graphon everywhere except on a curve emanating from the intersection point on the boundary; this curve ends at a ‘critical point’ in the interior of  $\Gamma$ , so there is only one phase in each of these models.<sup>5</sup> See Figure 5. The behavior of  $k$ -star models just above the Erdős–Rényi curve is common to many other models, including the edge/triangle model [19]. However this universality does not extend further from the Erdős–Rényi curve; in particular there is no transition in the edge/triangle model analogous to that in the  $k$ -star models.<sup>6</sup> (There is some confusion on this point coming from exponential random graph models.<sup>7</sup>)

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<sup>4</sup> The phase diagrams for  $k$ -star models are derived, but only for  $k \leq 30$ , in [18].

<sup>5</sup> The one phase is smooth except on the curve. Nonsmoothness on the curve has been proven for  $k = 2$ , and seen in simulation in  $k = 3$ , in [18].

<sup>6</sup> This is only known from simulation, but would not be expected because of the behavior of the edge/triangle model on the upper boundary of its phase space.

<sup>7</sup> Exponential random graph models are widely used, especially in the social sciences, to model graphs on a fixed, small number of nodes [24]. These models are sometimes considered Legendre transforms of the models being discussed in this report [31]. However, as was pointed out in [9], as the number of nodes gets large the parameters in the model become redundant, and this confuses any interpretation of phase transitions in such models. One way to understand the difficulty is that the constrained entropy in these models is not convex or concave, and the Legendre transform is not invertible [31].

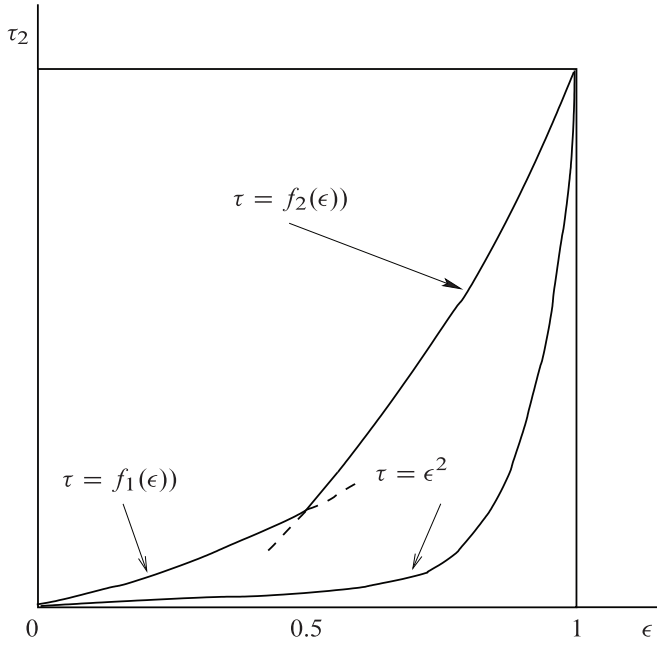


Figure 4. The phase space for the 2-star model.

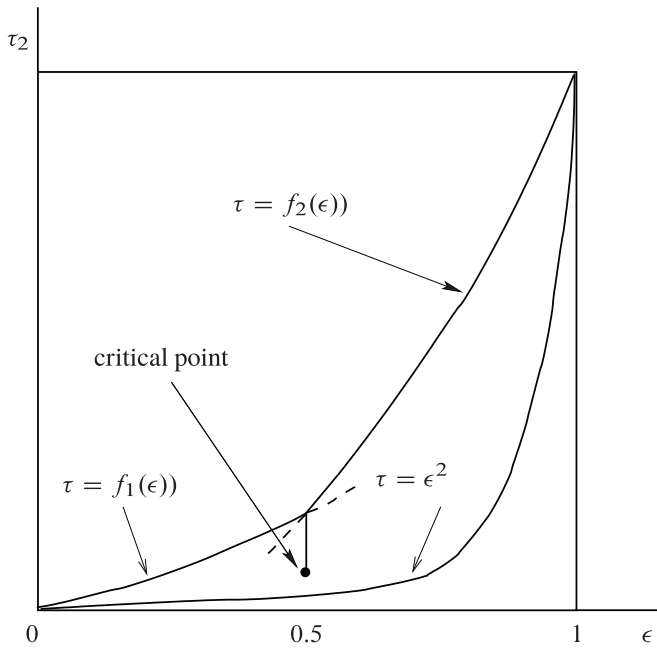


Figure 5. The critical point in the 2-star model.

**4.3. Half-blip model.** Finally we consider the half-blip model, where the constraints are a pair of signed densities, the signed 2-star density  $t_1$  and signed square density  $t_2$ , defined for graphons by:

$$t_1(q) = \int q(x, y)[1 - q(y, z)]dx dy dz; \quad (8)$$

$$t_2(q) = \int q(w, x)[1 - q(x, y)]q(y, z)[1 - q(z, w)]dw dx dy dz. \quad (9)$$

The phase space for this model is not fully known, but there is a lower edge corresponding to  $t_2 = 0$ , namely  $\{(t_1, 0) \mid 0 \leq t_1 \leq 1/6\}$ , with the following feature: as  $t_1$  increases from 0 the unique representing graphon is  $m$ -podal but with  $m \rightarrow \infty$  as  $t_1 \rightarrow 1/6$ . This feature is not so special, as it is shared with the edge/triangle model along its lower (scalloped) boundary as  $\epsilon \rightarrow 1$ . However in the half-blip model the unique graphon associated with  $(t_1, t_2) = (1/6, 0)$  is not multipodal – it is the graphon, with values 0 and 1, shown in Figure 6 – and this unusual circumstance is quite intriguing.

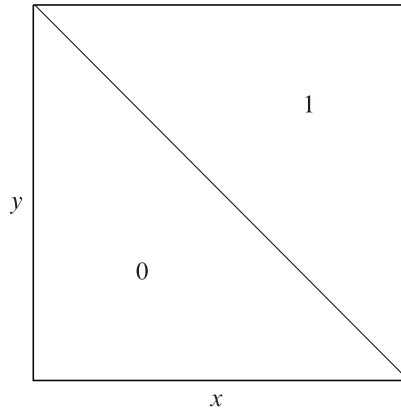


Figure 6. The half-blip graphon at  $(t_1, t_2) = (1/6, 0)$ .

There is much to learn about this model, both on the boundary and the interior of  $\Gamma$ . The model is an analog of statistical mechanics models of quasicrystals [28], which raises the question whether, in the half-blip model, there is a phase in the interior of  $\Gamma$  near  $(1/6, 0)$  without multipodal entropy optimizers. Indeed the analogous question has not yet been solved in statistical mechanics [3], but might well be easier to solve in this combinatorial setting.

We have discussed several models of large graphs, but all had two constraints. We do not know of new phenomena which become available with more constraints, though we note one model studied with three constraints, the taco model [18]. In the other direction, a model with only one constraining density reduces to the Erdős–Rényi family, which is very important but does not exhibit phases, or transitions, in the senses we have used the terms. There has been much work in Erdős–Rényi models on graphs where there are restrictions on which, or how many, vertices may be linked by an edge, for instance to exhibit percolation. Percolation is of course important, but seems to be exploring phenomena essentially different, say, from the emergence of the symmetric phase II in large graphs with edge/triangle constraints, as described in Section 4.1; see [34] concerning the effect of constraints.

## 5. Open problems

Two open problems for constrained graphs go to the heart of our understanding of phase emergence. The first is to understand why, in all models we have studied, there is a unique optimizer for the constrained entropy except off a set of constraints of lower dimension. As noted in Section 3.2, without this feature our method would not produce useful results. There is some analysis of this phenomenon in statistical mechanics, but the only results are uniqueness off a set of constraint values of category one, or of measure zero [38, 16], and while intuitively suggestive this is not of practical use.

Another basic problem is the origin of the multipodal structure of entropy optimizers. We have never found a nonmultipodal entropy optimizer in the interior of a phase space, i.e. in a phase, but there is no general proof that they cannot exist. (There are proofs in some regions of some models [18, 19], but they do not give any insight into the general situation.) An obvious candidate for exploring this is the half-blip model of Section 4.3, a model which had already been used to study the analogous phenomenon in extremal graph theory [23].

Multipodality can be understood in terms of a symmetry between nodes, as discussed in Section 2.2. Another, and related, open problem concerns phase II in the edge/triangle model. The symmetry of this phase, discussed in Section 4.1, is between the equivalence classes that define multipodal structure. What is the significance of this higher level of symmetry? Multipodal graphons are piecewise constant as functions on  $[0, 1]^2$ , and it is plausible that such uniformity originates from maximizing entropy, as was actually demonstrated in [18] for  $k$ -star models. But the higher level of symmetry of phase II in the edge/triangle model is in a

different category. One possible path to understanding this links the problem to an old open problem in statistical physics, to understand why there is not a critical point in the transition between solid and fluid phases of matter as there is between liquid and gas; see Figure 7.

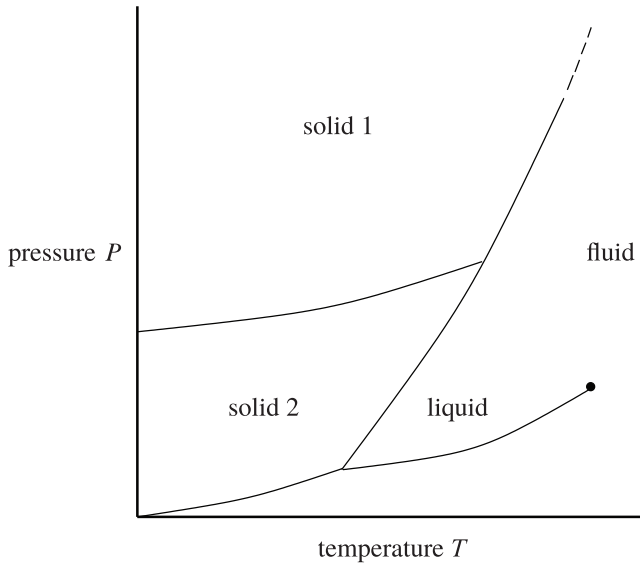


Figure 7. The phase diagram of a simple material.

Consider the traditional symmetry argument from physics [2]:

“It was Landau (Landau and Lifshitz, 1958) who, long ago, first pointed out the vital importance of symmetry in phase transitions. This, the First Theorem of solid-state physics, can be stated very simply: it is impossible to change symmetry gradually. A given symmetry element is either there or it is not; there is no way for it to grow imperceptibly. This means, for instance, that there can be no critical point for the melting curve as there is for the boiling point: it will never be possible to go continuously through some high-pressure phase from liquid to solid.”

This argument is not completely convincing [25], but the role of symmetry in the study of solids is pervasive and has been highly productive both in science and mathematics. And in support for linking the problems we note there is no critical point in the transition between phases II and III in Figure 2 where the graphons for phase II but not III have the higher symmetry, while there is a critical point in Figure 5, where the graphons do not exhibit the higher level symmetry.

## Appendix A. Phases in large constrained permutations

**A.1. Permutons and entropy.** Here we review some results in which the above style of analysis of phases is applied to large constrained permutations. We begin with a quick review of the asymptotic permuton formalism, introduced in [14, 15]. Given a labelled set of  $n$  objects, which we take to be  $\{1, 2, \dots, n\}$ , a permutation  $\pi$  in  $S_n$  is an invertible function from  $\{1, 2, \dots, n\}$  to itself, represented by its values  $(\pi_1, \pi_2, \dots, \pi_n)$ . It is commonly displayed as a square 0–1 matrix  $A_{j,k}$  with value 1 when  $\pi_j = k$ . This can be rescaled and reinterpreted as a function on  $[0, 1]^2$  which has values 0 or 1 on each square  $[(j-1)/n, j/n] \times [(k-1)/n, k/n]$ ,  $j, k = 1, 2, \dots, n$ , with value 1 when  $\pi_j = k$ . Since such functions are nonnegative and have integral 1, they can be reinterpreted as the densities of probability measures  $\gamma_\pi$  on  $[0, 1]^2$ , with the property of uniform marginals:

$$\gamma_\pi([a, b] \times [0, 1]) = b - a = \gamma_\pi([0, 1] \times [a, b]), \quad \text{for all } 0 \leq a \leq b \leq 1. \quad (10)$$

Permutons are then defined more generally to be probability measures on  $[0, 1]^2$  with uniform marginals. We put the usual weak topology of measure theory (or weak\* topology from functional analysis) on the compact space  $\mathbb{M}$  of permutons, and note that the set  $\cup_n \{\gamma_\pi \mid \pi \in S_n\}$  is dense in  $\mathbb{M}$  [14, 15, 13, 17].

We will be considering asymptotic conditional distributions on  $S_n$ , asymptotic as  $n \rightarrow \infty$ , and we choose the conditioning to mesh with the (extremal) study of pattern avoidance as indicated in the beginning of this report. This choice is a more serious decision in the study of permutations than conditioning by subgraph densities for graphs, because it emphasizes a *linear* ordering of the objects being permuted, which is quite restrictive; with another choice one might for instance use the permutations to model the mixing of objects in space. In any case, as we did with graphs we define the density  $\rho_\tau(\gamma)$  of a pattern  $\tau \in S_k$  in a permuton  $\gamma$  as an asymptotic form of its natural meaning for permutations, namely by the probability that when  $k$  points are selected independently from  $\gamma$  and their  $x$ -coordinates are ordered, the permutation induced by their  $y$ -coordinates is  $\tau$ . For example, for  $\gamma$  with probability density  $g(x, y) dx dy$ , the density of pattern  $12 \in S_2$  in  $\gamma$  is

$$\rho_{12}(\gamma) = 2 \int_{x_1 < x_2 \in [0, 1]} \int_{y_1 < y_2 \in [0, 1]} g(x_1, y_1) g(x_2, y_2) dx_1 dy_1 dx_2 dy_2. \quad (11)$$

It follows that if  $\gamma_{\pi_j}$  converges to  $\gamma$  then the density of  $\tau$  in  $\pi_j$  converges to  $\rho_\tau(\gamma)$ , and that two permutons are equal if they have the same pattern densities for all patterns. See [13] for background on permutons.



We now use pattern densities to condition permutations. Let  $\gamma$  be a permutation with probability density  $g$ . We define the Shannon entropy  $H(\gamma)$  of  $\gamma$  by:

$$H(\gamma) = \int_{[0,1]^2} -g(x, y) \ln g(x, y) \, dx dy, \tag{12}$$

where  $0 \ln 0$  is taken as 0. Then  $H$  is finite whenever  $g$  is bounded (and sometimes when it is not). In particular for any  $\pi \in S_k$ , we have  $H(\gamma_\pi) = -k(k \ln k / k^2) = -\ln k$  and therefore  $H(\gamma_\pi) \rightarrow -\infty$  for any sequence of increasingly large permutations even though  $H(\lim \gamma_\pi)$  may be finite. Note that  $H$  is 0 on the uniform permutation (where  $g(x, y) \equiv 1$ ) and negative (sometimes  $-\infty$ ) on all other permutations, since the function  $-z \ln z$  is concave downward. If  $\gamma$  has no probability density we define  $H(\gamma) = -\infty$ .

Fix some finite set  $\{\tau_1, \dots, \tau_k\}$  of patterns and let  $\alpha = (\alpha_1, \dots, \alpha_k)$  be a vector of their target densities. We then define two sets of permutations:

$$\Lambda^{\alpha, \delta} = \{\gamma \in \mathbb{M} \mid |\rho_{\tau_j}(\gamma) - \alpha_j| < \delta \text{ for each } 1 \leq j \leq k\}, \tag{13}$$

$$\Lambda^\alpha = \{\gamma \in \mathbb{M} \mid \rho_{\pi_j}(\gamma) = \alpha_j \text{ for each } 1 \leq j \leq k\}. \tag{14}$$

With that notation, and the understanding that  $\Lambda_n^{\alpha, \delta} = \Lambda^{\alpha, \delta} \cap \gamma(S_n)$ , where  $\gamma(\pi) = \gamma_\pi$ , we have:

**Theorem 2.** (*The variational principle for constrained permutations [17]*)

$$\lim_{\delta \rightarrow 0} \lim_{n \rightarrow \infty} \frac{1}{n} \ln \frac{|\Lambda_n^{\alpha, \delta}|}{n!} = \max_{\gamma \in \Lambda^\alpha} H(\gamma). \tag{15}$$

Constrained sets of permutations in  $S_n$  have cardinality of order  $e^{n \ln n + (c-n)}$  where  $c \in [-\infty, 0]$  is our target [17]. The function of  $\alpha$ ,  $\max_{\gamma \in \Lambda^\alpha} H(\gamma)$ , which is guaranteed by the theorem to exist but may be  $-\infty$ , is the *constrained entropy* and denoted by  $s(\alpha)$ . Theorem 2 was proven in [17] using the large deviations theorem from [42].

**A.2. Examples of constrained large permutations.** The general framework for the asymptotics of constrained permutations is thus analogous to that of constrained graphs. In detail the mathematics is quite different, but in terms of results about phase structure the main difference is in the depth of progress on examples, even on the boundary of their phase spaces, i.e. the extremal theory. The main examples in which relevant progress has been made concerning phases in constrained permutations are: the 12/123 model, star models, and the 123/321 model.

For the 12/123 model it has been shown [17] that the phase space is the same scalloped triangle which is the phase space for the edge/triangle of graphs Figure 1. For graphs the vertices of the scalloped triangle were shown to give rise to interesting phases and phase transitions, as indicated in Figure 2. However there is no evidence yet of an analogous phenomenon for the 12/123 model of permutations.

Star models of permutations use constraints of slightly different character than considered so far. Instead of a single pattern  $\tau \in S_k$  say, one replaces two or more of the symbols in  $\tau$  by a  $*$ , which is a place holder which can be filled by any unused symbols. For instance the constraint  $*2*$  fixes the density of the union of all consistent patterns in  $S_3$ , namely 123 and 321. For a class of models with a finite number of such constraints it is proven that constrained entropy is an analytic function of the constraint values, and that it has a unique optimal permutation at each point in its phase space [17].

Finally, for the 123/321 model there is proven [17] to be a phase transition on a curve emanating from the singularity at  $(0.278\dots, 0.278\dots)$  on its phase boundary (see Figure 8), of similar character to the one proven for the edge/2-star graph model (see Figure 4).

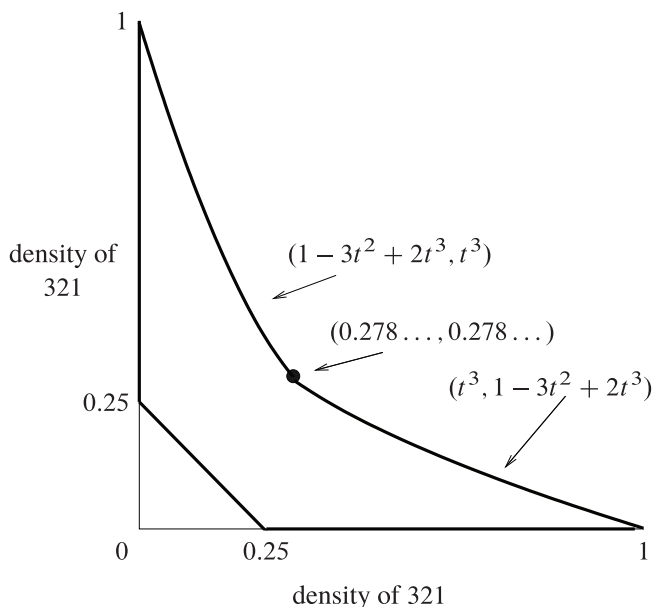


Figure 8. Phase space for density constraints on the patterns 123 and 321.

We conclude our discussion of the permutation theory by noting two topics in the asymptotics of constrained permutations which were omitted due to a lack of results on phase structure. One is the useful tool of insertion measures; see [17]. And finally, we have ignored work done with a single constraint because, as was noted in Section 4.3 for graphs, it does not seem to bear on the deeper issues of phases and phase transitions; however see [41] and references therein, and [35] for connection to other issues.

As an open problem we note that although the permuton formalism seems to apply well to pattern constraints, it leaves out a major aspect of permutations, their cycle structure, which makes use of permutation multiplication and avoids the linear structure used in patterns. It would be a significant advance to incorporate cycle structure in the formalism of pattern constraints.

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