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Two problems in extremal combinatorics

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DEDICATION

I would like to dedicate this thesis to my family, my closest friends, and of course my cat. Bruce, your advice guided me through the hardest of times, even though I sometimes forgot to ask. Mom and Dad, I made it this far thanks to the many sacrifices you made for my success. O'Neil and Carolyn, you filled my moments away from work with immeasurable happiness. Angus, when I needed it the most, you pulled my head of out the clouds with your unflinching demands for attention.

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ABSTRACT

In this thesis, we focus on two problems in extremal graph theory. Extremal graph theory consists of all problems related to optimizing parameters defined on graphs. The concept of "editing" appears in many key results and techniques in extremal graph theory, either as a means to account for error in structural results, or as a quantity to minimize or maximize. A typical problem in spectral extremal graph theory seeks relationships between the extremes of certain graph parameters and the extremes of eigenvalues commonly associated to graphs.

The *edit distance problem* asks the following problem: for any fixed "forbidden" graph F, how many "edits" are needed to ensure that any graph on n vertices can be made to contain no induced copies of F. If F is a complete graph, then Turán's Theorem, an early fundamental result in extremal graph theory, provides a precise answer. The *edit distance function* plays an essential role in answering this question and relates to the *speed* of a graph hereditary property $\mathcal{H}$ as well as the $\mathcal{H}$-chromatic number of a random graph. The main techniques revolve around so-called *colored regularity graphs (CRGs)*. We find an asymptotically almost sure formula for the edit distance function when F is an Erdős-Rényi random graph whose density lies in $[1-1/\phi, 1/\phi] \approx [0.382,0.618]$. As an intermediate step, we make several advances on the application of CRGs, such as the introduction and application of *p-prohibited CRGs*.

For any n-vertex graph G, its adjacency matrix $A = A_G$ is the $\{0,1\}$-valued $n \times n$ matrix whose (u, v) entry indicates whether uv is an edge of G. In 1999, Gregory, Hershkowitz, and Kirkland defined the *(adjacency) spread* of a graph as the difference between the maximum and minimum eigenvalues of its adjacency matrix. In their paper, since cited 68 times, the authors conjectured that the graph on n vertices which maximizes spread is the join of a complete graph on $\lfloor 2n/3 \rfloor$ vertices with an independent set on $\lceil n/3 \rceil$ vertices. We prove this claim for all n sufficiently large. As an intermediate step, we prove an analogous result for the eigenvalues of *graphons* (equivalently, kernel operators on symmetric functions $W : [0,1]^2 \to [0,1]$).

CHAPTER 1. GENERAL INTRODUCTION

In this chapter, we give a brief introduction to the topics, terminology, and notation common throughout this document.

1.1 General graph theory

In this section, we borrow many general terms from [4]. A *(simple, labeled)* graph G is an ordered pair (V, E) where V is a finite set of *vertices* and E is a set of *edges* which are unordered pairs of distinct elements from V. We also write $V(G)$ for the vertex set of G and $E(G)$ for the edge set of G when these sets are not specified in advance. Furthermore, $v(G) = |V(G)|$ is the *order* of G and $e(G) = |E(G)|$ is the *size* of G. The *complement* $H = G^c$ of G is the graph where $V(H) = V(G)$ and for all $u, v \in V(G)$ distinct, $uv \in E(H)$ if and only if $uv \notin E(G)$.

Given any two graphs G, H, an *isomorphism* is a bijection $\varphi : V(G) \to V(H)$ so that for all distinct $u, v \in V(G)$, $uv \in E(G)$ if and only if $\varphi(u)\varphi(v) \in E(H)$. When an isomorphism exists from graph G to graph H, then G and H are *isomorphic*. We treat isomorphic graphs as the same *unlabeled graph*. When necessary, we *label* the vertices of an unlabeled graph with some set V to form a labeled graph with the same name.

Let n be a nonnegative integer. For all $n \geq 0$, the n-vertex *complete graph* K_n is the n-vertex graph so that for all distinct $u, v \in V(K_n)$, $uv \in E(K_n)$, and K_n^c is the n-vertex *empty graph*. For all $n \geq 1$, the n-vertex *path graph* P_n has $V(P_n) = \{u_1, \ldots, u_n\}$ and $E(P_n) = \{u_1u_2, \ldots, u_{n-1}u_n\}$. For all $n \geq 3$, the n-vertex *cycle graph* has $V(C_n) = \{u_1, \ldots, u_n\}$ and $E(C_n) = E(P_n) \cup \{u_1u_n\}$.

Let G be a graph. If $\{u, v\} \in E(G)$, we write uv instead, for convenience, paying no attention to the order of the vertices. For any $uv \in E(G)$, we say that u and v are *adjacent*, u and v are the *endpoints* of uv, and the edge uv is incident to each of u and v. Moreover for any $u \in V(G)$, the *neighbors* of u are the vertices v so that $uv \in E(G)$, and the *neighborhood* of u is the set $N_G(u)$ consisting of all neighbors of u.

Let $S \subseteq V(G)$, the *induced subgraph* on S is the graph $H = G[S]$ where $V(G) = S$ and $E(H)$ is the set of all edges $uv \in E(G)$ so that $u, v \in S$. If $G[S]$ is a complete graph, then S is a *clique* and if $G[S]$ is an empty graph, then S is an *independent set.* The *clique number* $\omega(G)$ and *independence number* $\alpha(G)$ are the maximum cardinalities of a clique, and of an independent set, respectively. The *chromatic number* $\chi(G)$ is the minimum nonnegative integer k such that $V(G)$ admits a partition into k independent sets.

1.2 Spectral graph theory

Spectral graph theory is the area of interplay between linear algebra and graph theory. In *Spectra of Graphs*, Cvetković, Doob, and Sachs characterized the field as *"an attempt to utilize algebra... for the purposes of graph theory and its applications" with "characteristic features justifying it to be treated as a theory in its own right."*. In this section, we borrow many general terms from [2]. Let G be a graph and let $n = v(G)$. The *adjacency matrix* $A = A_G$ of G is the symmetric $n \times n$ so that for all $u, v \in V(G)$, the (u, v)-entry of A is 1 if and only if u, v are distinct and $uv \in E(G)$, and 0 otherwise. The *(adjacency) spectrum* $\Lambda(G)$ is the multiset whose elements are the eigenvalues $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$ of A.

1.3 Random graphs

In this subsection, we borrow terminology from [1]. For any nonnegative integer n and any $p \in (0, 1)$, the *Erdős-Rényi* random graph model $\mathbb{G}(n, p)$ assigns probability $p^{e(G)}(1-p)^{\binom{n}{2}-e(G)}$ to each graph G on vertex set $\{1, \ldots, n\}$. Equivalently, $\mathbb{G}(n, p)$ may be identified with a product probability space of $\binom{n}{2}$ identically distributed Bernoulli random variables, each corresponding to a candidate edge for G.

If $\{E_n\}_{n=1}^{\infty}$ is a sequence of $\{\mathcal{F}_n\}_{n=1}^{\infty}$-random variables and $(\Omega, \{\mathcal{F}_n\}_{n=1}^{\infty}, \mathbb{P})$ is a filtered probability space, then we say that $\{E_n\}_{n=1}^{\infty}$ holds *asymptotically almost surely (***a.a.s.***)* if and only if $\mathbb{P}[E_n] \to 1$ as $n \to \infty$. For example, we treat $\{\mathbb{G}(n, p)\}_{n=1}^{\infty}$ as a filtration on the product of $\mathbb{N}$ identically distributed Bernoulli random variables (each corresponding to an unordered pair of distinct nonnegative integers). If we abusively let $\mathbb{G}(n,p)$ denote a graph sampled according to $\mathbb{G}(n,p)$, then the event (or rather, sequence of events) $[e(\mathbb{G}(n,p)) > 100]$ holds **a.a.s.** for any $p \in (0,1)$.

1.4 Graph limits

In this section, we borrow terminology and discussion from [8]. A *graphon* W is a symmetric Lebesgue-measurable function from $[0,1]^2$ to $[0,1]$. We endow the space $\mathcal{W}_0 = \{W : W \text{ is a graphon}\}$ with the *cut metric* $\|\cdot\|_\square$, defined more generally on all bounded symmetric Lebesgue-measurable functions K by

$$\|K\|_\square := \left| \sup_{S,T \subseteq [0,1]} \int_{S \times T} K \right|.$$

For any n-vertex graph G (whose vertices are implicitly ordered somehow), the *pixel picture* of G is the graphon W_G defined by laying a uniformly spaced $n \times n$ grid on the unit square $[0,1]^2$ and setting W_G to be 1 (or 0) on the squares corresponding to the edges (or non-edges) of G. Two graphons W, U are *weakly isomorphic* if there exist measure-preserving transformations $\sigma, \tau : [0,1] \to [0,1]$ so that $W \circ (\sigma \otimes \sigma) = U \circ (\tau \otimes \tau)$. Graphons are of particular interest in graph theory due to the multitude of parameters, properties, and problems which translate to this analytic setting. We list three fundamental results:

1. *density:* for all $n \geq 1$, the pixel pictures for n-vertex graphs form an ε_n-net in $\mathcal{W}_0$, where $\varepsilon_n \to 0$ as $n \to \infty$.

2. *compactness:* the quotient of $\mathcal{W}_0$ under weak isomorphism is a compact metric space.

3. *continuity:* treating each $W \in \mathcal{W}_0$ as a kernel operator on $L_2[0,1]$, then for all $k \geq 1$, then when treated as a function on $\mathcal{W}_0$, the k-th maximum (or minimum) eigenvalue is continuous.

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CHAPTER 2. ON THE EDIT DISTANCE FUNCTION OF THE RANDOM GRAPH

A paper under review

Alex W. Neal Riasanovsky and Ryan R. Martin [1]

Abstract

Given a hereditary property of graphs $\mathcal{H}$ and a $p \in [0,1]$, the edit distance function $\mathrm{ed}_{\mathcal{H}}(p)$ is asymptotically the maximum proportion of edge-additions plus edge-deletions applied to a graph of edge density p sufficient to ensure that the resulting graph satisfies $\mathcal{H}$. The edit distance function is directly related to other well-studied quantities such as the speed function for $\mathcal{H}$ and the $\mathcal{H}$-chromatic number of a random graph.

Let $\mathcal{H}$ be the property of forbidding an Erdős-Rényi random graph $F \sim \mathbb{G}(n_0, p_0)$, and let φ represent the golden ratio. In this paper, we show that if $p_0 \in [1-1/\varphi, 1/\varphi]$, then **a.a.s.** as $n_0 \to \infty$,

$$\mathrm{ed}_{\mathcal{H}}(p) = (1+o(1))\,\frac{2\log n_0}{n_0} \cdot \min\left\{\frac{p}{-\log(1-p_0)}, \frac{1-p}{-\log p_0}\right\}.$$

Moreover, this holds for $p \in [1/3, 2/3]$ for any $p_0 \in (0,1)$.

2.1 Introduction

All graphs are finite and simple, i.e., without loops and multi-edges. A graph is *nonempty* if it has at least one edge. Denote P_n to be the path graph on n vertices.

For any $p \in [0,1]$ and any positive integer n, write $\mathbb{G}(n,p)$ to be the distribution of graphs according to the Erdős-Rényi random graph model with edge probability p. That is, $G \sim$

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$\mathbb{G}(n,p)$ means that the event that $uv \in E(G)$ for $uv \in \binom{\{1,\ldots,n\}}{2}$ are independent and identically distributed (i.i.d.) with common probability p. We write **a.a.s.** to mean that a sequence of events holds with probability approaching 1 under some implied limit. The limit will be clear by the context. All logarithms are natural unless explicitly stated otherwise.

2.1.1 Edit distance results and forbidding a random graph

The edit distance measures the minimum number of "edits" (that is, edge-additions plus edge-deletions) sufficient to turn one graph into another. This metric has been studied in contexts such as property testing and evolutionary biology (see [3, 11]). Formally, for any two n-vertex graphs G, H on the same vertex set,

$$\mathrm{dist}(G,H) = |E(G) \triangle E(H)| \cdot \binom{n}{2}^{-1}$$

where $\triangle$ is the symmetric difference operation for sets.

A graph property $\mathcal{H}$ is *hereditary* if $\mathcal{H}$ is closed under isomorphism and vertex deletion. For any family $\mathcal{F}$ of graphs, we may write $\mathrm{Forb}(\mathcal{F})$ for the hereditary property of graphs which do not contain an induced copy of F for any $F \in \mathcal{F}$. Any hereditary property is of the form $\mathrm{Forb}(\mathcal{F})$ for some $\mathcal{F}$. A hereditary property of the form $\mathrm{Forb}(\{F\})$ for a single graph F is called a *principal hereditary property* and we will write $\mathrm{Forb}(F)$ for simplicity.

A hereditary property $\mathcal{H}$ is *nontrivial* if, for every positive integer n, there exists a graph in $\mathcal{H}$ of order n. All hereditary properties in this paper are nontrivial. If $\mathcal{H}$ is a nontrivial hereditary property, then for all graphs G, we define

$$\mathrm{dist}(G,\mathcal{H}) = \min\{\mathrm{dist}(G,H) : H \in \mathcal{H} \text{ s.t. } V(H) = V(G)\}.$$

An early result that has motivated subsequent research is as follows:

Theorem 1 (Alon-Stav [2])**.** *For a nontrivial hereditary property $\mathcal{H}$, there exists a $p^* = p^*_{\mathcal{H}} \in [0,1]$ so that with $G \sim \mathbb{G}(n,p^*)$,*

$$\lim_{n\to\infty} \max_{|V(G)|=n} \mathrm{dist}(G,\mathcal{H}) = \mathbb{E}\left[\mathrm{dist}(G,\mathcal{H})\right] + o(1).$$

In other words, random graphs of density p^* asymptotically achieve the maximum distance to $\mathcal{H}$. For any $p \in [0,1]$ and any property $\mathcal{H}$ nontrivial and hereditary, let

$$\mathrm{ed}_{\mathcal{H}}(p) := \limsup_{n\to\infty} \max_{\substack{|V(G)|=n,\\ e(G)=\lfloor p\binom{n}{2}\rfloor}} \mathrm{dist}(G,\mathcal{H}). \tag{2.1}$$

We call $\mathrm{ed}_{\mathcal{H}}$ the *edit distance function of* $\mathcal{H}$. Theorem 2 below demonstrates that the maximum distance $\mathcal{H}$ among all density-p graphs is achieved asymptotically by Erdős-Rényi random graphs of expected density p.

Theorem 2 (Balogh-Martin [4])**.** *Let $\mathcal{H}$ be a nontrivial hereditary property. For all $p \in [0,1]$, if $G \sim \mathbb{G}(n,p)$, then*

$$\mathrm{ed}_{\mathcal{H}}(p) = \lim_{n\to\infty} \mathbb{E}[\mathrm{dist}(G,\mathcal{H})].$$

Moreover the function $\mathrm{ed}_{\mathcal{H}}$ is continuous and concave-down.

Proposition 3 below has several short proofs and follows from Bollobás' asymptotic result on the chromatic number of a random graph (see [5]), together with established techniques for computing edit distance functions (see [11]).

Proposition 3 (Alon-Stav [2])**.** *Let $F \sim \mathbb{G}(n_0, 1/2)$ and define $\mathcal{H} := \mathrm{Forb}(F)$. Then* **a.a.s.** *with $n_0 \to \infty$,*

$$\mathrm{ed}_{\mathcal{H}}(p) = (1+o(1))\,\frac{2\log_2 n_0}{n_0}\cdot \min\{p, 1-p\}.$$

Our main result extends Proposition 3 so that we are able to determine the edit distance function asymptotically for all p_0 in a relatively large open interval around $1/2$. Let $\varphi = (1+\sqrt{5})/2$ be the golden ratio. Note that $1-\varphi^{-1} \approx 0.381966$ and $\varphi^{-1} \approx 0.618034$.

Theorem 4. *Fix $p_0 \in (0,1)$, let $F \sim \mathbb{G}(n_0,p_0)$, and define $\mathcal{H} := \mathrm{Forb}(F)$. If $p_0 \in [1-\varphi^{-1}, \varphi^{-1}]$ then* **a.a.s.** *with $n_0 \to \infty$,*

$$\mathrm{ed}_{\mathcal{H}}(p) = (1+o(1))\,\frac{2\log n_0}{n_0}\cdot \min\left\{\frac{p}{-\log(1-p_0)}, \frac{1-p}{-\log p_0}\right\} \tag{2.2}$$

holds for all $p \in [0,1]$. If $p_0 \in [0, 1-\varphi^{-1})$, then **a.a.s.** *(2.2) holds for all $p \in [1/3, 1]$. If $p_0 \in (\varphi^{-1}, 1]$, then* **a.a.s.** *(2.2) holds for all $p \in [0, 2/3]$.*

In fact, the $o(1)$ error term depends only on the constant p_0 and holds uniformly for all p in each of the respective intervals.

The first author conjectured (see [11]) that for all $p_0 \in [0,1]$, (2.2) holds **a.a.s.** for all $p \in [0,1]$. Theorem 4 proves this for a range of p_0 of size ≈ 0.236068.

2.1.2 Equivalent parameters

The edit distance function is also interesting because of its connection to other parameters involving random graphs. For $\mathcal{H}$ any nontrivial hereditary property and any $p \in (0,1)$, the *speed* of $\mathcal{H}$ is

$$c_{\mathcal{H}}(p) := \lim_{k\to\infty} -\log_2\left(\mathbb{P}\left[\mathbb{G}(k,p) \in \mathcal{H}\right]\right) \cdot \binom{n}{2}^{-1}$$

Indeed, this limit does exist and a proof of that fact appears in [1] and in [6]. See also the survey [11].

The following observation was made by Thomason but it can be shown to follow from a prior result due to Bollobás and Thomason [6].

Theorem 5 (Thomason [13])**.** *Let $\mathcal{H}$ be a nontrivial hereditary property. Then for all $p \in (0,1)$,*

$$c_{\mathcal{H}}(p) = \left(-\log_2(p(1-p))\right) \cdot \mathrm{ed}_{\mathcal{H}}\left(\frac{\log(1-p)}{\log(p(1-p))}\right).$$

Note that the function $f : (0,1) \to (0,1)$ defined by

$$f(x) := \frac{\log(1-x)}{\log(x(1-x))}$$

on $x \in (0,1)$ is invertible. Since $\mathrm{ed}_{\mathcal{H}}$ is continuous, $c_{\mathcal{H}}$ can be computed from $\mathrm{ed}_{\mathcal{H}}$ and vice versa. As a result, combining Theorem 5 with Theorem 4 yields a result on the speed function of hereditary properties defined by random graphs.

Corollary 6. *Fix $p_0 \in (0,1)$, let $F \sim \mathbb{G}(n_0,p_0)$, and define $\mathcal{H} := \mathrm{Forb}(F)$. If $p_0 \in [1-\varphi^{-1},\varphi^{-1}]$ then* **a.a.s.** *with $n_0 \to \infty$,*

$$c_{\mathcal{H}}(p) = (1+o(1))\,\frac{2\log_2 n_0}{n_0} \cdot \min\left\{\frac{\log(1-p)}{\log(1-p_0)}, \frac{\log p}{\log p_0}\right\} \tag{2.3}$$

holds for all $p \in [0,1]$. If $p_0 \in [0,1-\varphi^{-1})$, then **a.a.s.** (2.3) *holds for all $p \in [1-\varphi^{-1},1]$. If $p_0 \in (\varphi^{-1},1]$, then* **a.a.s.** (2.3) *holds for all $p \in [0,\varphi^{-1}]$.*

For any hereditary property $\mathcal{H}$ and any graph G, let $\chi_{\mathcal{H}}(G)$ be the $\mathcal{H}$-*chromatic number* of G. This is the minimum nonnegative integer k for which there exists a partition $V(G) = V_1 \dot\cup \cdots \dot\cup V_k$ such that $G[V_i]$ satisfies $\mathcal{H}$ for all $i \in \{1, \ldots, k\}$. If $\mathcal{H}$ is the property of being an empty graph, then $\chi_{\mathcal{H}}(G)$ is the chromatic number of G.

Bollobás and Thomason established Theorem 7 for the $\mathcal{H}$-chromatic number of a random graph. In their paper, they assumed that all hereditary properties are nontrivial in our sense, and said that $\mathcal{H}$ is "nontrivial" if $\mathcal{H}$ is not the property satisfied by all graphs, i.e., $\mathcal{H} = \mathrm{Forb}(\mathcal{F})$ where $\mathcal{F}$ is a nonempty set of graphs. For convenience, we state this result in our language.

Theorem 7 (Bollobás-Thomason [6])**.** *Let $p \in (0,1)$ and let $\mathcal{H}$ be a nontrivial hereditary property where $\mathcal{H}$ is not the property satisfied by all graphs. Then* **a.a.s.** *with $G \sim \mathbb{G}(n,p)$,*

$$\chi_{\mathcal{H}}(G) = (1 + o(1))\, c_{\mathcal{H}}(p)\, \frac{n}{2 \log_2 n} \tag{2.4}$$

Bollobás' classic asymptotic result [5] on the chromatic number of the random graph can be derived from Theorem 7 by observing that if $\mathcal{H}_{\mathrm{em}}$ is the property of being an empty graph, then $c_{\mathcal{H}_{\mathrm{em}}}(p) = -\log_2(1-p)$ and so $\chi_{\mathcal{H}_{\mathrm{em}}}(G) = (1 + o(1))\,\frac{n}{2\log_{1/(1-p)} n}$ **a.a.s.**

However, the fact that $c_{\mathcal{H}_{\mathrm{em}}}(p) = -\log_2(1-p)$ can itself be derived from Theorem 5 and the entirely trivial observation that $\mathrm{ed}_{\mathcal{H}_{\mathrm{em}}}(p) = p$. In general, $\chi_{\mathcal{H}}$ has a close relationship with both $c_{\mathcal{H}}$ and $\mathrm{ed}_{\mathcal{H}}$.

The rest of the paper is organized as follows: In Section 2.2, we discuss colored regularity graphs (CRGs) and prove some basic results that have the potential to apply to a wide variety of edit distance results beyond the scope of this paper. In Section 2.3, we give the proof of Theorem 4. Section 2.4 includes a proof of the fact that for all $p \in [1 - \varphi^{-1}, \varphi^{-1}]$, $\mathrm{ed}_{\mathcal{H}}(p)$ can be computed by a set CRGs whose order is bounded by a constant depending only on $\mathcal{H}$. Section 2.4 also includes a discussion of the role paths play in CRGs. In Section 2.5, we discuss open questions and potential future work.

2.2 Colored regularity graphs

In this section, we address colored regularity graphs. In Section 2.2.1, we address background and basic facts about colored regularity graphs. Section 2.2.2 discusses the new notion of p-prohibited CRGs. Lemma 20 and Lemma 23 are important new results on p-prohibited CRGs. They are proven in Section 2.2.3 and Section 2.2.4, respectively.

2.2.1 Background on CRGs

The key element to studying the edit distance problem is the colored regularity graph, which was defined by Alon and Stav [2] but appeared as *types* in the prior literature by Bollobás and Thomason (see [6]).

Definition 8. *A* ***colored regularity graph*** *K is a complete graph, together with a partition $V(K) = \mathrm{VW}(K) \dot\cup \mathrm{VB}(K)$ of the vertex set into white and black vertices, and a partition $E(K) = \mathrm{EW}(K) \dot\cup \mathrm{EB}(K) \dot\cup \mathrm{EG}(K)$ of the edge set into white, black, and gray edges.*

A CRG K' is called a ***sub-CRG*** *of CRG K (denoted $K' \subseteq K$) if K' is obtained by deleting some vertices from K and all incident edges.*

CRGs approximate large graphs and we want to know whether a forbidden graph F is in a graph approximated by a given CRG. We express this in terms of embeddings of graphs into CRGs.

Definition 9. *A graph F* ***embeds into*** *CRG K (written $F \mapsto K$) if there exists a function $\phi : V(F) \to V(K)$ such that:*

- *If $uv \in E(F)$, then either $\phi(u) = \phi(v) \in \mathrm{VB}(K)$, or $\phi(u)\phi(v) \in \mathrm{EB}(K) \cup \mathrm{EG}(K)$*
- *If $uv \in E(F^c)$, then either $\phi(u) = \phi(v) \in \mathrm{VW}(K)$, or $\phi(u)\phi(v) \in \mathrm{EW}(K) \cup \mathrm{EG}(K)$.*

For any CRG K, we will treat the elements of $\mathbb{R}^{V(K)}$ both as functions on $V(K)$ and as vectors indexed by the vertices of K. For any two such $\mathbf{x}, \mathbf{y} \in \mathbb{R}^{V(K)}$, we define $\langle \mathbf{x}, \mathbf{y} \rangle := \sum_{u \in V(K)} \mathbf{x}(u)\mathbf{y}(u)$. We also let $M_K(p) \in \mathbb{R}^{V(K)\times V(K)}$ be the matrix whose uv-th entry is

$$m_{uv} := \begin{cases} p, & u \neq v \text{ and } uv \in \mathrm{EW}(K), \text{ or } u = v \text{ and } u \in \mathrm{VW}(K); \\ 1-p, & u \neq v \text{ and } uv \in \mathrm{EB}(K), \text{ or } u = v \text{ and } u \in \mathrm{VB}(K); \\ 0, & u \neq v \text{ and } uv \in \mathrm{EG}(K). \end{cases} \tag{2.5}$$

The all-ones vector $\mathbf{1} \in \mathbb{R}^{V(K)}$ is defined by $\mathbf{1}(u) = 1$ for all $u \in V(K)$ and the all-zeroes vector is just $\mathbf{0} = 0 \cdot \mathbf{1}$. Furthermore, we let $\triangle_K$ be the *standard simplex associated to K* which consists of all $\mathbf{x} \in \mathbb{R}^{V(K)}$ so that $\mathbf{x} \geq \mathbf{0}$ in the component-wise sense and $\langle \mathbf{x}, \mathbf{1} \rangle = 1$. The elements of $\triangle_K$ will be called *weight vectors*.

Now define

$$g_K(p, \mathbf{x}) := \langle \mathbf{x}, M_K(p)\mathbf{x} \rangle \text{ and}$$
$$g_K(p) := \min \{ g_K(p, \mathbf{x}) : \mathbf{x} \in \triangle_K \} .$$

A weight vector $\mathbf{x} \in \triangle_K$ is said to be *optimal for K* if $g_K(p, \mathbf{x}) = g_K(p)$. For any $p \in [0,1]$, a CRG K is said to be *p-core* if for any optimal weight vector $\mathbf{x}$, $\mathbf{x}(u) > 0$ for all $u \in V(K)$. It follows that for K a p-core CRG, there exists a unique optimal weight vector.

For any hereditary property $\mathcal{H} = \mathrm{Forb}(\mathcal{F})$ we define the following family of CRGs:

$$\mathcal{K}_{\mathcal{H}} := \{ K \text{ a CRG} : F \not\mapsto K \text{ for all } F \in \mathcal{F} \}.$$

Theorem 10 is the main technique for computing $\mathrm{ed}_{\mathcal{H}}(p)$, hence understanding the set $\mathcal{K}_{\mathcal{H}}$ is crucial to understanding $\mathrm{ed}_{\mathcal{H}}(p)$. The first equality was given by Balogh and Martin [4] and the second by Marchant and Thomason [10].

Theorem 10. *Let $\mathcal{H}$ be a nontrivial hereditary property. Then for all $p \in [0,1]$,*

$$\mathrm{ed}_{\mathcal{H}}(p) = \inf_{K \in \mathcal{K}_{\mathcal{H}}} g_K(p) = \min_{K \in \mathcal{K}_{\mathcal{H}}} g_K(p). \tag{2.6}$$

It follows by definition that the minimum in Theorem 10 is obtained by a p-core CRG and as Theorem 11 shows, p-core CRGs have a well-defined structure.

Theorem 11 (Marchant-Thomason [10])**.** *Let $p \in [0,1]$ and suppose K is a p-core CRG.*

(a) If $p \in [0,1/2]$, then $\mathrm{EB}(K) = \emptyset$ and for all $uv \in \mathrm{EW}(K)$, $u, v \in \mathrm{VB}(K)$.

(b) If $p \in [1/2,1]$, then $\mathrm{EW}(K) = \emptyset$ and for all $uv \in \mathrm{EB}(K)$, $u, v \in \mathrm{VW}(K)$.

To summarize, if $p \leq 1/2$, then a p-core CRG has no black edges and all white edges must be between black vertices. If $p \geq 1/2$, then a p-core CRG has no white edges and all black edges must be between white vertices. As a result, if $p = 1/2$, p-core CRGs have neither black nor white edges.

Remark 12. *A CRG K is $1/2$-core if and only if all edges of K are gray.*

2.2.2 p-prohibited CRGs

In this paper, we introduce the notion of a prohibited CRG.

Definition 13. *For any $p \in [0,1]$ and any CRG J, we say that J is p-**prohibited** if for any p-core CRG K, J is not a sub-CRG of K.*

For example, Theorem 11 shows that if $p \in [0,1/2)$, then the only 2-vertex CRGs that are not p-prohibited are those with a gray edge or the CRG with two black vertices and a white edge. See Figure 2.1.

Remark 14. *There is an abundance of CRGs which are neither p-core nor p-prohibited. For example, consider the CRGs K and K' defined as follows. Let K consist of 3 black vertices with 2 white edges and 1 gray edge. For all $p \in [0,1]$, K is not p-core. Now let K' be the CRG on 4 black vertices whose white edges induce a P_4 and all other edges are gray. Clearly K' contains K. It is an exercise to see that K' is p-core for all $p \in [0, 1-\varphi^{-1})$, so K is not p-prohibited on this interval.*

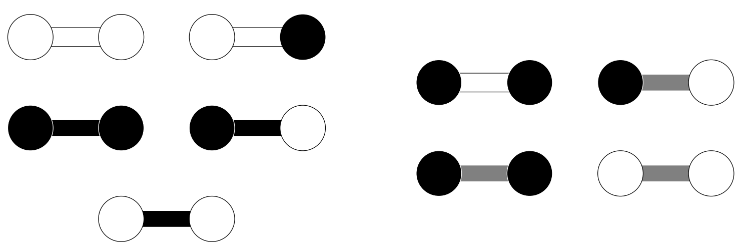

Figure 2.1 All two-vertex CRGs.

We also want to introduce the notion of the complement of a CRG.

Definition 15. *If K is a CRG, then the **complement** of K is the unique CRG $\overline{K}$, such that*

- $\mathrm{VW}(\overline{K}) = \mathrm{VB}(K)$, $\mathrm{VB}(\overline{K}) = \mathrm{VW}(K)$,
- $\mathrm{EW}(\overline{K}) = \mathrm{EB}(K)$, $\mathrm{EB}(\overline{K}) = \mathrm{EW}(K)$, *and* $\mathrm{EG}(\overline{K}) = \mathrm{EG}(K)$.

For a graph G, the notation is G^c is used to denote the graph complement, so as to avoid confusion. There is symmetry in the edit distance function about $p = 1/2$ with respect to complements.

Proposition 16. *If $p \in [0,1]$ and K is a CRG, then $g_K(p) = g_{\overline{K}}(1-p)$.*

Proof. This follows from the equality of the matrices $M_K(p) = M_{\overline{K}}(1-p)$:

$$\begin{aligned} g_K(p) &= \min\{\langle \mathbf{x}, M_K(p)\mathbf{x}\rangle : \mathbf{x} \in \triangle_K\} \\ &= \min\left\{\langle \mathbf{x}, M_{\overline{K}}(1-p)\mathbf{x}\rangle : \mathbf{x} \in \triangle_K\right\} = g_{\overline{K}}(1-p). \end{aligned}$$

□

There is also symmetry in the edit distance function about $p = 1/2$ when it comes to p-prohibition.

Proposition 17. *For all $p \in [0,1]$, a CRG J is p-prohibited if and only if $\overline{J}$ is $(1-p)$-prohibited.*

Proof. Suppose J is p-prohibited but $\overline{J}$ is not $(1-p)$-prohibited. Then, there is a $(1-p)$-core CRG $\overline{K}$ that contains $\overline{J}$ as a sub-CRG. If K is not p-core, then there is a $K' \subseteq K$ such that $g_{K'}(p) = g_K(p)$, but Proposition 16 gives that $g_{\overline{K'}}(1-p) = g_{\overline{K}}(1-p)$, a contradiction to $\overline{K}$ being $(1-p)$-core. □

Next, we introduce terminology which is useful in describing the structure of p-core and p-prohibited CRGs.

Definition 18. *Let K be a CRG.*

- *The **underlying graph** of K is the graph $G = (V(K), \mathrm{EB}(K) \cup \mathrm{EW}(K))$.*
- *A **component** of K is a component of the underlying graph of K.*
- *A **disjoint union** of vertex-disjoint CRGs J, K, denoted $J \oplus K$, is a CRG with vertex set $V_J \oplus V_K$, where the sub-CRG induced on V_J is isomorphic to J, the sub-CRG induced on V_K is isomorphic to K, and every edge incident to a vertex in each of V_J and in V_K has color gray. The disjoint union of k copies of K is $k \cdot K$.*
- *Let G be a nonempty graph. The CRG, K, **associated** to G is defined as follows: If $p \in [0,1/2]$, then $\mathrm{VW}(K) = \mathrm{EB}(K) = \emptyset$, $\mathrm{VB}(K) = V(G)$, $\mathrm{EW}(K) = E(G)$, and $\mathrm{EG}(K) = E(\overline{G})$. If $p \in (1/2,1]$, then $\mathrm{VB}(K) = \mathrm{EW}(K) = \emptyset$, $\mathrm{VW}(K) = V(G)$, $\mathrm{EB}(K) = E(G)$, and $\mathrm{EG}(K) = E(\overline{G})$.*

We associate CRGs to graphs for the purposes of discussing p-core CRGs. See Figure 2.2 for an example. Since 1/2-core CRGs are precisely those which have only gray edges, the definition of the CRG associated to a graph for $p = 1/2$ is made purely out of convenience.

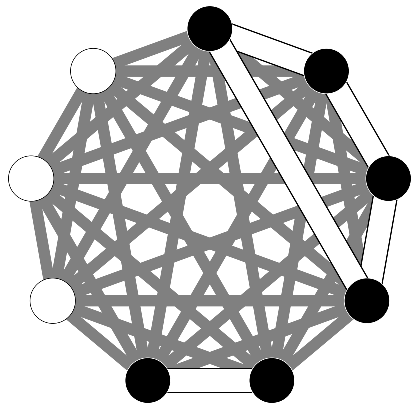

Figure 2.2 A CRG with 5 components. See Theorem 11.

In order to apply Lemma 20 below, we need the minimum adjacency eigenvalue to be at most -1. This occurs for all nonempty graphs. See [7] for a more detailed discussion about eigenvalues associated to graphs.

Proposition 19. *Every nonempty graph that is not disjoint cliques has minimum adjacency eigenvalue at most $-\sqrt{2}$. If a nonempty graph consists of disjoint cliques, its minimum adjacency eigenvalue is -1. An empty graph has all adjacency eigenvalues zero.*

Lemma 20. *Let G be a nonempty graph and let $\lambda \leq -1$ be the minimum eigenvalue of the adjacency matrix of G. The CRG associated to G is p-prohibited for all*

$$p \in \left[\frac{1}{1-\lambda}, 1 - \frac{1}{1-\lambda}\right].$$

In Section 2.2.3, we prove Lemma 20. First, we need some essential terms.

Definition 21. *For any positive integer t, the t-**dalmatian CRG** is the CRG, denoted D_t, consisting of t black vertices and all edges white. The ∞-**dalmatian CRG** is the CRG, denoted D_∞, which is a single white vertex. The set of CRGs denoted by $\mathcal{D}_p$ is as follows:*

- *If $p \in [0, 1/2)$, then $\mathcal{D}_p$ is the set of all CRGs whose components are dalmatian CRGs.*

- *If $p \in (1/2, 1]$, then $\mathcal{D}_p$ is the set of all CRGs whose components are complements of dalmatian CRGs.*
- *If $p = 1/2$, then $\mathcal{D}_{1/2}$ is the set of all CRGs whose components are single vertices.*

See Figure 2.3 for dalmatian CRGs of small order.

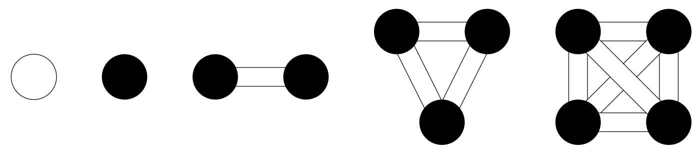

Figure 2.3 The dalmatian CRGs $D_\infty = \overline{D_1}$, $D_1 = \overline{D_\infty}$, D_2, D_3, and D_4.

Remark 22. *For all $p \in [0, 1]$ and each $K \in \mathcal{D}_p$, K is a p-core CRG. Moreover, if $p \in [0, 1/2]$, then $g_{D_\infty}(p) = p$ and for each positive integer t,*

$$g_{D_t}(p) = \min_{\mathbf{x} \in \triangle_{D_t}} \langle \mathbf{x}, M_{D_t}(p)\mathbf{x}\rangle = \frac{1}{t^2}\langle \mathbf{1}, M_{D_t}(p)\mathbf{1}\rangle = p + \frac{1-2p}{t}.$$

If $p \in [1/2, 1]$, then $g_{\overline{D_\infty}}(p) = 1 - p$ and for each positive integer t, $g_{\overline{D_t}}(p) = 1 - p + \frac{2p-1}{t}$.

In Lemma 23, we show that for all $p \in [1 - \varphi^{-1}, \varphi^{-1}]$, the *only* p-core CRGs are those that belong to $\mathcal{D}_p$.

Lemma 23. *For $p \in [0, 1]$, the CRG associated to P_3 is p-prohibited if and only if $p \in [1 - \varphi^{-1}, \varphi^{-1}]$. In particular for all $p \in [1 - \varphi^{-1}, \varphi^{-1}]$, a CRG K is p-core if and only if $K \in \mathcal{D}_p$.*

Remark 24. *Since the minimum eigenvalue of the adjacency matrix of P_3 is $-\sqrt{2}$, Lemma 20 gives that P_3 is prohibited for p in the interval $[\sqrt{2} - 1, 2 - \sqrt{2}] \approx [0.414, 0.586]$. Lemma 23, however, gives that P_3 is prohibited on the larger interval $[1 - \varphi^{-1}, \varphi^{-1}] \approx [0.382, 0.618]$.*

In Section 2.2.4, we prove Lemma 23.

2.2.3 Proof of Lemma 20

The result from Theorem 25 below was originally shown by Sidorenko [12] using different language and has appeared in several other forms throughout the study of hereditary properties. See [11] for a more detailed history. For convenience, we state it in the language of CRGs.

Theorem 25. *Let K be a p-core CRG with optimal weight vector $\mathbf{x} \in \triangle_K$. Then*

$$M_K(p)\,\mathbf{x} = g\,\mathbf{1}.$$

So, Theorem 25 establishes that the optimal weight vector produces a weighting that is balanced.

Lemma 26. *Let $0 \leq p \leq 1$ and J be a CRG. If there exists a nonzero vector $\boldsymbol{\delta} \in \mathbb{R}^{V(J)}$ so that $\langle \boldsymbol{\delta}, \mathbf{1} \rangle = 0$ and*

$$\langle \boldsymbol{\delta}, M_J(p)\,\boldsymbol{\delta} \rangle \leq 0, \tag{2.7}$$

then J is p-prohibited.

Proof. We proceed by contradiction. Suppose J is not p-prohibited and that there exists $\boldsymbol{\delta}$ as above. Then there exists a p-core CRG K containing J and we may let $\mathbf{x}$ denote the optimal weight vector for K. We extend $\boldsymbol{\delta}$ to a vector $\boldsymbol{\delta}' \in \mathbb{R}^{V(K)}$ by letting $\boldsymbol{\delta}'(u) := 0$ if $u \in V(K) \setminus V(J)$ and $\boldsymbol{\delta}'(u) := \boldsymbol{\delta}(u)$ if $u \in V(J)$. Note that $\langle \boldsymbol{\delta}', \mathbf{1} \rangle = 0$.

Since $\mathbf{x}$ is the optimal weight vector for the p-core CRG K, $\mathbf{x}(u) > 0$ for all $u \in V(K)$ and it follows that there exists some $\varepsilon > 0$ so that $\mathbf{x}' := \mathbf{x} + \varepsilon\boldsymbol{\delta}'$ lies in $\triangle_K$ and $\mathbf{x}'(u) = 0$ for some $u \in V(K)$. By the definition of $g_K(p)$, the fact that $\mathbf{x}$ is optimal, and Theorem 25,

$$\begin{aligned}
0 &< g_K(p, \mathbf{x}') - g_K(p, \mathbf{x}) \\
&= \langle \mathbf{x} + \varepsilon\boldsymbol{\delta}', M_K(p)(\mathbf{x} + \varepsilon\boldsymbol{\delta}') \rangle - \langle \mathbf{x}, M_K(p)\mathbf{x} \rangle \\
&= 2\varepsilon \langle \boldsymbol{\delta}, M_K(p)\mathbf{x} \rangle + \varepsilon^2 \langle \boldsymbol{\delta}', M_K(p)\boldsymbol{\delta}' \rangle \\
&= 2\varepsilon \langle \boldsymbol{\delta}', g_K(p)\mathbf{1} \rangle + \varepsilon^2 \langle \boldsymbol{\delta}, M_J(p)\boldsymbol{\delta} \rangle \\
&= \varepsilon^2 \langle \boldsymbol{\delta}, M_J(p)\boldsymbol{\delta} \rangle \leq 0,
\end{aligned}$$

a contradiction to the assumption that J is not p-prohibited. ∎

We include one more well-known fact about p-core CRGs.

Proposition 27 (See [11])**.** *Let $K_1, \ldots, K_\ell$ be CRGs and let $K = K_1 \oplus \cdots \oplus K_\ell$. Then for all $p \in [0, 1]$,*

$$g_K(p)^{-1} = \sum_{i=1}^{\ell} g_{K_i}(p)^{-1}. \tag{2.8}$$

In particular, K is p-core if and only if each of $K_1, \ldots, K_\ell$ are p-core.

Lemma 28. *Let $p \in [0,1]$. A CRG J is p-prohibited if and only if for all p-core CRGs K and all positive integers k, the CRG $(k \cdot J) \oplus K$ is p-prohibited.*

Proof. To prove the forward implication, if J is p-prohibited, then no p-core CRG can contain $k \cdot J$ because it would contain J. To prove the reverse implication, if J is not p-prohibited then there exists a p-core CRG, L, containing J. Then $J \oplus K$ is contained in $L \oplus K$, which is p-core by Proposition 27, as desired. □

With the primary tools of Lemmas 26 and 28 established, we now proceed to prove Lemma 20 itself.

Recall that J is the CRG associated to a nonempty graph G. If $p = 1/2$, then by Theorem 11, J is $1/2$-prohibited if and only if J has an edge that is not gray. Thus, any nonempty G gives that J is $1/2$-prohibited, settling the case where $p = 1/2$.

Now suppose $p \in (0, 1/2)$. Write A for the adjacency matrix of G and suppose $A\mathbf{x} = \lambda\mathbf{x}$ for some unit vector $\mathbf{x}$ where λ is the minimum eigenvalue of A. Then J is the the CRG on $V(G)$ with all vertices black, and where edge uv is white if $uv \in E(G)$, and uv is gray if $uv \in E(G^c)$. So $M_J(p) = (1-p)I + pA$.

For convenience, we write V_1 and V_2 for the vertex sets in $2 \cdot J$ corresponding to each copy of J. Let $\boldsymbol{\delta} \in \mathbb{R}^{V(2 \cdot J)}$ be defined by

$$\boldsymbol{\delta}(u) := \begin{cases} \mathbf{x}(u), & u \in V_1; \\ -\mathbf{x}(u), & u \in V_2. \end{cases}$$

By definition, $\langle \mathbf{1}, \boldsymbol{\delta} \rangle = 0$. Moreover note that

$$\begin{aligned} \langle \boldsymbol{\delta}, M_{2 \cdot J}(p)\boldsymbol{\delta} \rangle &= \langle \mathbf{x}, M_J(p)\mathbf{x} \rangle + \langle -\mathbf{x}, M_J(p)(-\mathbf{x}) \rangle \\ &= 2\langle \mathbf{x}, M_J(p)\mathbf{x} \rangle \\ &= 2\langle \mathbf{x}, ((1-p)I + pA)\mathbf{x} \rangle \\ &= 2(1-p)\langle \mathbf{x}, I\mathbf{x} \rangle + 2p\langle \mathbf{x}, A\mathbf{x} \rangle \\ &= 2(1-p)\langle \mathbf{x}, \mathbf{x} \rangle + 2p\lambda\langle \mathbf{x}, \mathbf{x} \rangle \\ &= 2 \cdot (1 - (1-\lambda)p) \cdot \langle \mathbf{x}, \mathbf{x} \rangle. \end{aligned}$$

If $p \geq 1/(1-\lambda)$, then $\langle \boldsymbol{\delta}, M_{2\cdot J}(p)\boldsymbol{\delta}\rangle \leq 0$. By Lemma 26, the CRG $2 \cdot J$ is p-prohibited and by Lemma 28, J itself is p-prohibited. This settles the case where $p \in (0, 1/2)$.

Finally, for the case of $p \in (1/2, 1)$, Proposition 17 gives that J is p-prohibited if and only if J is $(1-p)$-prohibited. This concludes the proof of Lemma 20.

2.2.4 Proof of Lemma 23

Lemma 29 below is a result in pure graph theory that is reminiscent of the theorem that categorizes $\{P_4, C_4, C_4^c\}$-free graphs as threshold graphs. A *dominant vertex* in a graph is one for which every other vertex is its neighbor.

Lemma 29. *If G is a connected $\{P_4, C_4\}$-free graph, then G has a dominant vertex.*

Proof. Let u be a vertex of G which attains the maximum degree $\Delta = \Delta(G)$ and let $A := N_G(u)$ and $B := V(G) \setminus (A \cup \{u\})$. If $B = \emptyset$, then u is the desired vertex, so we assume otherwise. Let $w \in B$. Since G avoids induced P_4-s, connectivity implies G has diameter at most 2.

In particular, $\mathrm{dist}_G(u, w) = 2$, so there exists some vertex $v \in A$ so that uvw is an induced path on 3 vertices. If v' is any vertex in $A \setminus \{v\}$, then $v'uvw$ is a path on 4 vertices. Since $uw \notin E(G)$ and G avoids both induced P_4-s and induced C_4-s, it follows that $vv' \in E(G)$. So v is adjacent to $\{u, w\} \cup (A \setminus \{v\})$ and has degree at least $\Delta + 1$, a contradiction. □

Lemma 29 yields a very strong structural theorem on CRGs, Lemma 30. Recall the definition of the underlying graph of CRG, K, in Definition 18: the graph whose vertices are the vertices of K and whose edges are the non-gray edges of K.

Lemma 30. *Let $p \in [1/3, 2/3]$. If a p-core CRG has an underlying graph which is $\{P_4, C_4\}$-free, then every component of the underlying graph is a clique. That is, every component of such a CRG must be a member of $\mathcal{D}_p$.*

Proof. If $p = 1/2$, then as we saw in Remark 12, a p-core CRG has only gray edges and so the underlying graph is empty.

Let $p \in [1/3, 1/2)$. Every trivial component of the underlying graph is simply a vertex in the CRG. Let K be a nontrivial component of the CRG. By Theorem 11, the vertices of K must be black and by Lemma 29, the underlying graph of K has a dominant vertex u.

Let $\mathbf{x} \in \triangle_K$ be the optimal weight vector for K and define $g := g_K(p)$. By Theorem 25, $M_K(p)\mathbf{x} = g\mathbf{1}$ and by inspecting the entry indexed by u,

$$g = (1-p)\mathbf{x}(u) + p \cdot \sum_{u \neq v \in V(K)} \mathbf{x}(v) = p + (1-2p)\mathbf{x}(u) > p.$$

For a contradiction, we now suppose K is not a dalmatian CRG. Hence, there exists some gray edge vw, and the sub-CRG K' on v and w is the disjoint union of two black vertices. Since K is p-core,

$$g < g_{K'}(p) = \min_{\mathbf{y} \in \triangle_{K'}} (1-p)(\mathbf{y}(v)^2 + \mathbf{y}(w)^2) = \frac{1-p}{2}.$$

Altogether, $p < g < (1-p)/2$ which implies that $p < 1/3$, a contradiction.

The case where $p \in (1/2, 2/3]$ follows by symmetry. □

We now prove Lemma 23 itself with the primary tool being Lemma 30. As mentioned in Remark 14, we leave it as an exercise to verify that the CRG associated with P_4 is p-core for $p \in (0, 1-\varphi^{-1}) \cup (\varphi^{-1}, 1)$. Hence, P_3 is not p-prohibited in this range, proving the forward implication.

For the reverse implication, let $p \in [1-\varphi^{-1}, \varphi^{-1}]$. Since the minimum eigenvalues of the adjacency matrices of C_4 and P_4 are -2 and $-\varphi^{-1}$ respectively, Lemma 20 implies that the CRGs associated with C_4 and P_4 are p-prohibited for $p \in [1-\varphi^{-1}, \varphi^{-1}]$.

Suppose K is a p-core CRG. Since $p \in [1/3, 2/3]$, it follows from Lemma 30 that the components of the underlying graph of K are cliques. No such graph contains an induced P_3 and so P_3 is p-prohibited for all $p \in [1-\varphi^{-1}, \varphi^{-1}]$, as desired.

For the second statement of the theorem, since P_3 is p-prohibited, the only underlying graphs of a p-core CRG can be disjoint cliques, which is exactly the condition of being in $\mathcal{D}_p$. As observed in Remark 22, all CRGs in $\mathcal{D}_p$ are p-core. This concludes the proof of Lemma 23.

2.3 Proof of the main result

To proceed with the proof of Theorem 4, we need some preparation. In Section 2.3.1, Lemma 31 shows that for all $p \in (1/3, 2/3)$ and for any CRG K, there exists a sub-CRG K'

of K so that $g_{K'}(p)$ is close to $g_K(p)$ and K' has components whose order is bounded by a function of p and a tolerance term ε.

For the remaining discussion, let $p_0 \in (0,1)$ and define

$$p^* := \frac{\log(1-p_0)}{\log(p_0(1-p_0))}. \tag{2.9}$$

In Section 2.3.2, we investigate when a random graph $F \sim \mathbb{G}(n_0, p_0)$ embeds into a CRG (i.e., when $F \mapsto K$). There we show that **a.a.s.**, if a CRG, K, has bounded components in the above sense and the random graph does not map into K, then $g_K(p^*)$ has to be at least the desired value to within a small tolerance. Applying Lemma 31, this is true even if the components of K are not bounded.

Finally in Section 2.3.3, we put together these ideas to prove our main result.

2.3.1 Trimming p-core CRGs

The main result in this subsection is Lemma 31, which establishes that, for $p \in (1/3, 2/3)$, a CRG has a sub-CRG with bounded component sizes and a negligible change in the value of the g-function.

Lemma 31. *Fix $p \in (1/3, 2/3)$ and $\varepsilon \in (0,1)$. There exists a positive integer $B = B(p,\varepsilon)$ such that the following holds: For all CRGs K, there exists a p-core sub-CRG K' whose components have order at most B, and $g_{K'}(p) \leq (1+\varepsilon) g_K(p)$.*

The first part of the proof is to remove vertices from a CRG K one-by-one in a way which does not affect $g_K(p)$ too much. Once enough vertices are removed, we show that each remaining vertex is incident to a bounded number of non-gray edges. Finally, we use Lemma 20 to bound the diameter of p-core CRGs on the interval $p \in (1/3, 2/3)$. The underlying graph has bounded degree and diameter, thus its connected components have bounded order.

The proof consists of a sequence of propositions:

Proposition 32. *Fix $p \in [0,1]$ and suppose K is a p-core CRG with least two vertices. If $\mathbf{x} \in \triangle_K$ is the optimal weight vector for K, i.e., $g = g_K(p) = g_K(p, \mathbf{x})$, then for all $u \in V(K)$,*

$$g_{K \setminus \{u\}}(p) \leq g + \frac{\mathbf{x}(u)^2}{(1-\mathbf{x}(u))^2}.$$

Proof. Let $K' := K \setminus \{u\}$. Since K is p-core with at least two vertices, $\mathbf{x}(u) < 1$ and we may define $\mathbf{x}' \in \triangle_K$ by

$$\mathbf{x}'(v) := \begin{cases} 0, & v = u \\ \dfrac{\mathbf{x}(v)}{1-\mathbf{x}(u)}, & \text{otherwise} \end{cases}.$$

In other words, if $\mathbf{e}_u \in \mathbb{R}^{V(K)}$ is the indicator vector for the vertex u, then $(1-\mathbf{x}(u))\mathbf{x}' = \mathbf{x} - \mathbf{x}(u)\mathbf{e}_u$. Recall that $M_K(p)$ denotes the weighted adjacency matrix of K. By Theorem 25, $M_K(p)\mathbf{x} = g\mathbf{1}$ and so

$$\begin{aligned}(1-\mathbf{x}(u))^2\langle \mathbf{x}', M_K(p)\mathbf{x}'\rangle &= \langle \mathbf{x} - \mathbf{x}(u)\mathbf{e}_u, M_K(p)(\mathbf{x} - \mathbf{x}(u)\mathbf{e}_u)\rangle \\ &= \langle \mathbf{x}, g\mathbf{1}\rangle - 2\mathbf{x}(u)\langle \mathbf{e}_u, g\mathbf{1}\rangle + \mathbf{x}(u)^2\langle \mathbf{e}_u, M_K(p)\mathbf{e}_u\rangle \\ &\le g - 2g\,\mathbf{x}(u) + \mathbf{x}(u)^2.\end{aligned}$$

By definition of $g_{K'}(p)$ and since $\mathbf{x}'(u) = 0$,

$$\begin{aligned}g_{K'}(p) &\le g_K(p, \mathbf{x}') \\ &= \frac{\langle \mathbf{x}', M_K(p)\mathbf{x}'\rangle}{(1-\mathbf{x}(u))^2} \\ &= \frac{g - 2g\,\mathbf{x}(u) + \mathbf{x}(u)^2}{(1-\mathbf{x}(u))^2} \\ &= g + \frac{(1-g)\mathbf{x}(u)^2}{(1-\mathbf{x}(u))^2} \\ &\le g + \frac{\mathbf{x}(u)^2}{(1-\mathbf{x}(u))^2},\end{aligned}$$

which completes the proof. □

Proposition 33. *Fix $p \in [0,1]$ and $\varepsilon \in (0,1)$. If K is a p-core CRG with $g = g_K(p)$, then there exists a p-core sub-CRG K' of K such that the following holds:*

1. *$|V(K')| \le 4/(\varepsilon g)$,*
2. *$g_{K'}(p) \le (1 + 17\varepsilon)g$, and*
3. *if $\mathbf{x}' \in \triangle_{K'}$ is the optimal weight vector for K', then*

$$\min_{u \in V(K')} \mathbf{x}'(u) \ge \varepsilon g.$$

Proof. Define a finite sequence of sub-CRGs

$$K = K_0 \supset K_1 \supset \cdots \supset K_\ell$$

as follows: First let $K := K_0$ and $g_0 := g_K(p)$. For any $k \geq 0$ so that $|V(K_k)| \geq 2$, do the following:

(i) Let $\mathbf{x}_k \in \triangle_{K_k}$ be the optimal weight vector for K_k, i.e., $g_{K_k}(p, \mathbf{x}_k) = g_{K_k}(p)$.

(ii) Let $u_k \in V(K_k)$ so that $\mathbf{x}_k(u_k) = \min \{\mathbf{x}_k(v) : v \in V(K_k)\}$.

(iii) Let K_{k+1} be any p-core sub-CRG of $K_k \setminus \{u_k\}$.

Since each step removes at least one vertex, $\ell \leq |V(K)|$. For each $k \in \{0, \ldots, \ell\}$, denote $g_k := g_{K_k}(p)$.

Let $a \in \{0, \ldots, \ell\}$ be the minimum index a so that $|V(K_a)| \leq 4/(\varepsilon g)$. By definition of a and by the fact that $\varepsilon, g < 1$,

$$\mathbf{x}_k(u_k) \leq 1/|V(K_k)| \leq (\varepsilon g)/4 \leq 1/4$$

for all $k \in \{0, \ldots, a-1\}$. By Proposition 32,

$$g_{k+1} \leq g_k + \frac{\mathbf{x}_k(u_k)^2}{(1-\mathbf{x}_k(u_k))^2} \leq g_k + \frac{\mathbf{x}_k(u_k)^2}{(3/4)^2} < g_k + \frac{2}{|V(K_k)|^2}.$$

Because $|V(K_k)| \geq |V(K_{a-1})| + (a-1-k)$ for all $k \in \{0, \ldots, a-1\}$,

$$\begin{aligned} g_a &< g + \sum_{k=0}^{a-1} \frac{2}{|V(K_k)|^2} \\ &\leq g + \sum_{k=0}^{a-1} \frac{2}{\left(|V(K_{a-1})| + (a-1-k)\right)^2} \\ &< g + \sum_{i=|V(K_{a-1})|}^{\infty} \frac{2}{i^2} \\ &< g + \int_{i=|V(K_{a-1})|-1}^{\infty} \frac{2}{x^2}\, dx \\ &= g + \frac{2}{|V(K_{a-1})| - 1} \\ &\leq g + \frac{2}{\lfloor 4/(\varepsilon g) \rfloor}. \end{aligned}$$

Since $\varepsilon g < 1$, it is the case that $\lfloor 4/(\varepsilon g) \rfloor > 2/(\varepsilon g)$. Consequently,

$$g_a \leq (1+\varepsilon)g. \tag{2.10}$$

Let b be the least index $a \leq b \leq \ell$ so that $\mathbf{x}_b(u) \geq \varepsilon g$ for all $u \in V(K_b)$. Note that b is well-defined since $\mathbf{x}_\ell(u) = 1 > \varepsilon g$ where x is the optimal weighting for K_ℓ, a CRG with a single vertex. For any $k \in \{a, \ldots, b-1\}$, it is the case that $\mathbf{x}_k(u_k) < \varepsilon g$ and that $\mathbf{x}_k(u_k) \leq 1/|V(K_k)| \leq 1/2$ and again by Proposition 32,

$$g_{k+1} \leq g_k + \frac{\mathbf{x}_k(u_k)^2}{(1-\mathbf{x}_k(u_k))^2} < g_k + \frac{(\varepsilon g)^2}{(1/2)^2} = g_k + 4\varepsilon^2 g^2.$$

Finally by (2.10) and since $b - a \leq |V(K_a)| \leq 4/(\varepsilon g)$,

$$g_b \leq g_a + \sum_{k=a}^{b-1} 4\varepsilon^2 g^2 \leq (1+\varepsilon)g + |V(K_a)| \cdot 4\varepsilon^2 g^2 \leq (1+17\varepsilon)g.$$

Letting $K' := K_b$, we have the desired sub-CRG. □

Proposition 34 below implies that we can decrease the degree of the underlying graph of a CRG K without changing $g_K(p)$ too much.

Proposition 34. *Fix $p \in (0,1)$ and $\varepsilon \in (0,1)$. If K is a p-core CRG, then there exists a p-core sub-CRG K' of K so that*

1. *$g_{K'}(p) \leq (1+\varepsilon)g_K(p)$, and*
2. *for each $u \in V(K')$, u is incident in K' to at most*

$$17\varepsilon^{-1} \cdot \max\left\{\frac{1}{p}, \frac{1}{1-p}\right\}$$

black or white edges.

Proof. We prove the claim for all $p \in (0, 1/2]$. By duality (that is, by replacing K with $\overline{K}$ and p with $1-p$) the claim holds also for all $p \in [1/2, 1)$. By Proposition 33 applied to K and $\varepsilon/17$, there exists a sub-CRG K' of K so that $g_{K'}(p) \leq (1+\varepsilon)g_K$ and whose optimal weight vector $\mathbf{x} \in \triangle_{K'}$ has $\mathbf{x}(u) \geq \varepsilon g/17$ for all $u \in V(K')$. By Theorem 11, the white vertices of K'

are incident to no white or black edges. So it suffices to prove the desired inequality for black vertices. Suppose $u \in \mathrm{VB}(K')$. By Theorem 25, $M_{K'}(p)\mathbf{x} = g\mathbf{1}$ and it follows that

$$\frac{g}{p} > \frac{g}{p} - \frac{1-p}{p}\mathbf{x}(u) = \sum_{uv \in \mathrm{EW}(K')} \mathbf{x}(v) \geq \frac{\varepsilon g}{17} \cdot \left|\{v : uv \in \mathrm{EW}(K')\}\right|.$$

So the number of vertices adjacent to a vertex via a non-gray edge is at most $17/(\varepsilon p)$, as desired. ☐

Next, we uniformly bound the diameter of all p-core CRGs, for each $p \in (1/3, 2/3)$.

Proposition 35. *For all positive integers d, the CRG associated to the path P_d on d vertices is p-prohibited for all*

$$p \in \left[\frac{1}{1 + 2\cos(\pi/(d+1))}, 1 - \frac{1}{1 + 2\cos(\pi/(d+1))}\right]. \tag{2.11}$$

Proof. It is a well-known fact from spectral graph theory that the spectrum of the adjacency matrix of P_d, the path on d vertices is the multiset $\left\{2\cos\left(\frac{\pi k}{d+1}\right) : k \in \{1, \ldots, d\}\right\}$. See, for example, [8]. In particular, the minimum such eigenvalue is $-2\cos(\pi/(d+1))$. Lemma 20 gives that P_d is p-prohibited for p in the stated range. ☐

Finally, we prove Lemma 31.

Proof of Lemma 31. Since the sequence $\left\{\frac{1}{1+2\cos(\pi/(d+1))}\right\}$ is monotone decreasing and converges to $1/3$, there exists a positive integer $d = d_p$ so that P_d is p-prohibited. Let K' be the sub-CRG from Proposition 34 and write G for its underlying graph. Then by construction, G has degree at most

$$D = 17\varepsilon^{-1} \cdot \max\left\{\frac{1}{p}, \frac{1}{1-p}\right\}.$$

Let C be any component of G. Since P_d is p-prohibited, C has diameter at most $d - 1$. It follows that

$$|C| \leq 1 + D + D(D-1) + \cdots + D(D-1)^{d-1} =: B(p, \varepsilon),$$

as desired. ☐

2.3.2 Forbidding a random graph

Now we proceed to prove our main result, Theorem 4. First, recall that Theorem 7 says that if $F' \sim \mathbb{G}(n_0', p_0)$ then **a.a.s.**,

$$\chi_H(F') = (1 + o(1))\, c_{\mathcal{H}}(p_0)\, \frac{n_0'}{2 \log_2 n_0'}.$$

This is useful because in the proof of Lemma 37, we repeatedly decompose induced subgraphs of a random graph of order $n_0 \gg n_0'$. An essential tool is the following restatement of a theorem of Bollobás and Thomason:

Lemma 36 (Lemma 5.1 from [6])**.** *Let K be a CRG and define $\mathcal{H}$ to be the hereditary property of graphs, G, such that $G \mapsto K$. For all $p_0 \in (0, 1)$,*

$$c_{\mathcal{H}}(p_0) = -\log_2(p_0(1 - p_0)) \cdot g_K\,(p^*)$$

Lemma 37. *Let p_0 and ε be fixed such that $p_0 \in (0, 1)$ and $\varepsilon \in (0, 1)$. Moreover, fix $\mathcal{B}$ to be a finite set of CRGs. If $F \sim \mathbb{G}(n_0, p_0)$, the following holds* **a.a.s.** *as $n_0 \to \infty$: For all CRGs K such that all components of K lie in $\mathcal{B}$ and $F \not\mapsto K$, then*

$$(1 + \varepsilon)\, g_K\,(p^*) \geq \frac{2 \log n_0}{-\log(p_0(1 - p_0)) \cdot n_0}. \tag{2.12}$$

Proof. For any function $\mu : \mathcal{B} \to \{0, 1, \dots\}$, define the CRG, K_μ as follows:

$$K_\mu := \bigoplus_{B \in \mathcal{B}} \mu(B) \cdot B.$$

That is, K_μ consists of a disjoint union of $\mu(B)$ copies of B, for all $B \in \mathcal{B}$. For any induced subgraph G of the random graph $F \sim \mathbb{G}(n_0, p_0)$ and any CRG K, we will denote the event that G embeds into K by $[G \mapsto K]$. Additionally, let

$$E_\mu := [F \mapsto K_\mu].$$

Let

$$\mathcal{B}_0 := \left\{ \mu : \mathcal{B} \to \{0, 1, \dots\} : (1 + \varepsilon) g_{K_\mu}(p^*) < \frac{2 \log n_0}{-\log(p_0(1 - p_0)) \cdot n_0} \right\}.$$

To prove the desired claim, it is equivalent to show that the probability that $F \not\mapsto K_\mu$ for all $\mu \in \mathcal{B}_0$ goes to zero. That is,

$$\lim_{n_0 \to \infty} \mathbb{P}\left[\bigcup_{\mu \in \mathcal{B}_0} \overline{E_\mu}\right] = 0. \tag{2.13}$$

Recall $F \sim \mathbb{G}(n_0, p_0)$. We will partition $V(F)$ by setting

$$C := \left\lceil 2|\mathcal{B}| \cdot \frac{1+\varepsilon/2}{\varepsilon/2} \right\rceil$$

and let $I_1, \ldots, I_C$ be an equipartition of $V(F)$, i.e., $|I_k| \in \{\lfloor n_0/C \rfloor, \lceil n_0/C \rceil\}$ for $k \in \{1, \ldots, C\}$. Let $n_0' = \lceil n_0/C \rceil$.

For any $B \in \mathcal{B}$, set

$$m_B := \left\lfloor \frac{(1+\varepsilon/2) \cdot (n_0/C) \cdot (-\log(p_0(1-p_0))) \cdot g_B(p^*)}{2\log(n_0/C)} \right\rfloor.$$

We expect to be able to $(m_B \cdot B)$-color a $\mathbb{G}(n_0', p_0)$ graph (hence a $\mathbb{G}(n_0'-1, p_0)$ graph as well). Now for any $k \in \{1, \ldots, C\}$ and any $B \in \mathcal{B}$, we define the event

$$E_{k,B} := [F[I_k] \mapsto m_B \cdot B].$$

In other words, $E_{k,B}$ is the event that the subgraph of F that is induced by vertices in I_k is colorable by m_B copies of the CRG B.

The induced subgraphs $F[I_1], \ldots, F[I_C]$ are each independently sampled according to the Erdős-Rényi random graph model $\mathbb{G}(n_0', p_0)$. Moreover, the number of events of the form $E_{k,B}$ is equal to $C \cdot |\mathcal{B}|$, which is bounded as a function of the constants p_0, ε, and $|\mathcal{B}|$.

For any $K \in \mathcal{B}$, the property of all graphs G such that $G \mapsto K$ is not satisfied by all graphs. Then by Theorem 7 and Lemma 36, since the number of vertices in each I_k uniformly tends to ∞,

$$\lim_{n_0 \to \infty} \mathbb{P}\left[\bigcup_{k \in \{1,\ldots,C\}} \bigcup_{B \in \mathcal{B}} \overline{E_{k,B}}\right] = 0. \tag{2.14}$$

It suffices to show that

$$\bigcup_{\mu \in \mathcal{B}_0} \overline{E_\mu} \subseteq \bigcup_{k \in \{1,\ldots,C\}} \bigcup_{B \in \mathcal{B}} \overline{E_{k,B}},$$

because then (2.14) will imply (2.13) and complete the proof.

Indeed, suppose $\mu \in \mathcal{B}_0$ and suppose $\varphi_{k,B}$ are embeddings defined by the events $E_{k,B}$, for all $k \in \{1, \dots, C\}$ and all $B \in \mathcal{B}$. Further, for any $B \in \mathcal{B}$, let

$$M_B := \left\lfloor \frac{\mu(B)}{m_B} \right\rfloor.$$

We will show that if $\sum_{B \in \mathcal{B}} M_B \geq C$, then F can be colored by M_B copies of $m_B \cdot B$, over all $B \in \mathcal{B}$, and so $F \mapsto K_\mu$. We begin by summing the M_B's.

$$\begin{aligned}
\sum_{B \in \mathcal{B}} M_B &= \sum_{B \in \mathcal{B}} \left\lfloor \frac{\mu(B)}{m_B} \right\rfloor \\
&\geq \sum_{B \in \mathcal{B}} \left(\frac{\mu(B)}{m_B} - 1 \right) \\
&= -|\mathcal{B}| + \sum_{B \in \mathcal{B}} \frac{\mu(B) \cdot 2 \log(n_0/C)}{(1 + \varepsilon/2) \cdot (n_0/C) \cdot (-\log(p_0(1-p_0))) \cdot g_B(p^*)} \\
&= -|\mathcal{B}| + \frac{2C \log(n_0/C)}{(1+\varepsilon/2) n_0} \cdot \sum_{B \in \mathcal{B}} \frac{\mu(B)}{-\log(p_0(1-p_0)) \cdot g_B(p^*)}.
\end{aligned}$$

By Proposition 27,

$$\sum_{B \in \mathcal{B}} M_B = -|\mathcal{B}| + \frac{2C \log(n_0/C)}{(1+\varepsilon/2) n_0} \cdot \frac{1}{-\log(p_0(1-p_0)) \cdot g_{K_\mu}(p^*)}.$$

By (2.12),

$$\begin{aligned}
\sum_{B \in \mathcal{B}} M_B &\geq -|\mathcal{B}| + \frac{2C \log(n_0/C)}{(1+\varepsilon/2) n_0} \cdot \frac{(1+\varepsilon) n_0}{2 \log n_0} \\
&= -|\mathcal{B}| + C \left(1 - \frac{\log C}{\log n_0} \right) \left(1 + \frac{\varepsilon}{2+\varepsilon} \right) \\
&= C + C \left(\frac{\varepsilon}{2+\varepsilon} - \frac{2+2\varepsilon}{2+\varepsilon} \cdot \frac{\log C}{\log n_0} \right) - |\mathcal{B}|
\end{aligned}$$

With ε fixed and $n_0 \gg C \gg |\mathcal{B}|$, we have $\sum_{B \in \mathcal{B}} M_B \geq C$, as desired. Thus, the index set $\{1, \dots, C\}$ may be partitioned as

$$\{1, \dots, C\} = \dot{\bigcup_{B \in \mathcal{B}}} S_B$$

so that $|S_B| \leq M_B$, for each $B \in \mathcal{B}$. Also, for each $B \in \mathcal{B}$, we combine the embeddings $\varphi_{B,k}$ for all $k \in S_B$ to form an embedding

$$F \left[\dot{\bigcup_{k \in S_B}} I_k \right] \mapsto (|S_B| \cdot m_B) \cdot B \subseteq \mu(B) \cdot B.$$

Combining all such embeddings, $F \mapsto K_\mu$, as desired. So

$$\bigcap_{k\in\{1,\dots,C\}} \bigcap_{B\in\mathcal{B}} E_{k,B} \subseteq \bigcap_{\mu\in\mathcal{B}_0} E_\mu \qquad \Longleftrightarrow \qquad \bigcup_{\mu\in\mathcal{B}_0} \overline{E_\mu} \subseteq \bigcup_{k\in\{1,\dots,C\}} \bigcup_{B\in\mathcal{B}} \overline{E_{k,B}}.$$

This completes the proof of the desired claim. □

Finally, we are ready to prove Theorem 4.

2.3.3 Proof of Theorem 4

Formally, our goal is to show that for each $\varepsilon \in (0,1)$, the following occurs **a.a.s.** as $n_0 \to \infty$:

$$\sup_{p\in I} \left| \mathrm{ed}_{\mathcal{H}}(p) \left(\frac{2\log n_0}{n_0} \cdot \min\left\{ \frac{p}{-\log(1-p_0)}, \frac{1-p}{-\log p_0} \right\} \right)^{-1} - 1 \right| < \varepsilon, \tag{2.15}$$

where

$$I = \begin{cases} [0,1], & \text{if } p^* \in [1-\varphi^{-1}, \varphi^{-1}]; \\ [1/3,1], & \text{if } p^* \in [0, 1-\varphi^{-1}); \\ [0,2/3], & \text{if } p^* \in (\varphi^{-1}, 1]. \end{cases}$$

We first establish an upper bound for $\mathrm{ed}_{\mathcal{H}}(p)$ for all $p \in [0,1]$. By the main result in [5], if $F \sim \mathbb{G}(n_0, p_0)$, then **a.a.s.** as $n_0 \to \infty$,

$$\chi(F) - 1 \geq (1-\varepsilon/2)\, \frac{n_0}{2\log_{1/(1-p_0)} n_0},$$
$$\chi(F^c) - 1 \geq (1-\varepsilon/2)\, \frac{n_0}{2\log_{1/p_0} n_0}.$$

Clearly F does not map into $\chi(F)-1$ white vertices or $\chi(F^c)-1$ black vertices. By, for example Theorem 10, and the fact that $1/(1-\varepsilon/2) < 1+\varepsilon$, then the following occurs **a.a.s.**:

$$\begin{aligned} \mathrm{ed}_{\mathcal{H}}(p) &\leq (1+\varepsilon)\ \min\left\{ \frac{p}{n_0/(2\log_{1/(1-p_0)} n_0)}, \frac{1-p}{n_0/(2\log_{1/p_0} n_0)} \right\} \\ &= (1+\varepsilon)\, \frac{2\log n_0}{n_0} \cdot \min\left\{ \frac{p}{-\log(1-p_0)}, \frac{1-p}{-\log p_0} \right\}. \end{aligned} \tag{2.16}$$

We now find a lower bound to match Inequality (2.16) over the interval I as stated above. We will do this by finding the lower bound for $p \in (1/3, 2/3)$ and then use concavity show how this extends to I in the various cases.

We will choose a $\tilde{p} \in (1/3, 2/3)$ depending on the case:

$$\tilde{p} := \begin{cases} p^*, & \text{if } p^* \in (1/3, 2/3); \\ 1/3 + \varepsilon/9, & \text{if } p^* \in (0, 1/3]; \\ 2/3 - \varepsilon/9, & \text{if } p^* \in [2/3, 1). \end{cases}$$

Let $K = K(\tilde{p}) \in \mathcal{K}_{\mathcal{H}}$ be a $\tilde{p}$-core CRG that satisfies $\mathrm{ed}_{\mathcal{H}}(\tilde{p}) = g_K(\tilde{p})$, as guaranteed by Theorem 10.

Since $\tilde{p} \in (1/3, 2/3)$, Lemma 31 gives that there exists a sub-CRG $K' = K'(\tilde{p}, \varepsilon/4)$ of K so that

$$g_K(\tilde{p}) \leq g_{K'}(\tilde{p}) \leq (1 + \varepsilon/4)\, g_K(\tilde{p}) \tag{2.17}$$

and whose components lie in some finite set $\mathcal{B} = \mathcal{B}(\tilde{p}, \varepsilon/4)$ of CRGs.

The function $g_{K'} : [0,1] \to [0,1]$ is concave-down. To see this, let $M_{K'}(p)$ be the matrix defined by the CRG K. Let $p_1, p_2 \in [0,1]$, $t \in [0,1]$, and let $\mathbf{x} \in \Delta_{K'}$ be the vector that witnesses the value of $g_{K'}$ at $tp_1 + (1-t)p_2$,

$$\begin{aligned} g_{K'}\left(tp_1 + (1-t)p_2\right) &= \langle \mathbf{x}, M_{K'}\left(tp_1 + (1-t)p_2\right)\mathbf{x} \rangle \\ &= t \cdot \langle \mathbf{x}, M_{K'}(p_1)\mathbf{x} \rangle + (1-t) \cdot \langle \mathbf{x}, M_{K'}(p_2)\mathbf{x} \rangle \\ &\geq t \cdot g_{K'}(p_1) + (1-t) \cdot g_{K'}(p_2), \end{aligned}$$

establishing the concavity of $g_{K'}$. Since $g_{K'}(0), g_{K'}(1) \geq 0$, the graph of $g_{K'}$ lies above the line segment from $(0,0)$ to $(\tilde{p}, g_{K'}(\tilde{p}))$ to $(1,0)$. So

$$g_{K'}(p) \geq g_{K'}(p^*) \cdot \min\left\{\frac{p}{p^*}, \frac{1-p}{1-p^*}\right\} \tag{2.18}$$

Also by Lemma 37 (recall the definition of p^* from (2.9)), the following is true **a.a.s.**:

$$g_{K'}(p^*) \geq (1 - \varepsilon/4) \cdot \frac{2 \log n_0}{-\log(p_0(1-p_0)) \cdot n_0}. \tag{2.19}$$

Combining (2.17), (2.18), and (2.19),

$$\begin{aligned}
\mathrm{ed}_{\mathcal{H}}(\tilde{p}) &= g_K(\tilde{p}) \\
&\geq \frac{1}{1+\varepsilon/4}\, g_{K'}(\tilde{p}) \\
&\geq \frac{1}{1+\varepsilon/4}\, g_{K'}(p^*) \cdot \min\left\{\frac{\tilde{p}}{p^*}, \frac{1-\tilde{p}}{1-p^*}\right\} \\
&\geq \frac{1-\varepsilon/4}{1+\varepsilon/4} \cdot \frac{2\log n_0}{-\log(p_0(1-p_0)) \cdot n_0} \cdot \min\left\{\frac{\tilde{p}}{p^*}, \frac{1-\tilde{p}}{1-p^*}\right\} \\
&\geq (1-\varepsilon/2)\, \frac{2\log n_0}{-\log(p_0(1-p_0)) \cdot n_0} \cdot \min\left\{\frac{\tilde{p}}{p^*}, \frac{1-\tilde{p}}{1-p^*}\right\} \qquad (2.20)
\end{aligned}$$

Case 1. $p_0 \in (1-\varphi^{-1}, \varphi^{-1}) \iff p^* \in (1/3, 2/3)$. In this case, $\tilde{p} = p^*$. By (2.20) and the concavity of $\mathrm{ed}_{\mathcal{H}}(p)$,

$$\begin{aligned}
\mathrm{ed}_{\mathcal{H}}(p^*) &\geq (1-\varepsilon/2)\, \frac{2\log n_0}{-\log(p_0(1-p_0)) \cdot n_0} \\
\mathrm{ed}_{\mathcal{H}}(p) &\geq (1-\varepsilon/2)\, \frac{2\log n_0}{-\log(p_0(1-p_0)) \cdot n_0} \cdot \min\left\{\frac{p}{p^*}, \frac{1-p}{1-p^*}\right\} \\
&= (1-\varepsilon/2)\, \frac{2\log n_0}{n_0} \cdot \min\left\{\frac{p}{-\log(1-p_0)}, \frac{1-p}{-\log p_0}\right\}.
\end{aligned}$$

This satisfies (2.15) for all $p \in [0,1]$, completing the proof in this case.

Case 2. $p_0 \in (0, 1-\varphi^{-1}] \iff p^* \in (0, 1/3]$. In this case, $\tilde{p} = 1/3 + \varepsilon/9 > p^*$. By (2.20) and the concavity of $\mathrm{ed}_{\mathcal{H}}$,

$$\begin{aligned}
\mathrm{ed}_{\mathcal{H}}(\tilde{p}) &\geq (1-\varepsilon/2)\, \frac{2\log n_0}{-\log(p_0(1-p_0)) \cdot n_0} \cdot \frac{1-\tilde{p}}{1-p^*} \\
\mathrm{ed}_{\mathcal{H}}(p) &\geq (1-\varepsilon/2)\, \frac{2\log n_0}{-\log(p_0(1-p_0)) \cdot n_0} \cdot \frac{1-\tilde{p}}{1-p^*} \cdot \min\left\{\frac{p}{\tilde{p}}, \frac{1-p}{1-\tilde{p}}\right\}.
\end{aligned}$$

Substituting $\tilde{p} = 1/3 + \varepsilon/9$ and $p = 1/3$,

$$\begin{aligned}
\mathrm{ed}_{\mathcal{H}}(1/3) &\geq (1-\varepsilon/2)\, \frac{2\log n_0}{-\log(p_0(1-p_0)) \cdot n_0} \cdot \frac{2/3-\varepsilon/9}{1-p^*} \cdot \frac{1/3}{1/3+\varepsilon/9} \\
&= \frac{(1-\varepsilon/2)(1/3-\varepsilon/18)}{1/3+\varepsilon/9} \cdot \frac{2\log n_0}{n_0} \cdot \frac{2/3}{-\log p_0} \\
&\geq (1-\varepsilon)\, \frac{2\log n_0}{n_0} \cdot \frac{2/3}{-\log p_0}.
\end{aligned}$$

Again by concavity,

$$\mathrm{ed}_{\mathcal{H}}(p) \geq (1-\varepsilon)\, \frac{2\log n_0}{n_0} \cdot \frac{2/3}{-\log p_0} \cdot \min\left\{\frac{p}{1/3}, \frac{1-p}{2/3}\right\}.$$

This matches the upper bound (2.16) for all $p \in [1/3, 1]$ and, in fact, if $p^* = 1/3$, then it matches the upper bound for all $p \in [0, 1]$. This completes the proof in this case.

Case 3. $p_0 \in [\varphi^{-1}, 1) \iff p^* \in [2/3, 1)$. This case may be shown with a similar argument as Case 2. In this case, $\tilde{p} = 2/3 - \varepsilon/9 < p^*$. By (2.20) and the concavity of $\mathrm{ed}_{\mathcal{H}}$,

$$\mathrm{ed}_{\mathcal{H}}(p) \geq (1-\varepsilon)\,\frac{2\log n_0}{n_0} \cdot \frac{1/3}{-\log p_0} \cdot \min\left\{\frac{p}{2/3}, \frac{1-p}{1/3}\right\}.$$

This matches the upper bound (2.16) for all $p \in [0, 2/3]$ and if $p^* = 2/3$, then it matches the upper bound for all $p \in [0, 1]$. This completes the proof in this case and the proof of Theorem 4.

2.4 Discussion

In the process of proving the main result, Theorem 4, we have developed a number of observations that apply generally to computing edit distance functions. Lemma 20 gives a general condition for which a CRG is p-prohbited and Lemma 23 shows that for $p \in [1-\varphi^{-1}, \varphi^{-1}]$, the only CRGs that need to be considered are dalmatian sets and their complements.

In this section, we discuss some other general results.

2.4.1 Defining the edit distance function with a finite set of CRGs

The following was conjectured by the first author:

Conjecture 38 ([11])**.** *Let $\mathcal{H}$ be a nontrivial hereditary property. For every $\varepsilon > 0$ there exists a finite set of CRGs $\mathcal{K}' = \mathcal{K}'(\varepsilon, \mathcal{H})$ such that*

$$\mathrm{ed}_{\mathcal{H}}(p) = \min\left\{g_K(p) : K \in \mathcal{K}'\right\}, \qquad \text{for all } p \in (\varepsilon, 1-\varepsilon).$$

Note that this is stronger than the Marchant-Thomason result in Theorem 10 which says that, for every p there is a finite set of CRGs that define $\mathrm{ed}_{\mathcal{H}}(p)$. Conjecture 38 asserts that a single finite set will define $\mathrm{ed}_{\mathcal{H}}(p)$ for all p an arbitrary open interval in $(0, 1)$. In Theorem 39, we provide a partial answer by showing that the conjecture is true for $\varepsilon \geq 1 - \varphi^{-1}$.

Theorem 39. *Let $\mathcal{H}$ be a nontrivial hereditary property. There exists a finite set of CRGs, $\mathcal{K}' = \mathcal{K}'(\mathcal{H})$, such that*

$$\mathrm{ed}_{\mathcal{H}}(p) = \min\left\{g_K(p) : K \in \mathcal{K}'\right\}, \qquad \textit{for all } p \in [1-\varphi^{-1}, \varphi^{-1}].$$

Proof. By Lemma 23, the only p-core CRGs are denoted $\mathcal{D}_p$ and consist of components which are dalmatian CRGs if $p \in [1-\varphi^{-1}, 1/2)$, complements of dalmatian CRGs if $p \in (1/2, \varphi^{-1}]$, and CRGs with only gray edges if $p = 1/2$.

It is easy to see that if $p = 1/2$ and $\mathcal{H} = \mathrm{Forb}(\mathcal{F})$, then for any $F \in \mathcal{F}$ such that $F \not\mapsto K$, the number of vertices of K is bounded by $\chi(F) + \chi(F^c)$, so the number of such CRGs is finite. We will now show that a finite set of CRGs suffice for $p \in [1-\varphi^{-1}, 1/2)$. The case $p \in (1/2, \varphi^{-1}]$ follows by symmetry. Note that $\mathcal{D}_p$ is the same for all $p \in [0, 1/2)$ (that is, CRGs whose components are all dalmatian CRGs) so we denote $\mathcal{D}_{0,\mathcal{H}} := \mathcal{D}_p \cap \mathcal{K}_{\mathcal{H}}$.

Write $\mathcal{H} = \mathrm{Forb}(\mathcal{F})$ and, for a contradiction, let $\{p_k\}_{k=1}^{\infty} \subset [1-\varphi^{-1}, 1/2)$ be an infinite set and let $\mathcal{K}' := \{K_k\}_{k=1}^{\infty} \subset \mathcal{D}_{0,\mathcal{H}}$ an infinite set of CRGs such that K_k is p_k-core and $g_{K_k}(p_k) = \mathrm{ed}_{\mathcal{H}}(p_k)$.

For all $k \geq 1$, with D_i denoting a dalmatian CRG of order i, we may write

$$K_k = D_{c_k^{(1)}} \oplus \cdots \oplus D_{c_k^{(\ell_k)}} \oplus (w_k \cdot D_\infty) \tag{2.21}$$

where $w_k, \ell_k, c_k^{(1)}, \ldots, c_k^{(\ell_k)}$ are nonnegative integers and $c_k^{(1)} \geq \cdots \geq c_k^{(\ell_k)}$.

For all $k \geq 1$, $w_k + \ell_k \leq |V(F)|$ for any $F \in \mathcal{F}$ because otherwise $F \mapsto K_k$ by embedding each vertex of F into a different component of K_k. Thus, ℓ_k is bounded by an absolute constant $\ell = \ell(\mathcal{H})$. So we associate each K_k in (2.21) with the $(\ell+1)$-tuple

$$\left(c_k^{(1)}, \ldots, c_k^{(\ell)}; w_k\right),$$

where $c_k^{(\ell_k+1)} = \cdots = c_k^{(\ell)} = 0$ if $\ell > \ell_k$.

Because $\mathcal{K}'$ is infinite, there exists a maximum $m \in \{1, \ldots, \ell\}$ such that $\sup_k\{c_k^{(1)}\} = \cdots = \sup_k\{c_k^{(m)}\} = \infty$. That is, if $m < \ell$, then $\sup_k\{c_k^{(m+1)}\} < \infty$. Thus, there is a fixed (possibly empty) tuple $\left(c_*^{(m+1)}, \ldots, c_*^{(\ell)}; w_*\right)$ and an infinite subsequence $k_1, k_2, \ldots$ such that K_{k_i} is associated with $(\ell+1)$-tuple $\left(c_{k_i}^{(1)}, \ldots, c_{k_i}^{(m)}, c_*^{(m+1)}, \ldots, c_*^{(\ell)}; w_*\right)$.

With this choice of $\left(c_*^{(m+1)}, \ldots, c_*^{(\ell)}; w_*\right)$, if ℓ' is the largest entry such that $c_*^{(\ell')} \geq 1$, then define

$$K_* = D_{c_k^{(m+1)}} \oplus \cdots \oplus D_{c_k^{(\ell')}} \oplus ((m + w_*) \cdot D_\infty).$$

We claim that $K_* \in \mathcal{D}_{0,\mathcal{H}} \subseteq \mathcal{K}_\mathcal{H}$.

If not, then there exists some $F \in \mathcal{F}$ and some embedding $\phi : V(F) \to V(K_*)$. Let $A_1, \ldots, A_m$ be the preimages of the first m copies of D_∞ under φ, respectively. Then $A_1, \ldots, A_m$ are independent sets in F.

Let k be sufficiently large so that $c_1^k, \ldots, c_m^k \geq |V(F)|$. Then we define $\phi' : V(F) \to V(K_k)$ by instead sending the vertices of A_i to distinct vertices of the dalmatian set $D_{c_i^k}$, for each $i \in \{1, \ldots, m\}$. As a result, ϕ' is an embedding of F into K_k, a contradiction.

Finally by Proposition 27 and Remark 22, for all $p \in (0, 1/2)$ and k chosen as above,

$$\begin{aligned} g_{K_k}(p)^{-1} &= \frac{w}{p} + \sum_{i=1}^{m} \frac{1}{p + (1-2p)/c_i^k} + \sum_{i=1}^{\ell - m} \frac{1}{p + (1-2p)/c_i} \\ &< \frac{w+m}{p} + \sum_{i=1}^{\ell - m} \frac{1}{p + (1-2p)/c_i} \\ &= g_{K_*}(p)^{-1} \end{aligned}$$

The fact that $g_{K_*}(p_k) < g_{K_k}(p_k) = \mathrm{ed}_\mathcal{H}(p_k)$ contradicts $K_* \in \mathcal{K}_\mathcal{H}$, hence the original assumption that $\mathcal{K}'$ is infinite.

□

2.4.2 Paths

In Proposition 35, it is established that P_d is p-prohibited for $p \in \left[\frac{1}{1+2\cos(\pi/(d+1))}, 1 - \frac{1}{1+2\cos(\pi/(d+1))}\right]$. In the case of $d = 3$, P_3 is p-prohibited for p in the interval

$$[\sqrt{2} - 1, 2 - \sqrt{2}] \approx [0.414214, 0.585786].$$

However, Lemma 23 establishes that P_3 is p-prohibited if and only if p is in the interval

$$[1 - \varphi^{-1}, \varphi^{-1}] = \left[\frac{3 - \sqrt{5}}{2}, \frac{\sqrt{5} - 1}{2}\right] \approx [0.381966, 0.618034].$$

d	$(1+2\cos(\pi/(d+1)))^{-1}$		$1-(1+2\cos(\pi/(d+1)))^{-1}$	
3	$\sqrt{2}-1$	≈ 0.414214	$2-\sqrt{2}$	≈ 0.585786
4	$(3-\sqrt{5})/2$	≈ 0.381966	$(\sqrt{5}-1)/2$	≈ 0.618034
5	$(\sqrt{3}-1)/2$	≈ 0.366025	$(3-\sqrt{3})/2$	≈ 0.633975
6		≈ 0.356896		≈ 0.643104
7		≈ 0.351153		≈ 0.648847
8		≈ 0.347296		≈ 0.652704
9		≈ 0.344577		≈ 0.655423
10		≈ 0.342585		≈ 0.657415
11		≈ 0.341081		≈ 0.658919
12		≈ 0.339918		≈ 0.660082
13		≈ 0.339000		≈ 0.661000
14		≈ 0.338261		≈ 0.661739
15		≈ 0.337659		≈ 0.662341

Table 2.1 Table for endpoints of an interval where P_d is prohibited.

We ask whether P_d is p-prohibited over a larger interval than given in (2.11). See Table 2.1 for small values.

Question 40. *For $d \geq 4$, what is the largest interval over which P_d is p-prohibited?*

2.5 Questions and future work

2.5.1 p-core CRGs

Lemma 23 classifies all p-core CRGs on the interval $[1-\varphi^{-1}, \varphi^{-1}]$.

Question 41. *For which $a \in (0, 1-\varphi^{-1})$ does there exist an elementary classification of all p-core CRGs for all $p \in [a, 1-a]$? Additionally, are all sufficiently large connected p-core CRGs either dalmatian CRGs (if $p \leq 1/2$) or the complement of a dalmatian CRG (if $p \geq 1/2$)?*

A crucial part of the proof of Theorem 4 is Lemma 31, which establishes that, for $p \in (1/3, 2/3)$, a p-core CRG can be approximated so that the g function does not increase by much, but the components are bounded.

Question 42. *Does Lemma 31 hold if the interval $(1/3, 2/3)$ is widened to $(a, 1-a)$ for some $a \in (0, 1/3)$?*

2.5.2 Inhomogeneous random graphs

Since the development of graph limits, inhomogeneous generalizations $\mathbb{G}(n, W)$ of the Erdős-Rényi random graph models have emerged as a topic of research interest (see [9]). Here, $W : \Omega^2 \to [0, 1]$ is a *graphon*, which is a symmetric measurable function where Ω is a probability space, frequently $[0, 1]$ equipped with the Lebesgue measure. To form a W-random graph $G \sim \mathbb{G}(n, W)$, sample n elements $x_1, \ldots, x_n \sim \Omega$ independently and form a graph on $\{1, \ldots, n\}$ by adding edge ij independently with probability $W(x_i, x_j)$. We may also generate a sequence of W-random graphs $(G_n)_{n=1}^{\infty} \sim \mathbb{G}(\mathbb{N}, W)$ adding the vertices corresponding to $x_1, x_2, \ldots$, one at a time.

There are several questions we may ask related to the edit distance problem and inhomogeneous random graphs.

First, note that Theorem 4 implies that with $p_0 \in [1 - \varphi^{-1}, \varphi^{-1}]$ and $(F_n) \sim \mathbb{G}(\mathbb{N}, p_0)$, then **a.a.s.** as $n_0 \to \infty$,

$$\mathrm{ed}_{\mathrm{Forb}(F_n)} = (1 + o(1))\, r(n_0) \cdot s(p), \tag{2.22}$$

where $r : \mathbb{N} \to [0, 1]$ and $s : [0, 1] \to [0, 1]$ are some functions.

Question 43. *If W is a graphon, does Equation (2.22)* **a.a.s.** *hold for $(F_n) \sim \mathbb{G}(\mathbb{N}, W)$ with some suitable functions $r = r_W$ and $s = s_W$?*

For the next question, we note the following expression for the distance from a homogeneous random graph to a hereditary property. Combining Theorems 2 and 10, we see that if $\mathcal{H}$ is a (fixed) nontrivial hereditary property and $p \in [0, 1]$, then with $G_n \sim \mathbb{G}(n, p)$,

$$\lim_{n\to\infty} \mathbb{E}[\mathrm{dist}(G_n, \mathcal{H})] = \inf_{K \in \mathcal{K}_{\mathcal{H}}} g_K(p) = \min_{K \in \mathcal{K}_{\mathcal{H}}} g_K(p). \tag{2.23}$$

Question 44. *If instead $G_n \sim \mathbb{G}(n, W)$, is there a similar expression for $\limsup_{n\to\infty} \mathbb{E}[\mathrm{dist}(G_n, \mathcal{H})]$? In particular, can we extend the functions $g_K(\cdot)$ from $[0, 1]$ to the set of all graphons so that Equation (2.23) holds?*

2.5.3 Acknowledgements

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CHAPTER 3. THE MAXIMUM SPREAD OF GRAPHS

A paper in preparation

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Abstract

Given a graph G with adjacency matrix A, the *(adjacency) spread* of G is the difference between the maximum and minimum eigenvalues of A. In 2001, Gregory, Hershkowitz, and Kirkland [5] conjectured that the maximum spread among all n-vertex graphs is attained by the join of a clique on $\lfloor 2n/3 \rfloor$ vertices and an independent set on $\lceil n/3 \rceil$ vertices. Since then, this problem has been cited more than 60 times in the literature on spectral graph theory. In this work, we prove this conjecture for all n sufficiently large. As an intermediate step, we prove an analogous statement for symmetric kernel operators of the form $W : [0,1]^2 \to [0,1]$.

3.1 Introduction

Let $\mathcal{G}_n$ be the set of all simple undirected graphs of order n; that is, graphs with a vertex set $V(G)$ of order n. The adjacency matrix A of a graph $G \in \mathcal{G}_n$ is the matrix whose rows and columns are indexed by the vertices of G, with entries defined as

$$A_{u,v} = \begin{cases} 1 & \text{if } u \sim v; \\ 0 & \text{if } u \nsim v. \end{cases}$$

Since A is a real symmetric matrix, its eigenvalues are real, and can be ordered $\lambda_1(G) \geq \lambda_2(G) \geq \cdots \geq \lambda_n(G)$.

The spread $s(M)$ of an arbitrary $n \times n$ complex matrix M is given by the diameter of its spectrum; that is,

$$s(M) := \max_{i,j} |\lambda_i - \lambda_j|,$$

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where the maximum is taken over all pairs of eigenvalues of M. When the matrix is the adjacency matrix of some graph G, the spread is simply the distance between $\lambda_1(G)$ and $\lambda_n(G)$, denoted by

$$s(G) := \lambda_1(G) - \lambda_n(G).$$

In this instance, $s(G)$ is referred to as the *spread of the graph*.

In [5], the authors investigated a number of properties regarding the spread of a graph, determining upper and lower bounds on $s(G)$. Furthermore, they made two key conjectures. Let us denote the maximum spread over all graphs $G \in \mathcal{G}_n$ by $s(n)$, the maximum spread over all graphs $G \in \mathcal{G}_n$ of size e by $s(n,e)$, and the maximum spread over all bipartite graphs $G \in \mathcal{G}_n$ of size e by $s_b(n,e)$. Let K_k be the clique of order k and $G(n,k) := K_k \vee \bar{K}_{n-k}$ be the join of the clique K_k and the independent set $\bar{K}_{n-k}$. The conjectures addressed in this article are as follows.

Conjecture 1 ([5], Conjecture 1.3))**.** *For any positive integer n, the graph of order n with maximum spread is $G(n, \lfloor 2n/3 \rfloor)$; that is, $s(n)$ is attained only by $G(n, \lfloor 2n/3 \rfloor)$.*

Conjecture 2 ([5], Conjecture 1.4))**.** *If G is a graph with n vertices and e edges attaining the maximum spread $s(n,e)$, and if $e \le \lfloor n^2/4 \rfloor$, then G must be bipartite. That is, $s_b(n,e) = s(n,e)$ for all $e \le \lfloor n^2/4 \rfloor$.*

Conjecture 1 is referred to as the Spread Conjecture, and Conjecture 2 is referred to as the Bipartite Spread Conjecture.

3.2 Properties of spread-extremal graphs

In this section, we review what has already been proven about spread-extremal graphs in [5], where the original conjectures were made. We then prove a number of properties of spread-extremal graphs (n vertex graphs with spread $s(n)$), and properties of the eigenvectors associated with the maximum and minimum eigenvalues of a spread-extremal graph.

Let G be a graph, and let A be the adjacency matrix of G, with eigenvalues $\lambda_1 \ge \cdots \ge \lambda_n$. For unit vectors $\mathbf{x}$, $\mathbf{y} \in \mathbb{R}^n$, we have

$$\lambda_1 \ge \mathbf{x}^T A \mathbf{x} \quad \text{and} \quad \lambda_n \le \mathbf{y}^T A \mathbf{y}.$$

Hence (as it is observed in [5]), the spread of a graph can be expressed

$$s(G) = \max_{\mathbf{x},\mathbf{z}} \sum_{u\sim v} (\mathbf{x}_u\mathbf{x}_v - \mathbf{z}_u\mathbf{z}_v)$$

where the maximum is taken over all unit vectors $\mathbf{x}, \mathbf{z}$. Furthermore, this maximum is attained only for $\mathbf{x}, \mathbf{z}$ orthonormal eigenvectors corresponding to the eigenvalues λ_1, λ_n, respectively. We refer to such a pair of vectors $\mathbf{x}, \mathbf{z}$ as *extremal eigenvectors* of G. We restate the following lemma from [5] to refer to later.

Lemma 3.2.1. ([5, Lemma 3.4]) *If G is a spread-extremal graph (i.e. $s(G) = s(n)$), and $\mathbf{x}, \mathbf{z}$ are extremal eigenvectors of G, then for any two vertices u, v of G, u and v are adjacent whenever $\mathbf{x}_u\mathbf{x}_v - \mathbf{z}_u\mathbf{z}_v > 0$ and u and v are nonadjacent whenever $\mathbf{x}_u\mathbf{x}_v - \mathbf{z}_u\mathbf{z}_v < 0$.*

For any two vectors $\mathbf{x}$, $\mathbf{z}$ in $\mathbb{R}^n$, let $G(\mathbf{x}, \mathbf{z})$ denote the graph for which distinct vertices u, v are adjacent if and only if $\mathbf{x}_u\mathbf{x}_v - \mathbf{z}_u\mathbf{z}_v \geq 0$. Then from the above, the spread-extremal graph must be some graph $G(\mathbf{x}, \mathbf{z})$ with $\mathbf{x}$, $\mathbf{z}$ orthonormal and $\mathbf{x}$ positive ([5, Lemma 3.5]). These observations from [5] indicate that the spread-extremal graph must be the join of two graphs; in particular, if $G = G(\mathbf{x}, \mathbf{z})$ is a spread-extremal graph, then $G = G_1 \vee G_2$, where G_1 is the subgraph induced by the vertices $v \in V(G)$ with $\mathbf{z}_v > 0$, and G_2 is the subgraph induced by the vertices $v \in V(G)$ with $\mathbf{z}_v \leq 0$. Henceforth, we will denote the vertices of G_1 as P and the vertices of G_2 as N.

Our first result shows that if $G = G_1 \vee G_2$ is a spread-extremal graph, then both G_1 and G_2 are in fact *threshold graphs* [11].

Definition 3.2.2. A *threshold graph* is a graph that can be constructed by starting from a one-vertex graph and repeatedly adding either a single isolated vertex or a single dominating vertex.

Theorem 3.2.3. *Let $G = G_1 \vee G_2$ be a spread-extremal graph. Then G_1 and G_2 are both threshold graphs.*

Note that to prove Theorem 3.2.3, we will consider graphs that result from repeated applications of a graph operation known as a *Kelmans transformation*. In [3], the author determines an upper bound for the sum of the spectral radius of a graph and its complement $\rho(G)+\rho(\overline{G})$ using a sequence of Kelmans transformations and their threshold graphs (originally introduced in [7]). This follows from observing that performing such a transformation on a graph increases both its adjacency spectral radius and the spectral radius of the adjacency matrix of its graph complement; thus the extremal graph for the above quantity must be one which is invariant under further Kelmans transformations. We will use a similar approach in the proof of Theorem 3.2.3.

Let G be a graph with vertex set $V(G)$ and edge set $E(G)$, and let u and v be two vertices in G. A Kelmans transformation on G involving vertices u, v with u as the *beneficiary* produces a graph $\hat{G}$ in which for all $w \in V(G)$ such that $vw \in E(G)$ and $uw \notin E(G)$, we have $vw \notin E(\hat{G})$ and $uw \in E(\hat{G})$. That is, $\hat{G}$ is obtained by deleting all edges between v and $N(v)\setminus(N(u)\cup\{u\})$, and instead adding edges between u and every vertex in $N(v)\setminus(N(u)\cup\{u\})$.

It is clear that by performing a Kelmans transformation on a graph G with vertices u, v and u as the beneficiary, u *dominates* v in the resulting graph; that is $N_{\hat{G}}(u) \supseteq N_{\hat{G}}(v)$. One can repeatedly perform these Kelmans transformations and obtain a graph where any further Kelmans transformation produces an isomorphic graph. Moreover, as observed in [3, Thm 2.2], these graphs resulting from repeated application of this operation satisfy the condition that the vertices may be ordered in such a way that whenever $i < j$, v_i dominates v_j. Note that an alternate characterization of threshold graphs is that they are the graphs that do not have as induced subgraphs a path on 3 edges, a C_4, or a 2-edge matching. Thus it is clear that any graph with nested neighborhoods as described above must also be a threshold graph.

Proof of Theorem 3.2.3. Let G be the join of two graphs G_1 and G_2, and let $\lambda_1(G)$, $\lambda_n(G)$ denote the largest and smallest eigenvalues of the adjacency matrix of G, respectively. Let $\mathbf{x}$ be a positive eigenvector corresponding to $\lambda_1(G)$, and $\mathbf{z}$ an eigenvector corresponding to $\lambda_n(G)$, both of norm 1.

Now suppose that $\widehat{G}$ is obtained from G by Kelmans transformation with u, v either both in G_1 or both in G_2, and u as beneficiary. We will show that the spread of $\hat{G}$ is always at least the spread of G.

$$\begin{aligned}\lambda_1(\widehat{G}) &= \max_{\|\mathbf{y}\|=1} \mathbf{y}^\top \hat{A}\mathbf{y} \\ &\geq \mathbf{x}^\top \hat{A}\mathbf{x} \\ &= \mathbf{x}^\top A\mathbf{x} + 2(\mathbf{x}_u - \mathbf{x}_v)\sum_{\substack{w\sim v\\ w\nsim u}} \mathbf{x}_w.\end{aligned}$$

Since $\mathbf{x}$ is positive, $\lambda_1(\widehat{G}) \geq \lambda_1(G)$ if $\mathbf{x}_u \geq \mathbf{x}_v$.

Furthermore, note that a Kelmans transformation on G involving u and v with u as beneficiary produces the graph $\hat{G}_u$, which is isomorphic to $\widehat{G}_v$, the graph produced by a Kelmans transformation with v as beneficiary instead. Therefore for any Kelmans transformation on G, the spectral radius is increased (see [3]).

Next, consider $\lambda_n(\widehat{G})$.

$$\begin{aligned}\lambda_n(\widehat{G}) &= \min_{\|\mathbf{y}\|=1} \mathbf{y}^\top \hat{A}\mathbf{y} \\ &\leq \mathbf{z}^\top \hat{A}\mathbf{z} \\ &= \mathbf{z}^\top A\mathbf{z} + 2(\mathbf{z}_u - \mathbf{z}_v)\sum_{\substack{w\sim v\\ w\nsim u}} \mathbf{z}_w.\end{aligned}$$

If $u, v \in G_1$, then the set $\{w \mid w \sim v, w \nsim u\}$ is a subset of the vertices of G_1, and so the summation $\sum \mathbf{z}_w$ is nonnegative, and $\lambda_n(\widehat{G}) \leq \lambda_n(G)$ if $\mathbf{z}_u \leq \mathbf{z}_v$. If $u, v \in G_2$, then the set $\{w \mid w \sim v, w \nsim u\}$ is a subset of the vertices of G_2, and so the summation $\sum \mathbf{z}_w$ is nonpositive, and $\lambda_n(\widehat{G}) \leq \lambda_n(G)$ if $\mathbf{z}_u \geq \mathbf{z}_v$.

Again, since choosing either u or v as beneficiary produces isomorphic graphs, we can conclude that any Kelmans transformation involving vertices either both in G_1 or both in G_2 will produce a graph whose minimum adjacency eigenvalue has not increased.

Hence any such Kelmans transformation increases the spread of the graph, and thus the extremal graph must be one for which the subgraphs G_1 and G_2 are threshold graphs with respect to this operation.

□

The next lemma shows that both P and N have linear size.

Lemma 3.2.4. *If G is a spread-extremal graph, then both P and N have size at least $\frac{n}{100}$.*

Proof. First, since G is extremal it has spread more than $1.1n$ and hence has smallest eigenvalue $\lambda_n < \frac{-n}{10}$. Without loss of generality, for the remainder of this proof we will assume that $|P| \leq |N|$, that $\mathbf{z}$ is normalized to have infinity norm 1, and that v is a vertex satisfying $|\mathbf{z}_v| = 1$. By way of contradiction, assume that $|P| < \frac{n}{100}$.

If $v \in N$, then we have

$$\lambda_n \mathbf{z}_v = -\lambda_n = \sum_{u \sim v} \mathbf{z}_u \leq \sum_{u \in P} \mathbf{z}_u \leq |P| < \frac{n}{100},$$

contradicting that $\lambda_n < \frac{-n}{10}$. Therefore, assume that $v \in P$. Then

$$\lambda_n^2 \mathbf{z}_v = \lambda_n^2 = \sum_{w \sim u} \sum_{u \sim v} \mathbf{z}_w \leq \sum_{\substack{w \sim u \\ w \in P}} \sum_{u \sim v} \mathbf{z}_w \leq |P||N| + 2e(P) \leq |P||N| + |P|^2 \leq \frac{99n^2}{100^2} + \frac{n^2}{100^2}.$$

This gives $|\lambda_n| \leq \frac{n}{10}$, a contradiction. □

Lemma 3.2.5. *If* $\mathbf{x}$ *and* $\mathbf{z}$ *are unit eigenvectors for* λ_1 *and* λ_n*, then* $\|\mathbf{x}\|_\infty = O(n^{-1/2})$ *and* $\|\mathbf{z}\|_\infty = O(n^{-1/2})$.

Proof. During this proof we will assume that $\hat{u}$ and $\hat{v}$ are vertices satisfying $\|\mathbf{x}\|_\infty = \mathbf{x}_{\hat{u}}$ and $\|\mathbf{z}\|_\infty = -\mathbf{z}_{\hat{v}}$ and without loss of generality that $\hat{v} \in N$. We will use the weak estimates that $\lambda_1 > \frac{n}{2}$ and $\lambda_n < \frac{-n}{10}$. Define sets

$$A = \left\{ w : \mathbf{x}_w > \frac{\mathbf{x}_{\hat{u}}}{4} \right\}$$
$$B = \left\{ w : |\mathbf{z}_w| > \frac{-\mathbf{z}_{\hat{v}}}{20} \right\}.$$

It suffices to show that A and B both have size $\Omega(n)$, for then there exists a constant $\epsilon > 0$ such that

$$1 = \mathbf{x}^T \mathbf{x} \geq \sum_{w \in A} \mathbf{x}_w^2 \geq |A| \frac{\|\mathbf{x}\|_\infty^2}{16} \geq \epsilon n \|\mathbf{x}\|_\infty^2,$$

and similarly

$$1 = \mathbf{z}^T \mathbf{z} \geq \sum_{w \in B} \mathbf{z}_w^2 \geq |B| \frac{\|\mathbf{z}\|_\infty^2}{400} \geq \epsilon n \|\mathbf{z}\|_\infty^2.$$

We now give a lower bound on the sizes of A and B using the eigenvalue-eigenvector equation and the weak bounds on λ_1 and λ_n.

$$\frac{n}{2} \|\mathbf{x}\|_\infty = \frac{n}{2} \mathbf{x}_{\hat{u}} < \lambda_1 \mathbf{x}_{\hat{u}} = \sum_{w \sim \hat{u}} \mathbf{x}_w \leq \|\mathbf{x}\|_\infty \left(|A| + \frac{1}{4}(n - |A|) \right),$$

giving that $|A| > \frac{n}{3}$. Similarly,

$$\frac{n}{10}\|\mathbf{z}\|_\infty = -\frac{n}{10}\mathbf{z}_{\hat{v}} < \lambda_n \mathbf{z}_{\hat{v}} = \sum_{w\sim\hat{v}} \mathbf{z}_w \leq \|\mathbf{z}\|_\infty \left(|B| + \frac{1}{20}(n - |B|)\right),$$

and so $|B| > \frac{n}{19}$.

□

Lemma 3.2.6. *Assume that* $\mathbf{x}$ *and* $\mathbf{z}$ *are unit vectors. Then there exists a constant* C *such that for any pair of vertices* u *and* v*, we have*

$$(\lambda_1 \mathbf{x}_u^2 - \lambda_n \mathbf{z}_u^2) - (\lambda_1 \mathbf{z}_v^2 - \lambda_n \mathbf{z}_v^2) < \frac{C}{n}.$$

Proof. Let u and v be vertices, and create a graph $\tilde{G}$ by deleting u and cloning v. That is, $V(\tilde{G}) = \{v'\} \cup V(G) \setminus \{u\}$ and

$$E(\tilde{G}) = E(G \setminus \{u\}) \cup \{v'w : vw \in E(G)\}.$$

Note that $v \not\sim v'$. Let $\tilde{A}$ be the adjacency matrix of $\tilde{G}$. Define two vectors $\tilde{\mathbf{x}}$ and $\tilde{\mathbf{z}}$ by

$$\tilde{\mathbf{x}}_w = \begin{cases} \mathbf{x}_w & w \neq v' \\ \mathbf{x}_v & w = v', \end{cases}$$

and

$$\tilde{\mathbf{z}}_w = \begin{cases} \mathbf{z}_w & w \neq v' \\ \mathbf{z}_v & w = v. \end{cases}$$

Then $\tilde{\mathbf{x}}^T\tilde{\mathbf{x}} = 1 - \mathbf{x}_u^2 + \mathbf{x}_v^2$ and $\tilde{\mathbf{z}}^T\tilde{\mathbf{z}} = 1 - \mathbf{z}_u^2 + \mathbf{z}_v^2$. Similarly,

$$\begin{aligned} \tilde{\mathbf{x}}^T\tilde{A}\tilde{\mathbf{x}} &= \lambda_1 - 2\mathbf{x}_u \sum_{uw\in E(G)} \mathbf{x}_w + 2\mathbf{x}_{v'} \sum_{vw\in E(G)} \mathbf{x}_w - 2A_{uv}\mathbf{x}_v\mathbf{x}_u \\ &= \lambda_1 - 2\lambda_1\mathbf{x}_u^2 + 2\lambda_1\mathbf{x}_v^2 - 2A_{uv}\mathbf{x}_u\mathbf{x}_v, \end{aligned}$$

and

$$\begin{aligned} \tilde{\mathbf{z}}^T\tilde{A}\tilde{\mathbf{z}} &= \lambda_n - 2\mathbf{z}_u \sum_{uw\in E(G)} \mathbf{z}_w + 2\mathbf{z}_{v'} \sum_{vw\in E(G)} \mathbf{z}_w - 2A_{uv}\mathbf{z}_v\mathbf{z}_u \\ &= \lambda_n - 2\lambda_n\mathbf{z}_u^2 + 2\lambda_n\mathbf{z}_v^2 - 2A_{uv}\mathbf{z}_u\mathbf{z}_v. \end{aligned}$$

By optimality of G we have

$$\begin{aligned}
0 &\geq \left(\frac{\tilde{\mathbf{x}}^T\tilde{A}\tilde{\mathbf{x}}}{\tilde{\mathbf{x}}^T\tilde{\mathbf{x}}} - \frac{\tilde{\mathbf{z}}^T\tilde{A}\tilde{\mathbf{z}}}{\tilde{\mathbf{z}}^T\tilde{\mathbf{z}}}\right) - (\lambda_1 - \lambda_n) \\
&= \left(\frac{\lambda_1 - 2\lambda_1\mathbf{x}_u^2 + 2\lambda_1\mathbf{x}_v^2 - 2A_{uv}\mathbf{x}_u\mathbf{x}_v}{1 - \mathbf{x}_u^2 + \mathbf{x}_v^2} - \frac{\lambda_n - 2\lambda_n\mathbf{z}_u^2 + 2\lambda_n\mathbf{z}_v^2 - 2A_{uv}\mathbf{z}_u\mathbf{z}_v}{1 - \mathbf{z}_u^2 - \mathbf{z}_v^2}\right) - (\lambda_1 - \lambda_n) \\
&= \frac{\lambda_1\mathbf{x}_u^2 - \lambda_1\mathbf{x}_v^2 - 2A_{ij}\mathbf{x}_u\mathbf{x}_v}{1 - \mathbf{x}_u^2 - \mathbf{x}_v^2} - \frac{\lambda_n\mathbf{z}_u^2 - \lambda_n\mathbf{z}_v^2 - 2A_{ij}\mathbf{z}_u\mathbf{z}_v}{1 - \mathbf{z}_u^2 - \mathbf{z}_v^2}.
\end{aligned}$$

By Lemma 3.2.5, we have that $|\mathbf{x}_u|$, $|\mathbf{x}_v|$, $|\mathbf{z}_u|$, and $|\mathbf{z}_v|$ are all $O(n^{-1/2})$, and so it follows that

$$(\lambda_1\mathbf{x}_u^2 - \lambda_1\mathbf{x}_v^2) - (\lambda_n\mathbf{z}_u^2 - \lambda_n\mathbf{z}_v^2) < \frac{C}{n},$$

for some absolute constant C. Rearranging gives the result. □

Next we show that an asymptotic upper bound of $cn + o(n)$ actually implies an upper bound of cn for all n.

Theorem 3.2.7. *Let*

$$c = \limsup_{n\to\infty} \frac{s(n)}{n}.$$

Then for all positive integers n, $s(n) \leq cn$.

Proof. By way of contradiction, assume that there is a graph G on m vertices such that $s(G) = cm + \delta$ for some positive δ. Let G^t be the t-blowup of G. That is G^t is the graph on mt vertices where each vertex in G is replaced by an independent set of size t and each edge is replaced by a $K_{t,t}$ between the two independent sets. One can check that $\lambda_1(G^t) = t\lambda_1(G)$ and $\lambda_n(G^t) = t\lambda_n(G)$, and so

$$s(G^t) = ts(G) = t(cm + \delta) = c(mt) + \frac{\delta}{m}mt.$$

Letting t go to infinity gives a sequence of graphs on $n = mt$ vertices satisfying $s(G) = (c + \delta/m)n$, contradicting the hypothesis. □

3.3 The spread-extremal problem for graphons

Graphons (or graph functions) are analytical objects which may be used to study the limiting behaviour of large, dense graphs, and were originally introduced in [2] and [9].

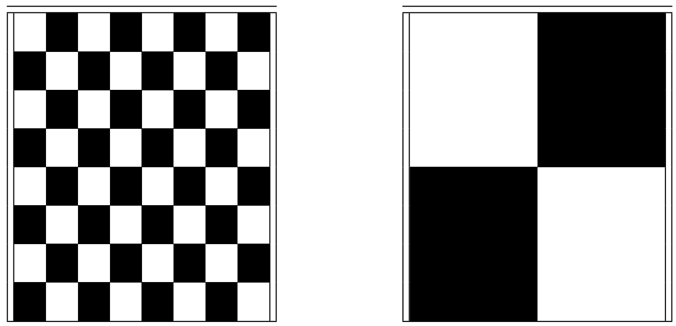


Figure 3.1 Two presentations of a bipartite graph as a stepfunction.

3.3.1 Introduction to graphons

Consider the set $\mathcal{W}$ of all bounded symmetric measurable functions $W : [0,1]^2 \to [0,1]$ (by symmetric, we mean $W(x,y) = W(y,x)$ for all $(x,y) \in [0,1]^2$. A function $W \in \mathcal{W}$ is called a *stepfunction* if there is a partition of $[0,1]$ into subsets $S_1, S_2, \ldots, S_m$ such that W is constant on every block $S_i \times S_j$. Every graph has a natural representation as a stepfunction in $\mathcal{W}$ taking values either 0 or 1 (such a graphon is referred to as a *stepgraphon*). In particular, given a graph G on n vertices indexed $\{1, 2, \ldots, n\}$, we can define a measurable set $K_G \subseteq [0,1]^2$ as

$$K_G = \bigcup_{u \sim v} \left[\frac{u-1}{n}, \frac{u}{n}\right] \times \left[\frac{v-1}{n}, \frac{v}{n}\right],$$

and this represents the graph G as a bounded symmetric measurable function W_G which takes value 1 on K_G and 0 everywhere else.

This representation of a graph as a measurable subset of $[0,1]^2$ lends itself to a visual presentation sometimes referred to as a *pixel picture*; see, for example, Fig. 3.3.1 for two representations of a bipartite graph as a measurable subset of $[0,1]^2$. Clearly, this indicates that such a representation is not unique; neither is the representation of a graph as a stepfunction. Using an equivalence relation on $\mathcal{W}$ derived from the so-called *cut metric*, we can identify graphons that are equivalent up to relabelling, and up to any differences on a set of measure zero (i.e. equivalent *almost everywhere*).

Given $W \in \mathcal{W}$, the following norm is defined:

$$\|W\|_{\square} = \sup_{S,T \subseteq [0,1]} \left| \int_{S \times T} W(x,y)\, dx\, dy \right|.$$

This is referred to as the *cut norm.* One can also define a semidistance $\delta_\square$ on $\mathcal{W}$. To account for 'relabeling', consider the set $\mathcal{S}$ of all measure-preserving bijections of $[0,1]$, and define

$$\delta_\square(W_1, W_2) = \inf_{\phi\in\mathcal{S}}\{\|W_1 - W_2 \circ \phi\|_\square\}.$$

We denote by $\hat{\mathcal{W}}$ the quotient space of $\mathcal{W}$ under the equivalence relation

$$W_1 \sim W_2 \Leftrightarrow \delta_\square(W_1, W_2) = 0.$$

On $\hat{\mathcal{W}}$, $\delta_\square$ is a metric, and by [10, Theorem 5.1], $\hat{\mathcal{W}}$ is a compact space.

Given $W \in \mathcal{W}$, define the linear operator $A_W : \mathscr{L}^2[0,1] \to \mathscr{L}^2[0,1]$ as

$$A_W f(x) = \int_0^1 W(x,y) f(y)\, dy.$$

Since $W(x,y) = W(y,x)$ for a.e. $(x,y) \in [0,1]^2$, A_W is self-adjoint. Moreover since W is bounded, A_W is compact and has a discrete, real spectrum whose only possible accumulation point is 0 (c.f. [1]). In particular, we can consider the largest and smallest eigenvalues of this operator as the maximum and minimum elements of the spectrum. Let $\mu(W)$ and $\nu(W)$ be the maximum and minimum eigenvalue of A_W respectively. Thus we may define the spread of W as

$$\operatorname{spr}(W) = \mu(W) - \nu(W).$$

By the Min-Max Theorem , we have that

$$\mu(W) = \max_{\|f\|_2=1} \int_0^1 \int_0^1 W(x,y) f(x) f(y)\, dx\, dy,$$

and

$$\nu(W) = \min_{\|f\|_2=1} \int_0^1 \int_0^1 W(x,y) f(x) f(y)\, dx\, dy.$$

By Theorem 11.54 from [8], μ and ν are continuous functions with respect to $\delta_\square$ and if $W \sim W'$ then $\mu(W) = \mu(W')$ and $\nu(W) = \nu(W')$. By defining the quotient space $\hat{\mathcal{W}} := \mathcal{W}/\sim$, we may consider the optimization problem:

$$\operatorname{spr}(\hat{\mathcal{W}}) = \max_{W\in\hat{\mathcal{W}}} \operatorname{spr}(W).$$

Since $\hat{\mathcal{W}}$ is a compact space and s is a continuous function with respect to $\delta_\square$, $\operatorname{spr}(\hat{\mathcal{W}})$ is well-defined and there is a $W \in \hat{\mathcal{W}}$ that attains the maximum. Since every graph is represented by

$W_G \in \hat{\mathcal{W}}$, this allows us to give an upper bound for $s(n)$ in terms of $\operatorname{spr}(\hat{\mathcal{W}})$ using the following lemma.

Lemma 3.3.1. *Let G be a graph on n vertices. Then*

$$\lambda_1(G) = n\mu(W_G),$$

and

$$\lambda_n(G) = n\nu(W_G).$$

Hence, we have by Lemma 3.3.1,

$$s(n) \leq n\operatorname{spr}(\hat{\mathcal{W}}). \tag{3.1}$$

For convenience, we recall the following theorem.

Theorem 3.3.2 (c.f. Theorem 6.6 from [2] or Theorem 11.54 in [8])**.** *Let $\{W_i\}_i$ be a sequence of graphons converging to W with respect to $\delta_\square$. Then as $n \to \infty$,*

$$\mu(W_n) \to \mu(W) \quad \text{and} \quad \nu(W_n) \to \nu(W).$$

3.3.2 Properties of spread-extremal graphons

Our main objective in the next sections is to solve the maximum spread problem for graphons in order to determine this upper bound for $s(n)$. As such, in this subsection we set up some preliminaries to the solution which largely comprise a translation of what is known in the graph setting (see Section 3.2). Specifically, we define what it means for a graphon to be connected, and show that spread-extremal graphons must be connected. We then prove a standard corollary of the Perron-Frobenius theorem. Finally, we prove graphon versions of Lemma 3.2.1, Theorem 3.2.3, and Lemma 3.2.6.

Let W_1 and W_2 and let α_1, α_2 be positive real numbers with $\alpha_1 + \alpha_2 = 1$. We define the *direct sum* of W_1 and W_2 with weights α_1 and α_2, denoted $W = \alpha_1 W_1 \oplus \alpha_2 W_2$, as follows. Let φ_1 and φ_2 be the increasing affine maps which send $J_1 := [0, \alpha_1]$ and $J_2 := [\alpha_1, 1]$ to $[0, 1]$, respectively. Then for all $(x, y) \in [0, 1]^2$, let

$$W(x, y) := \begin{cases} W_i(\varphi_i(x), \varphi_i(y)), & \text{if } (x, y) \in J_i \times J_i \text{ for some } i \in \{1, 2\} \\ 0, & \text{otherwise} \end{cases}.$$

A graphon W is *connected* if W is not weakly isomorphic to a direct sum $\alpha_1 W_1 \oplus \alpha_2 W_2$ where $\alpha_1 \neq 0, 1$. Equivalently, W is connected if there does not exist a measurable subset $A \subseteq [0,1]$ of positive measure such that $W(x,y) = 0$ for a.e. $(x,y) \in A \times A^c$.

Proposition 3.3.3. *Suppose W_1, W_2 are graphons and α_1, α_2 are positive real numbers summing to 1. Let $W := \alpha_1 W_1 \oplus \alpha_2 W_2$. Then as multisets,*

$$\Lambda(W) = \{\alpha_1 u : u \in \Lambda(W_1)\} \cup \{\alpha_2 v : v \in \Lambda(W_2)\}.$$

Moreover, spr$(W) \leq \alpha_1$spr$(W_1)+\alpha_2$spr(W_2) with equality if and only W_1 or W_2 is the all-zeroes graphon.

Proof. For convenience, let $\Lambda_i := \{\alpha_i u : u \in \Lambda(W_i)\}$ for each $i \in \{1,2\}$ and $\Lambda := \Lambda(W)$. The first claim holds simply by considering the restriction of eigenfunctions to the intervals $[0, \alpha_1]$ and $[\alpha_1, 1]$.

For the second claim, we first write $\text{spr}(W) = \alpha_i \mu - \alpha_j \nu$ for some $i,j \in \{1,2\}$. Let $I_i := [\min(\Lambda_i), \max(\Lambda_i)]$ for each $i \in \{1,2\}$ and $I := [\min(\Lambda), \max(\Lambda)]$. Clearly $\alpha_i \text{spr}(W_i) = \text{diam}(I_i)$ for each $i \in \{1,2\}$ and $\text{spr}(W) = \text{diam}(I)$. Moreover, $I = I_1 \cup I_2$. Since $0 \in I_1 \cap I_2$, $\text{diam}(I) \leq \text{diam}(I_1) + \text{diam}(I_2)$ with equality if and only if either I_1 or I_2 equals $\{0\}$. So the desired claim holds. □

Furthermore, the following basic corollary of the Perron-Frobenius holds. For completeness, we prove it here.

Proposition 3.3.4. *Let W be a connected graphon and write f for an eigenfunction corresponding to $\mu(W)$. Then f is nonzero with constant sign a.e.*

Proof. Let $\mu = \mu(W)$. Since

$$\mu = \max_{\|h\|_2 = 1} \int_{(x,y)\in[0,1]^2} W(x,y)h(x)h(y),$$

it follows without loss of generality that $f \geq 0$ a.e. on $[0,1]$. Let $Z := \{x \in [0,1] : f(x) = 0\}$. Then for a.e. $x \in Z$,

$$0 = \mu f(x) = \int_{y\in[0,1]} W(x,y)f(y) = \int_{y \in Z^c} W(x,y)f(y).$$

Since $f > 0$ on Z^c, it follows that $W(x,y) = 0$ a.e. on $Z \times Z^c$. Clearly $\lambda(Z) \neq 0$. If $\lambda(Z^c) = 0$ then the desired claim holds, so without loss of generality, $0 < \lambda(Z), \lambda(Z^c) < 1$. It follows that W is disconnected, a contradiction to our assumption, which completes the proof of the desired claim. □

Lemma 3.3.5. *Suppose W is a graphon achieving maximum spread and let f, g be eigenfunctions for the maximum and minimum eigenvalues for W, respectively. Then the following claims hold:*

(i) For a.e. $(x,y) \in [0,1]^2$,

$$W(x,y) = \begin{cases} 1, & f(x)f(y) > g(x)g(y) \\ 0, & \textit{otherwise} \end{cases} .$$

(ii) $f(x)f(y) - g(x)g(y) \neq 0$ for a.e. $(x,y) \in [0,1]^2$.

Proof. We proceed in the following order:

- Prove Item (i) holds for a.e. $(x,y) \in [0,1]^2$ such that $f(x)f(y) \neq g(x)g(y)$. We will call this Item (i)*.
- Prove Item (ii).
- Deduce Item (i) also holds.

By Propositions 3.3.3 and 3.3.4, we may assume without loss of generality that $f > 0$ a.e. on $[0,1]$. For convenience, we define the quantity $d(x,y) := f(x)f(y) - g(x)g(y)$. To prove Item (i)*, we first define a graphon W' by

$$W'(x,y) = \begin{cases} 1, & d(x,y) > 0 \\ 0, & d(x,y) < 0 \\ W(x,y) & \text{otherwise} \end{cases} .$$

Then by inspection,

$$\begin{aligned}\operatorname{spr}(W') &\geq \int_{(x,y)\in[0,1]^2} W'(x,y)(f(x)f(y) - g(x)g(y)) \\ &= \int_{(x,y)\in[0,1]^2} W(x,y)(f(x)f(y) - g(x)g(y)) \\ &\quad + \int_{d(x,y)>0} (1 - W(x,y))d(x,y) - \int_{d(x,y)<0} W(x,y)d(x,y) \\ &= \operatorname{spr}(W) + \int_{d(x,y)>0} (1 - W(x,y))d(x,y) - \int_{d(x,y)<0} W(x,y)d(x,y).\end{aligned}$$

Since W maximizes spread, Item (i)* holds.

Now, we prove Item (ii). For convenience, we define U to be the set of all pairs $(x, y) \in [0, 1]^2$ so that $d(x, y) = 0$. Now let W' be any graphon which differs from W only on U. Then

$$\begin{aligned}\operatorname{spr}(W') &\geq \int_{(x,y)\in[0,1]^2} W'(x,y)(f(x)f(y) - g(x)g(y)) \\ &= \int_{(x,y)\in[0,1]^2} W(x,y)(f(x)f(y) - g(x)g(y)) \\ &\quad + \int_{(x,y)\in U} (W'(x,y) - W(x,y))(f(x)f(y) - g(x)g(y)) \\ &= \operatorname{spr}(W).\end{aligned}$$

Since $\operatorname{spr}(W) \geq \operatorname{spr}(W')$, f and g are eigenfunctions for W' and we may write μ' and ν' for the corresponding eigenvalues. Now, we define

$$\begin{aligned}I_{W'}(x) &:= (\mu' - \mu)f(x) \\ &= \int_{y\in[0,1]} (W'(x,y) - W(x,y))f(y) \\ &= \int_{y\in[0,1],\,(x,y)\in U} (W'(x,y) - W(x,y))f(y).\end{aligned}$$

Similarly, we define

$$\begin{aligned}J_{W'}(x) &:= (\nu' - \nu)g(x) \\ &= \int_{y\in[0,1]} (W'(x,y) - W(x,y))g(y) \\ &= \int_{y\in[0,1],\,(x,y)\in U} (W'(x,y) - W(x,y))g(y).\end{aligned}$$

Since f and g are orthogonal,

$$0 = \int_{x\in[0,1]} I_{W'}(x)J_{W'}(x).$$

Before proceeding, we make the following observation. For a.e. $(x,y) \in U$, $0 = d(x,y) = f(x)f(y) - g(x)g(y)$. In particular, since $f(x), f(y) > 0$ for a.e. $(x,y) \in [0,1]^2$, then a.e. $(x,y) \in U$ has $g(x)g(y) > 0$. So by letting

$$\begin{aligned} U_+ &:= \{(x,y) \in U : g(x), g(y) > 0\}, \\ U_- &:= \{(x,y) \in U : g(x), g(y) < 0\}, \text{ and} \\ U_0 &:= U \setminus (U_+ \cup U_-), \end{aligned}$$

U_0 has measure 0.

First, let W' be the graphon defined by

$$W'(x,y) = \begin{cases} 1, & (x,y) \in U_+ \\ W(x,y), & \text{otherwise} \end{cases}.$$

For this choice of W',

$$\begin{aligned} I_{W'}(x) &= \int_{y\in[0,1],\,(x,y)\in U_+} (1 - W(x,y))f(y), \text{ and} \\ J_{W'}(x) &= \int_{y\in[0,1],\,(x,y)\in U_+} (1 - W(x,y))g(y). \end{aligned}$$

Clearly $I_{W'}$ and $J_{W'}$ are nonnegative functions so $I_{W'}(x)J_{W'}(x) = 0$ for a.e. $x \in [0,1]$. Since $f(y)$ and $g(y)$ are positive for a.e. $(x,y) \in U$, $W(x,y) = 1$ for a.e. on U_+.

If instead we let $W'(x,y)$ be 0 for all $(x,y) \in U_+$, it follows by a similar argument that $W(x,y) = 0$ for a.e. $(x,y) \in U_+$. So U_+ has measure 0. Repeating the same argument on U_-, we similarly conclude that U_- has measure 0. This completes the proof of Item (ii).

Finally we note that Items (i)* and (ii) together imply Item (i). This completes the proof of the desired claims. □

From here, it is easy to see that any graphon maximizing the spread is a join of two threshold graphons.

Lemma 3.3.6. *If W is a graphon achieving the maximum spread with corresponding eigenfunctions f, g, then $\mu f^2 - \nu g^2 = \mu - \nu$ almost everywhere.*

Proof. Let $\varphi : [0,1] \to [0,1]$ be an arbitrary homeomorphism which is *orientation-preserving* in the sense that $\varphi(0) = 0$ and $\varphi(1) = 1$. Then φ is a continuous strictly monotone increasing function which is differentiable almost everywhere. Now let $\tilde{f} := \varphi' \cdot (f \circ \varphi)$, $\tilde{g} := \varphi' \cdot (g \circ \varphi)$ and $\tilde{W} := \{(x,y) \in [0,1]^2 : (\varphi(x), \varphi(y)) \in K\}$. Using the substitutions $u = \varphi(x)$ and $v = \varphi(y)$,

$$
\begin{aligned}
\tilde{f}\tilde{W}\tilde{f} &= \int_{(x,y)\in[0,1]^2} \chi_{(\varphi(x),\varphi(y))\in W}\ \varphi'(x)\varphi'(y) \cdot f(\varphi(x)) f(\varphi(y)) dx\, dy \\
&= \int_{(x,y)\in[0,1]^2} \chi_{(x,y)\in W}\ f(u)f(v) du\, dv \\
&= \mu.
\end{aligned}
$$

Similarly, $\tilde{g}\tilde{W}\tilde{g} = \nu$.

Note however that the L_2 norms of $\tilde{f}, \tilde{g}$ may not be 1. Indeed using the substitution $u = \varphi(x)$,

$$
\|\tilde{f}\|_2^2 = \int_{x\in[0,1]} \varphi'(x)^2 f(\varphi(x))^2\, dx = \int_{u\in[0,1]} \varphi'(\varphi^{-1}(u)) \cdot f(u)^2\, du.
$$

We exploit this fact as follows. Suppose I, J are disjoint subintervals of $[0,1]$ of the same positive length $\lambda(I) = \lambda(J) = \ell > 0$ and for any $\varepsilon > 0$ sufficiently small (in terms of ℓ), let φ be the (unique) piecewise linear function which stretches I to length $(1+\varepsilon)\lambda(I)$, shrinks J to length $(1-\varepsilon)\lambda(J)$, and shifts only the elements in between I and J. Note that for a.e. $x \in [0,1]$,

$$
\varphi'(x) = \begin{cases} 1+\varepsilon, & x \in I \\ 1-\varepsilon, & x \in J \\ 1, & \text{otherwise.} \end{cases}
$$

Again with the substitution $u = \varphi(x)$,

$$
\begin{aligned}
\|\tilde{f}\|_2^2 &= \int_{x\in[0,1]} \varphi'(x)^2 \cdot f(\varphi(x))^2\, dx \\
&= \int_{u\in[0,1]} \varphi'(\varphi^{-1}(u)) f(u)^2\, du \\
&= 1 + \varepsilon \cdot (\|\chi_I f\|_2^2 - \|\chi_J f\|_2^2).
\end{aligned}
$$

The same equality holds for $\tilde{g}$ instead of $\tilde{f}$. After normalizing $\tilde{f}$ and $\tilde{g}$, by optimality of W, we get a difference of Rayleigh quotients as

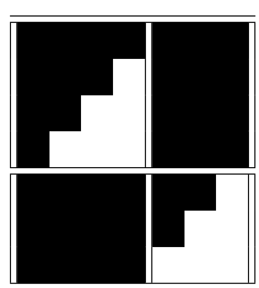
$$\begin{aligned}
0 &\leq \frac{\tilde{f}\tilde{W}\tilde{f}}{\|\tilde{f}\|_2^2} - \frac{\tilde{g}\tilde{W}\tilde{g}}{\|\tilde{g}\|_2^2} - (fWf - gWg) \\
&= \frac{\mu\varepsilon \cdot (\|\chi_I f\|_2^2 - \|\chi_J f\|_2^2)}{1 + \varepsilon \cdot (\|\chi_I f\|_2^2 - \|\chi_J f\|_2^2)} - \frac{\nu\varepsilon \cdot (\|\chi_I g\|_2^2 - \|\chi_J g\|_2^2)}{1 + \varepsilon \cdot (\|\chi_I g\|_2^2 - \|\chi_J g\|_2^2)} \\
&= (1 + o(\varepsilon))\varepsilon \cdot \left(\int_I (\mu f(x)^2 - \nu g(x)^2) dx - \int_J (\mu f(x)^2 - \nu g(x)^2) dx \right)
\end{aligned}$$

as $\varepsilon \to 0$. It follows that for all disjoint intervals $I, J \subseteq [0,1]$ of the same length that the corresponding integrals are the same. Taking finer and finer partitions of $[0,1]$, it follows that the integrand $\mu f(x)^2 - \nu g(x)^2$ is constant almost everywhere. Since the average of this quantity over all $[0,1]$ is $\mu - \nu$, the desired claim holds. □

3.4 From graphons to stepgraphons

The main result of this section is as follows.

Theorem 3.4.1. *Suppose W maximizes spr$(\hat{\mathcal{W}})$. Then W is a stepfunction taking values 0 and 1 of the following form*

 .

Here the internal divisions separate according to the sign of the eigenfunction corresponding to the minimum eigenvalue of W.

In Section 3.4.1, we show how the extreme eigenvalues can change under L_2 averaging and vertex cloning and in Section 3.4.2, we prove Theorem 3.4.1.

3.4.1 Averaging

For convenience, we introduce some terminology. For U a measurable subset of $[0,1]$, let $m(U)$ denote the Lebesgue measure of U. For any graphon W with λ-eigenfunction h, we say that $x \in [0,1]$ is *typical* (with respect to W and h) if

$$\lambda \cdot h(x) = \int_{y \in [0,1]} W(x,y)h(y).$$

Note that a.e. $x \in [0,1]$ is typical. Additionally if $U \subseteq [0,1]$ is measurable with positive measure, then we say that $x_0 \in U$ is *average* (on U, with respect to W and h) if

$$h(x_0)^2 = \frac{1}{m(U)} \int_{y \in U} h(y)^2.$$

Given W, h, U, and x_0 as above, we define the $L_2[0,1]$ function $\mathrm{av}_{U,x_0} h$ by setting

$$(\mathrm{av}_{U,x_0} h)(x) := \begin{cases} h(x_0), & x \in U \\ h(x), & \text{otherwise} \end{cases}.$$

Clearly $\|\mathrm{av}_{U,x_0} h\|_2 = \|h\|_2$. Additionally, we define the graphon $\mathrm{av}_{U,x_0} W$ by setting

$$\mathrm{av}_{U,x_0} W = \begin{cases} 0, & (x,y) \in U \times U \\ W(x_0,y), & (x,y) \in U \times U^c \\ W(x,x_0), & (x,y) \in U^c \times U \\ W(x,y), & (x,y) \in U^c \times U^c \end{cases}.$$

In the graph setting, this is analogous to replacing U with an independent set whose vertices are clones of x_0. The following lemma indicates how this cloning affects the eigenvalues.

Lemma 3.4.2. *Suppose W is a graphon with h a λ-eigenfunction and suppose there exist disjoint measurable subsets $U_1, U_2 \subseteq [0,1]$ of positive measures α and β, respectively. Let $U := U_1 \cup U_2$. Moreover, suppose $W = 0$ a.e. on $(U \times U) \setminus (U_1 \times U_1)$. Additionally, suppose $x_0 \in U_2$ is typical and average on U, with respect to W and h. Let $\tilde{h} := av_{U,x_0} h$ and $\tilde{W} := av_{U,x_0} W$. Then for a.e. $x \in [0,1]$,*

$$(A_{\tilde{W}} \tilde{h})(x) = \lambda \tilde{h}(x) + \begin{cases} 0, & x \in U \\ m(U) \cdot W(x_0,x)h(x_0) - \int_{y \in U} W(x,y)h(y), & \textit{otherwise} \end{cases}. \tag{3.2}$$

Furthermore,

$$\langle A_{\tilde{W}}\tilde{h}, \tilde{h}\rangle = \sigma + \int_{(x,y)\in U_1\times U_1} W(x,y)h(x)h(y). \tag{3.3}$$

Proof. We first prove Equation (3.2). Note that for a.e. $x \in U$, Then

$$\begin{aligned}
(A_{\tilde{W}}\tilde{h})(x) &= \int_{y\in[0,1]} \tilde{W}(x,y)\tilde{h}(y) \\
&= \int_{y\in U} \tilde{W}(x,y)\tilde{h}(y) + \int_{y\in[0,1]\setminus U} \tilde{W}(x,y)\tilde{h}(y) \\
&= \int_{y\in[0,1]\setminus U} W(x_0,y)h(y) \\
&= \int_{y\in[0,1]} W(x_0,y)h(y) - \int_{y\in U} W(x_0,y)h(y) \\
&= \lambda h(x_0) \\
&= \lambda\tilde{h}(x),
\end{aligned}$$

as desired. Now note that for a.e. $x \in [0,1] \setminus U$,

$$\begin{aligned}
(A_{\tilde{W}}\tilde{h})(x) &= \int_{y\in[0,1]} \tilde{W}(x,y)\tilde{h}(y) \\
&= \int_{y\in U} \tilde{W}(x,y)\tilde{h}(y) + \int_{y\in[0,1]\setminus U} \tilde{W}(x,y)\tilde{h}(y) \\
&= \int_{y\in U} W(x_0,x)h(x_0) + \int_{y\in[0,1]\setminus U} W(x,y)h(y) \\
&= m(U)\cdot W(x_0,x)h(x_0) + \int_{y\in[0,1]} W(x,y)h(y) - \int_{y\in U} W(x,y)h(y) \\
&= \lambda h(x) + m(U)\cdot W(x_0,x)h(x_0) - \int_{y\in U} W(x,y)h(y).
\end{aligned}$$

So again, the claim holds and this completes the proof of Equation (3.2). Now we prove

Equation (3.3). Indeed by Equation (3.2),

$$\begin{aligned}
\langle (A_{\tilde{W}}\tilde{h}), \tilde{h}\rangle &= \int_{x\in[0,1]} (A_{\tilde{W}}\tilde{h})(x)\tilde{h}(x) \\
&= \int_{x\in[0,1]} \lambda\tilde{h}(x)^2 \\
&\quad + \int_{x\in[0,1]\setminus U} \left(m(U)\cdot W(x_0,x)h(x_0) - \int_{y\in U} W(x,y)h(y)\right)\cdot h(x) \\
&= \lambda + m(U)\cdot h(x_0)\left(\int_{x\in[0,1]} W(x_0,x)h(x) - \int_{x\in U} W(x_0,x)h(x)\right) \\
&\quad - \int_{y\in U}\left(\int_{x\in[0,1]} W(x,y)h(x) - \int_{x\in U} W(x,y)h(x)\right)\cdot h(y) \\
&= \lambda + m(U)\cdot h(x_0)\left(\lambda h(x_0) - \int_{y\in U} 0\right) \\
&\quad - \int_{y\in U}\left(\lambda h(y)^2 - \int_{x\in U} W(x,y)h(x)h(y)\right) \\
&= \lambda + \lambda m(U)\cdot h(x_0)^2 - \lambda\int_{y\in U} h(y)^2 + \int_{(x,y)\in U\times U} W(x,y)h(x)h(y) \\
&= \lambda + \int_{(x,y)\in U_1\times U_1} W(x,y)h(x)h(y),
\end{aligned}$$

and this completes the proof of desired claims. □

We have the following useful corollary.

Corollary 3.4.3. *Suppose spr*$(W) =$ *spr*$(\hat{\mathcal{W}})$ *with maximum and minimum eigenvalues* μ^*, ν^* *corresponding respectively to eigenfunctions* f^*, g^**. Moreover, suppose that there exist disjoint subsets* $A, B \subseteq [0,1]$ *and* $x_0 \in B$ *so that the conditions of Lemma 3.4.2 are met for* W *with* $\lambda = \mu^*$, $h = f^*$, $U_1 = A$, *and* $U_2 = B$*. Then,*

(i) $W(x,y) = 0$ *for a.e.* $(x,y) \in U^2$, *and*

(ii) f^* *is constant on* U*.*

Proof. Without loss of generality, we assume that $\|f\|_2 = \|g\|_2 = 1$. Write $\tilde{W}$ for the graphon and $\tilde{f}, \tilde{g}$ for the corresponding functions produced by Lemma 3.4.2. By Lemma 3.3.4, we may assume without loss of generality that $f > 0$ a.e. on $[0,1]$. We first prove Item (i). Note that

$$\begin{aligned}\operatorname{spr}(\tilde{W}) &\geq \int_{(x,y)\in[0,1]^2} W'(x,y)(f'(x)f'(y) - g'(x)g'(y)) \\ &= (\mu - \nu) + \int_{(x,y)\in A\times A} W(x,y)(f(x)f(y) - g(x)g(y)) \\ &= \operatorname{spr}(W) + \int_{(x,y)\in A\times A} W(x,y)(f(x)f(y) - g(x)g(y)). \end{aligned} \tag{3.4}$$

Since $\operatorname{spr}(W) \geq \operatorname{spr}(W')$, Lemma 3.3.5.(ii), implies that $f(x)f(y) - g(x)g(y) > 0$ for a.e. $(x,y) \in A \times A$ such that $W(x,y) \neq 0$. Item (i) follows.

For Item (ii), we first note that f^* is a μ-eigenfunction for $\tilde{W}$. Indeed, if not, then the inequality in (3.4) holds strictly, a contradiction to the fact that $\operatorname{spr}(W) \geq \operatorname{spr}(\tilde{W})$. Again by Lemma 3.4.2,

$$m(U) \cdot W(x_0, x) f(x_0) = \int_{y\in U} W(x,y) f(y)$$

for a.e. $x \in [0,1] \setminus U$. Let $S_1 := \{x \in [0,1] \setminus U : W(x_0, x) = 1\}$ and $S_0 := [0,1] \setminus (U \cup S_1)$. We claim that $m(S_1) = 0$. Assume otherwise. By Lemma 3.4.2 and by Cauchy-Schwarz, for a.e. $x \in S_1$,

$$\begin{aligned} m(U) \cdot f(x_0) &= m(U) \cdot W(x_0, x) f(x_0) \\ &= \int_{y\in U} W(x,y) f(y) \\ &\leq \int_{y\in U} f(y) \\ &\leq m(U) \cdot f(x_0), \end{aligned}$$

and by sandwiching, $W(x,y) = 1$ and $f(y) = f(x_0)$ for a.e. $y \in U$. Since $m(S_1) > 0$, it follows that $f(y) = f(x_0) = 0$ for a.e. $y \in U$, as desired.

So we assume otherwise, that $m(S_1) = 0$. Then for a.e. $x \in [0,1] \setminus U$, $W(x_0, x) = 0$ and

$$0 = m(U) \cdot W(x_0, x) f(x_0) = \int_{y\in U} W(x,y) f(y).$$

Since $f > 0$ a.e. on $[0,1]$, it follows that $W(x,y) = 0$ for a.e. $y \in U$. So altogether, $W(x,y) = 0$ for a.e. $(x,y) \in ([0,1] \setminus U) \times U$. So W is disconnected, a contradiction to Fact 3.3.3. So the desired claim holds. $\square$

3.4.2 Proof of Theorem 3.4.1

Proof. For convenience, we write $\mu := \mu(W)$ and $\nu := \nu(W)$ and let f, g denote the corresponding unit eigenfunctions. Moreover by Proposition 3.3.4, we may assume without loss of generality that $f > 0$.

First, we show without loss of generality that f, g are monotone on the sets $P := \{x \in [0,1] : g(x) \geq 0\}$ and $N := [0,1] \setminus P$. Indeed, we define a total ordering $\preccurlyeq$ on $[0,1]$ as follows. For all x and y, we let $x \preccurlyeq y$ if:

(i) $g(x) \geq 0$ and $g(y) < 0$, or

(ii) Item (i) does not hold and $f(x) < f(y)$, or

(iii) Item (i) does not hold, $f(x) = f(y)$, and $x \leq y$.

By inspection, the function $\varphi : [0,1] \to [0,1]$ defined by

$$\varphi(x) := m(\{y \in [0,1] : y \preccurlyeq x\}).$$

is a weak isomorphism between W and its entrywise composition with φ. By invariance of $\operatorname{spr}(\cdot)$ under weak isomorphism, we make the above replacement and write f, g for the replacement eigenfunctions. That is, we are assuming that our graphon is relabeled so that $[0,1]$ respects $\preccurlyeq$.

As above, let $P := \{x \in [0,1] : g(x) \geq 0\}$ and $N := [0,1] \setminus P$. By Lemma 3.3.6, f and $-g$ are monotone nonincreasing on P. Additionally, f and g are monotone nonincreasing on N. Without loss of generality, we may assume that W is of the form from Theorem 3.2.3. Now we let $C := \{x \in [0,1] : f(x) < g(x)\}$, $B := [0,1] \setminus C$. We first prove the following claim.

Claim A: Except on a set of measure 0, f takes on at most 2 values on $P \cap C$, and at most 2 values on $N \cap C$.

We first prove this claim for f on $P \cap C$. Let D be the set of all discontinuities of f on the interior of the interval $P \cap C$. Clearly D consists only of jump-discontinuities. By the Darboux-Froda Theorem, D is at most countable and moreover, $(P \cap C) \setminus D$ is a union of at most countably many disjoint intervals $\mathcal{I}$. Moreover, f is continuous on the interior of each $I \in \mathcal{I}$.

We show now that f is piecewise constant on the interiors of each $I \in \mathcal{I}$. Indeed, let $I \in \mathcal{I}$. Since f is a μ-eigenfunction function for W,

$$\mu f(x) = \int_{y \in [0,1]} W(x,y) f(y)$$

for a.e. $x \in [0,1]$ and by continuity of f on the interior of I, this equation holds everywhere on the interior of I. Additionally since f is continuous on the interior of I, by the Mean Value Theorem, there exists some x_0 in the interior of I so that

$$f(x_0)^2 = \frac{1}{m(U)} \int_{x \in U} f(x)^2.$$

By Corollary 3.4.3, f is constant on the interior of U, as desired.

If $|\mathcal{I}| \leq 2$, the desired claim holds, so we may assume otherwise. Then there exists distinct $I_1, I_2, I_3 \in \mathcal{I}$. Moreover, f equals a constant f_1, f_2, f_3 on the interiors of I_1, I_2, and I_3, respectively. Additionally since I_1, I_2, and I_3 are separated from each other by at least one jump discontinuity, we may assume without loss of generality that $f_1 < f_2 < f_3$. It follows that there exists a measurable subset $U \subseteq I_1 \cup I_2 \cup I_3$ of positive measure so that

$$f_2^2 = \frac{1}{m(U)} \int_{x \in U} f(x)^2.$$

By Corollary 3.4.3, f is constant on U, a contradiction. So Claim A holds on $P \cap C$. For Claim A on $N \cap C$, we may repeat this argument with P and N interchanged, and g and $-g$ interchanged.

Now we show the following claim.

Claim B: For a.e. $(x,y) \in (P \times P) \cup (N \times N)$ such that $f(x) \geq f(y)$, we have that for a.e. $z \in [0,1]$, $W(x,z) = 0$ implies that $W(y,z) = 0$.

We first prove the claim for a.e. $(x,y) \in P \times P$. Indeed, suppose $W(y,z) = 0$. Then for a.e. such x, y, by Lemma 3.3.6, $g(x) \leq g(y)$. By Lemma 3.3.5.(i), $W(x,z) = 0$ implies that $f(x)f(z) < g(x)g(z)$. Clearly in this case, $z \in P$. Since $f(x) \geq f(y)$ and $g(x) \leq g(y)$, $f(y)f(z) < g(y)g(z)$. Again by Lemma 3.3.5.(i), $W(y,z) = 0$ for a.e. such x, y, z, as desired. So the desired claim holds for a.e. $(x,y) \in P \times P$ such that $f(x) \geq f(y)$. We may repeat the argument for a.e. $(x,y) \in N \times N$ to arrive at the same conclusion.

The next claim follows directly from Lemma 3.3.6.

Claim C: For a.e. $x \in [0,1]$, $x \in B$ if and only if $f(x) \geq 1$, if and only if $|g(x)| \leq 1$.

Finally, we show the following claim.

Claim D: f takes on at most 3 values on $P \cap B$, and on $N \cap B$.

For a proof, we first write $P \cap C = C_1 \cup C_2$ so that C_1, C_2 are disjoint and f equals some constant f_1 a.e. on C_1 and f equals some constant f_2 a.e. on C_2. By Lemma 3.3.6, g equals some constant g_1 a.e. on C_1 and g equals some constant g_2 a.e. on C_2. By definition of P, $g_1, g_2 \geq 0$. Now suppose $x \in P \cap B$ so that

$$\mu f(x) = \int_{y \in [0,1]} W(x,y) f(y).$$

Then by Lemma 3.3.5.(i),

$$\mu f(x) = \int_{y \in (P \cap B) \cup N} f(y) + \int_{y \in C_1} W(x,y) f(y) + \int_{y \in C_2} W(x,y) f(y).$$

By Claim B, this expression for $\mu f(x)$ may take on at most 3 values. So the desired claim holds on $P \cap B$. Repeating the same argument, the claim also holds on $N \cap B$.

We are nearly done with the proof of the theorem. We now partition $P \cap B, P \cap C, N \cap B$, and $N \cap C$ so that f and g are constant a.e. on each part as:

- $P \cap B = U_1 \cup U_2 \cup U_3$,
- $P \cap C = U_4 \cup U_5$,
- $N \cap B = U_6 \cup U_7 \cup U_8$, and
- $N \cap C = U_9 \cup U_{10}$.

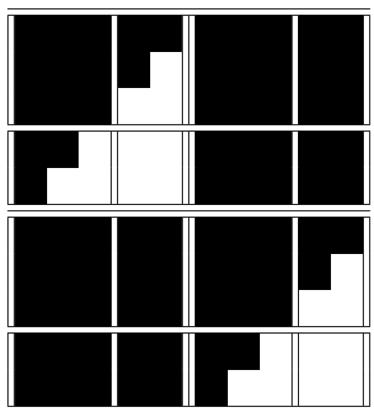
Then by Lemma 3.3.5.(i), there exists a matrix $(m_{ij})_{i,j \in [10]}$ so that for all $(i,j) \in [10] \times [10]$,

- $m_{ij} \in \{0,1\}$,
- $W(x,y) = m_{ij}$ for a.e. $(x,y) \in U_i \times U_j$,
- $m_{ij} = 1$ if and only if $f_i f_j > g_i g_j$, and

- $m_{ij} = 0$ if and only if $f_i f_j < g_i g_j$.

Additionally, we set $\alpha_i = m(U_i)$ and also denote by f_i and g_i the constant values of f, g on each U_i, respectively, for each $i = 1, \ldots, 10$. Furthermore, we assume without loss of generality that that $f_1 > f_2 > f_3 \geq 1 > f_4 > f_5$ and that $f_6 > f_7 > f_8 \geq 1 > f_9 > f_{10}$. Also by Lemma 3.3.6, $0 \leq g_1 < g_2 < g_3 \leq 1 < g_4 < g_5$ and $0 \leq -g_1 < -g_2 < -g_3 \leq 1 < -g_4 < -g_5$. Also, by Claim B, no two columns of m are identical within the sets $\{1, 2, 3, 4, 5\}$ and within $\{6, 7, 8, 9, 10\}$. Shading $m_{ij} = 1$ black and $m_{ij} = 0$ white, we let

$M =$



.

Therefore, W is a stepgraphon with values determined by M and the size of each block determined by the α_i.

We claim that $0 \in \{\alpha_3, \alpha_4, \alpha_5\}$ and $0 \in \{\alpha_8, \alpha_9, \alpha_{10}\}$. Indeed, otherwise there there exists some $x_4 \in U_4$ such that

$$\mu f_4 = \mu f(x_0) = \int_{y \in [0,1]} W(x, y) f(y).$$

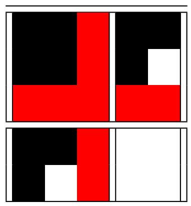
Moreover, there exist measurable subsets $U_3' \subseteq U_3$ and $U_5' \subseteq U_5$ of positive measure such that

$$f(x_4)^2 = \frac{1}{m(U)} \int_{y \in U_3' \cup U_4 \cup U_5'} f(y)^2.$$

The conditions of Corollary 3.4.3 are met for W with $A = U_3', x_0 = x_3, \mu^* = \mu$, $\nu^* = \nu, f^* = f$, and $g^* = g$. Since $\int_{A \times A} W(x, y) f(x) f(y) > 0$, this is a contradiction to the corollary, so the desired claim holds. The same argument may be used to prove that $0 \in \{\alpha_8, \alpha_9, \alpha_{10}\}$.

We now form the principal submatrix M' by removing the i-th row and column from M if and only if $\alpha_i = 0$. Since $\alpha_i = 0$, W is a stepgraphon with values determined by M'. Let M_P'

denote the principal submatrix of M' corresponding to the indices $i \in \{1, \ldots, 5\}$ so that $\alpha_i > 0$. We use red to indicate rows and columns present in M but not M'_P. Since $0 \in \{\alpha_3, \alpha_4, \alpha_5\}$, it follows that M'_P is a principal submatrix of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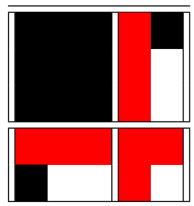
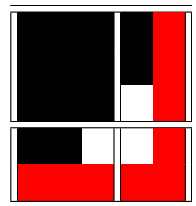

, or

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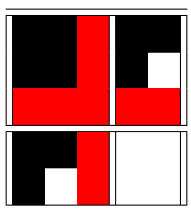
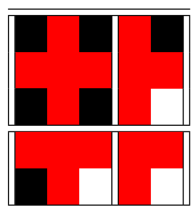
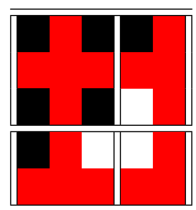
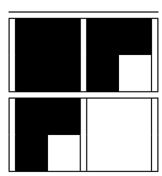
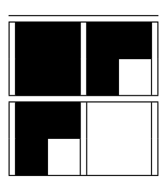
In the second case, columns 2 and 3 are identical in M', and in the third case, columns 1 and 2 are identical in M'. So without loss of generality, M'_P is a principal submatrix of one of


,

, or

.

In each case, M'_P is a principal submatrix of


.

An identical argument shows that the principal submatrix of M' on the indices $i \in \{6, \ldots, 10\}$ such that $\alpha_i > 0$ is a principal submatrix of


.

Finally, we note that $0 \in \{\alpha_1, \alpha_6\}$. Indeed otherwise the corresponding columns are identical in M', a contradiction. So without loss of generality, row and column 6 were also removed from M to form M'. This completes the proof of the theorem. $\square$

3.5 Spread maximum graphons

In this section, we complete the proof of the graphon version of the spread conjecture of Gregory, Hershkowitz, and Kirkland from [5]. In particular, we prove the following theorem. For convenience and completeness, we state this result in the following level of detail.

Theorem 3.5.1. *If W is a graphon that maximizes spread, then W may be represented as follows. For all $(x,y) \in [0,1]^2$,*

$$W(x,y) = \begin{cases} 0, & (x,y) \in [2/3, 1]^2 \\ 1, & \textit{otherwise} \end{cases}$$

and

$$\mu = \frac{1+\sqrt{3}}{3} \quad \textit{and} \quad \nu = \frac{1-\sqrt{3}}{3}$$

are the maximum and minimum eigenvalues of W, respectively. Furthermore if f, g are unit eigenfunctions associated to μ, ν, respectively, then, up to a change in sign, they may be written as follows. For every $x \in [0,1]$,

$$f(x) = \frac{1}{2\sqrt{3+\sqrt{3}}} \cdot \begin{cases} 3+\sqrt{3}, & x \in [0, 2/3] \\ 2\cdot\sqrt{3} & \textit{otherwise} \end{cases}, \quad \textit{and}$$

$$g(x) = \frac{1}{2\sqrt{3-\sqrt{3}}} \cdot \begin{cases} 3-\sqrt{3}, & x \in [0, 2/3] \\ -2\cdot\sqrt{3} & \textit{otherwise} \end{cases}.$$

To help outline our proof of Theorem 3.5.1, we first let G^* be the graph (with loops) whose adjacency matrix matches the array in Theorem 3.4.1, as shown in Figure 3.2. We proceed in the following steps.

1. In Section 3.5.1, we reduce the proof of Theorem 3.5.1 to 17 cases, each corresponding to a subset of $V(G^*)$. We also define and discuss the maximization problems SPR_S associated to each case.

2. In Section 3.5.2, we appeal to interval arithmetic to translate these optimization problems into algorithms. Based on the output of the 17 programs we wrote, we eliminate 15 of

the 17 cases. We address the multitude of formulas used throughout and relocate their statements and proofs to Appendix 3.7.1.

3. Finally in Section 3.5.3, we complete the proof of Theorem 3.5.1 by analyzing the 2 remaining cases. Here, we apply Viète's Formula for roots of cubic equations and make a direct argument.

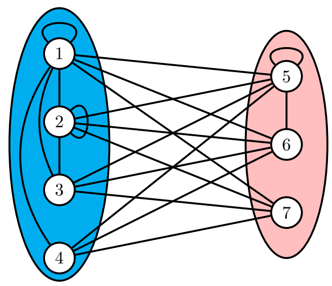


Figure 3.2 The graph G^*.

3.5.1 Stepgraphon case analysis

For concreteness, we define G^* on the vertex set $\{1, \ldots, 7\}$. Explicitly, the neighborhoods $N_1, \ldots, N_7$ are:

$$\begin{aligned} &N_1 = \{1,2,3,4,5,6,7\} && N_2 = \{1,2,3,5,6,7\} \\ &N_3 = \{1,2,5,6,7\} && N_4 = \{1,5,6,7\} \\ &N_5 = \{1,2,3,4,5,6\} && N_6 = \{1,2,3,4,5\} \\ &N_7 = \{1,2,3,4\} \end{aligned}.$$

More compactly, we may note that

$$\begin{aligned} N_1 = \{1,\ldots,7\} \quad & N_2 = N_1 \setminus \{4\} \quad N_3 = N_2 \setminus \{3\} \quad N_4 = N_3 \setminus \{2\} \\ & N_5 = N_1 \setminus \{7\} \quad N_6 = N_5 \setminus \{5\} \quad N_7 = N_6 \setminus \{4\} \end{aligned}.$$

Now, we introduce the following specialized notation. For any nonempty set $S \subseteq V(G^*)$ and any labeled partition $(I_i)_{i\in S}$ of $[0,1]$, we define the stepgraphon $W_{\mathcal{I}}$ as follows. For all $i,j \in S$, $W_{\mathcal{I}}$ equals 1 on $I_i \times I_j$ if and only if ij is an edge (or loop) of G^*, and 0 otherwise. If $\alpha = (\alpha_i)_{i\in S}$ where $\alpha_i = m(I_i)$ for all $i \in S$, we may W_α denote the graphon $W_{\mathcal{I}}$ up to weak isomorphism.

Next, let $\mathcal{A} := [1, +\infty]$, $\mathcal{B} := [0, 1]$, $\mathcal{C} := [-1, 0]$, and $\mathcal{D} := [-\infty, -1]$. For each $i \in V(G^*)$, we define the intervals F_i and G_i by

$$(F_i, G_i) := \begin{cases} (\mathcal{A}, \mathcal{B}), & i \in \{1, 2\} \\ (\mathcal{B}, \mathcal{A}), & i \in \{3, 4\} \\ (\mathcal{A}, \mathcal{C}), & i = 5 \\ (\mathcal{B}, \mathcal{D}), & i \in \{6, 7\} \end{cases}.$$

Given that the set S and the quantities $(\alpha_i, f_i, g_i)_{i \in S}$ are clear from context, we label the following equation:

$$\sum_{i \in S} \alpha_i = \sum_{i \in S} \alpha_i f_i^2 = \sum_{i \in S} \alpha_i g_i^2 = 1. \tag{3.5}$$

Furthermore when $i \in S$ is understood from context, we define the equations

$$\mu f_i^2 - \nu g_i^2 = \mu - \nu \tag{3.6}$$

$$\sum_{j \in N_i \cap S} \alpha_j f_j = \mu f_i \tag{3.7}$$

$$\sum_{j \in N_i \cap S} \alpha_j g_j = \nu f_i \tag{3.8}$$

Additionally, we consider the following inequalities. For all $S \subseteq V(G^*)$ and all distinct $i, j \in S$,

$$f_i f_j - g_i g_j \begin{cases} \geq 0, & ij \in E(G^*) \\ \leq 0, & ij \notin E(G^*) \end{cases} \tag{3.9}$$

Finally, for all nonempty $S \subseteq V(G^*)$, we define the constrained-optimization problem SPR_S by:

$$(\text{SPR}_S): \begin{cases} \max & \mu - \nu \\ \text{s.t} & \text{Equation (3.5)} \\ & \text{Equations (3.6), (3.7), and (3.8)} \quad \text{for all } i \in S \\ & \text{Inequality (3.9)} \quad \text{for all distinct } i, j \in S \\ & (\alpha_i, f_i, g_i) \in [0, 1] \times F_i \times G_i \quad \text{for all } i \in S \\ & \mu, \nu \in \mathbb{R} \end{cases}.$$

For completeness, we state and prove the following observation.

Proposition 3.5.2. *Let $W \in \mathcal{W}$ such that $spr(W) = \max_{U \in \mathcal{W}} spr(U)$ and write μ, ν for the maximum and minimum eigenvalues of W, with some corresponding unit eigenfunctions f, g. Then for some nonempty set $S \subseteq V(G^*)$, the following holds. There exists a triple $(I_i, f_i, g_i)_{i \in S}$, where $(I_i)_{i \in S}$ is a labeled partition of $[0, 1]$ with parts of positive measure and $f_i, g_i \in \mathbb{R}$ for all $i \in S$, such that:*

(i) $W = W_{\mathcal{I}}$.

(ii) Allowing the replacement of f by $-f$ and of g by $-g$, for all $i \in S$, f and g equal f_i and g_i a.e. on I_i.

(iii) With $\alpha_i := m(I_i)$ for all $i \in S$, SPR_S is solved by μ, ν, and $(\alpha_i, f_i, g_i)_{i \in S}$.

Proof. First we prove item (i). By Theorem 3.4.1 and the definition of G^*, there exists a nonempty set $S \subseteq V(G^*)$ and a labeled partition $\mathcal{I} = (I_i)_{i \in S}$ such that $W = W_{\mathcal{I}}$. By merging any parts of measure 0 into some part of positive measure, we may assume without loss of generality that $m(I_i) > 0$ for all $i \in S$. So item (i) holds.

Finally, we prove item (iii), we first prove that for all $i \in V(G^*)$, $(f_i, g_i) \in F_i \times G_i$. By Lemma 3.3.6,

$$\mu f_i^2 - \nu g_i^2 = \mu - \nu$$

for all $i \in S$. In particular, either $f_i^2 \leq 1 \leq g_i^2$ or $g_i^2 \leq 1 \leq f_i^2$. By Lemma 3.3.5, for all $i, j \in S$, $f_i f_j - g_i g_j \neq 0$ and $ij \in E(G)$ if and only if $f_i f_j - g_i g_j > 0$. Note that the loops of G^* are $1, 2$, and 5. It follows that for all $i \in S$, $f_i^2 > 1 > g_i^2$ if and only if $i \in \{1, 2, 5\}$, and $g_i^2 > 1 > f_i^2$, otherwise. Since f is positive on $[0, 1]$, this completes the proof that inspection, $f_i \in F_i$ for all $i \in S$. Similarly since g is positive on $\bigcup_{i \in \{1,2,3,4\} \cap S} I_i$ and negative on $\bigcup_{i \in \{5,6,7\}} I_i$, by inspection $g_i \in G_i$ for all $i \in S$. Similarly, Inequalities (3.9) follow directly from Lemma 3.3.5.

Continuing, we note the following. Since W is a stepgraphon, if $\lambda \neq 0$ is an eigenvalue of W, there exists a λ-eigenfunction h for W such that for all $i \in S$, $h = h_i$ on I_i for some $h_i \in \mathbb{R}$. Moreover for all $i \in S$, since $m(I_i) > 0$,

$$\lambda h_i = \sum_{i \in S} \alpha_i h_i.$$

In particular, any solution to SPR_S is at most $\mu-\nu$. Since f, g are eigenfunctions corresponding to W and the eigenvalues μ, ν, respectively, Equations (3.7), and (3.8) hold. Finally since $(I_i)_{i\in S}$ is a partition of $[0,1]$ and since $\|f\|_2^2 = \|g\|_2^2 = 1$, Equation (3.5) holds. So μ, ν, and $(\alpha_i, f_i, g_i)_{i\in S}$ lie in the domain of SPR_S. This completes the proof of item (iii), and the desired claim. □

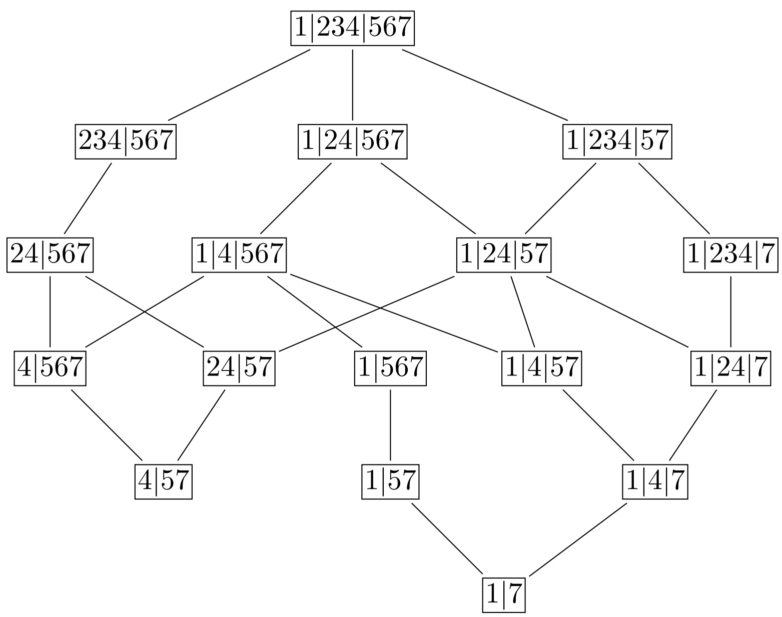


Figure 3.3 The set $\mathcal{S}_{17}$, as a poset ordered by inclusion. See Lemma 3.5.3.

Following the same convention as Figure 3.3, we suppress braces and commons when writing sets $S \subseteq V(G^*)$, and use vertical bars to partition S according to its intersections with the sets $\{1\}$, $\{2,3,4\}$, and $\{5,6,7\}$. Now we let

$$\mathcal{S}_{17} := \left\{ \begin{array}{c} 1|234|567, 1|24|567, 1|234|57, 1|4|567, 1|24|57, 1|234|7, 234|567, \\ 24|567, 4|567, 24|57, 1|567, 1|4|57, 1|2|47, 1|57, 4|57, 1|4|7, 1|7 \end{array} \right\}.$$

We enhance Proposition 3.5.2 as follows.

Lemma 3.5.3. *Proposition 3.5.2 holds with the added assumption that $S \in \mathcal{S}_{17}$.*

Proof. We begin our proof with the following claim.

Claim A: Suppose $i \in S$ and $j \in V(G^*)$ are distinct such that $N_i \cap S = N_j \cap S$. Then Proposition 3.5.2 holds with the set $S' := (S \setminus \{i\}) \cup \{j\}$ replacing S.

First, we define the following quantities. For all $k \in S' \setminus \{j\}$, let $(f'_k, g'_k, I'_k) := (f_k, g_k, I_k)$, and also let $(f'_j, g'_j) := (f_i, g_i)$. If $j \in S$, let $I'_j := I_i \cup I_j$, and otherwise, let $I'_j := I_i$. Additionally let $\mathcal{I}' := (I'_k)_{k \in S'}$ and for each $k \in S'$, let $\alpha'_k := m(I'_k)$. By the criteria from Proposition 3.5.2, the domain criterion $(\alpha'_k, f'_k, g'_k) \in [0,1] \times F_k \times G_k$ as well as Equation (3.6) holds for all $k \in S'$. Since we are reusing μ, ν, the constraint $\mu, \nu \in \mathbb{R}$ also holds.

It suffices to show that Equation (3.5) holds, and that Equations (3.7) and (3.8) hold for all $k \in S'$. To do this, we first note that for all $k \in S'$, $f = f'_k$ and $g = g'_k$ on I'_k. By definition, $f = f_k$ and $g = g_k$ on $I'_k = I_k$ for all $k \in S' \setminus \{j\}$ as needed by Claim A. Now suppose $j \notin S$. Then $f = f_i = f'_j$ and $g = g_i = g'_j$ and $I'_j = I_i$ on the set $I_i = I'_j$, matching Claim A. Finally, suppose $j \in S$. Note by definition that $f = f_i = f'_j$ and $g = g_i = g'_j$ on I_i. Since and $I'_j = I_i \cup I_j$, it suffices to prove that $f = f'_j$ and $g = g'_j$ on I_j. We first show that $f_j = f_i$ and $g_j = g_i$. Indeed,

$$\mu f_j = \sum_{k \in N_j \cap S} \alpha_k f_k = \sum_{k \in N_i \cap S} \alpha_k f_k = \mu f_i$$

and since $\mu \neq 0$, $f_j = f_i$. Similarly, $g_j = g_i$. So $f = f_j = f_i = f'_j$ and $g = g_j = g_i = g'_j$ on the set $I'_j = I_i \cup I_j$. This completes the proof of Claim A.

Finally, we claim that $W_{\mathcal{I}'} = W$. Indeed, this follows directly from Lemma 3.3.5 and the fact that $W = W_{\mathcal{I}}$. Since $\mathcal{I}'$ is a partition of $[0,1]$ and since f, g are unit eigenfunctions for W Equation (3.5) holds, and Equations (3.7) and (3.8) hold for all $k \in S'$. This completes the proof of Claim A.

Next, we prove the following claim.

Claim B: If S satisfies the criteria of Proposition 3.5.2, then the following holds.

(a) If there exists some $i \in S$ such that $N_i = S$, then $i = 1$.

(b) $S \cap \{1, 2, 3, 4\} \neq \emptyset$.

(c) $S \cap \{2, 3, 4\}$ is one of $\emptyset, \{4\}, \{2, 4\}$, and $\{2, 3, 4\}$.

(d) $S \cap \{5, 6, 7\}$ is one of $\{7\}, \{5, 7\}$, and $\{5, 6, 7\}$.

Since $N_1 \cap S = S = N_i$, item (a) follows from Claim A applied to the pair $(i, 1)$. Since f, g are orthogonal and f is positive on $[0, 1]$, g is positive on a set of positive measure, so item (b) holds.

To prove item (c), we have 3 cases. If $S \cap \{2, 3, 4\} = \{2\}$, then $N_2 \cap S = N_1 \cap S$ and we may apply Claim A to the pair $(2, 1)$. If $S \cap \{2, 3, 4\} = \{3\}$, then $N_3 \cap S = N_4 \cap S$ and we may apply Claim A to the pair $(3, 4)$. If $S \cap \{2, 3, 4\} = \{2, 3\}$, then $N_2 \cap S = N_1 \cap S$ and we may apply Claim A to the pair $(2, 1)$. So item (c) holds. For item (d), we reduce $S \cap \{5, 6, 7\}$ to one of $\emptyset$, $\{7\}$, $\{5, 7\}$, and $\{5, 6, 7\}$ in the same fashion. To eliminate the case where $S \cap \{5, 6, 7\} = \emptyset$, we simply note that since f and g are orthogonal and f is positive on $[0, 1]$, g is negative on a set of positive measure. This completes the proof of Claim B.

	$\emptyset$	$\{4\}$	$\{2,4\}$	$\{2,3,4\}$
$\{7\}$	$1\|7$	$4\|7$ $1\|4\|7$	$24\|7$ $1\|24\|7$	$234\|7$ $1\|234\|7$
$\{5,7\}$	$1\|57$	$4\|57$ $1\|4\|57$	$24\|57$ $1\|24\|57$	$234\|57$ $1\|234\|57$
$\{5,6,7\}$	$1\|567$	$4\|567$ $1\|4\|567$	$24\|567$ $1\|24\|567$	$234\|567$ $1\|234\|567$

Table 3.1 The 21 sets which arise from repeated applications of Claim B.

After repeatedly applying Claim B, we may replace S with one of the cases found in Table 3.1. Let $\mathcal{S}_{21}$ denote the sets in Table 3.1. By definition,

$$\mathcal{S}_{21} = \mathcal{S}_{17} \bigcup \{\{4, 7\}, \{2, 4, 7\}, \{2, 3, 4, 7\}, \{2, 3, 4, 5, 7\}\}.$$

Finally, we eliminate the 4 cases in $\mathcal{S}_{21} \setminus \mathcal{S}_{17}$. If $S = \{4, 7\}$, then W is a bipartite graphon, hence $\text{spr}(W) \leq 1$, a contradiction since $\max_{U \in \mathcal{W}} \text{spr}(W) > 1$.

For the three remaining cases, let τ be the permutation on $\{2, \ldots, 7\}$ defined as follows. For all $i \in \{2, 3, 4\}$, $\tau(i) := i + 3$ and $\tau(i + 3) := i$. If S is among $\{2, 4, 7\}, \{2, 3, 4, 7\}, \{2, 3, 4, 5, 7\}$, we apply τ to S in the following sense. Replace g with $-g$ and replace $(\alpha_i, I_i, f_i, g_i)_{i\in S}$ with $(\alpha_{\tau(i)}, I_{\tau(i)}, f_{\tau(i)}, -g_{\tau(i)})_{i\in\tau(S)}$. By careful inspection, it follows that $\tau(S)$ satisfies the criteria from Proposition 3.5.2. Since $\tau(\{2, 4, 7\}) = \{4, 5, 7\}$, $\tau(\{2, 3, 4, 7\}) = \{4, 5, 6, 7\}$, and $\tau(\{2, 3, 4, 5, 7\}) = \{2, 4, 5, 6, 7\}$, this completes the proof. $\square$

3.5.2 Interval arithmetic

Interval arithmetic is a computational technique which bounds errors that accumulate during computation. For convenience, let $\mathbb{R}^* := [-\infty, +\infty]$ be the extended real line. To enhance order floating point arithmetic, we replace extended real numbers with unions of intervals which are guaranteed to contain them. Moreover, we extend the basic arithmetic operations $+, -, \times, \div$, and $\sqrt{}$ to operations on unions of intervals. This technique has real-world applications in the hard sciences, but has also been used in computer-assisted proofs. For two famous examples, we refer the interested reader to [6] for Hales' proof of the Kepler Conjecture on optimal sphere-packing in $\mathbb{R}^2$, and to [13] for Warwick's solution of Smale's 14th problem on the Lorenz attractor as a strange attractor.

As stated before, we consider extensions of the binary operations $+, -, \times$, and $\div$ as well as the unary operation $\sqrt{}$ defined on $\mathbb{R}$ to operations on unions of intervals of extended real numbers. For example if $[a, b], [c, d] \subseteq \mathbb{R}$, then we may use the following extensions of $+, -$, and $\times$:

$$\begin{aligned}
&[a, b] + [c, d] = [a + c, b + d], \\
&[a, b] - [c, d] = [a - d, b - c], \text{and} \\
&[a, b] \times [c, d] = [\min\{ac, ad, bc, bd\}, \max\{ac, ad, bc, bd\}] .
\end{aligned}$$

For $\div$, we must address the cases $0 \in [c, d]$ and $0 \notin [c, d]$. Here, we take the extension

$$[a, b] \div [c, d] = \left[\min\left\{\frac{a}{c}, \frac{a}{d}, \frac{b}{c}, \frac{b}{d}\right\}, \max\left\{\frac{a}{c}, \frac{a}{d}, \frac{b}{c}, \frac{b}{d}\right\}\right]$$

where

$$1 \div [c, d] = \begin{cases} \left[\min\{c^{-1}, d^{-1}\}, \max\{c^{-1}, d^{-1}\}\right], & 0 \notin [c, d] \\ \left[d^{-1}, +\infty\right], & \text{c=0} \\ \left[-\infty, c^{-1}\right], & d = 0 \\ \left[-\infty, \frac{1}{c}\right] \cup \left[\frac{1}{d}, +\infty\right], & c < 0 < d \end{cases} .$$

Additionally, we may let

$$\sqrt{[a, b]} = \begin{cases} \emptyset, & b < 0 \\ \left[\sqrt{\max\{0, a\}}, \sqrt{b}\right], & \text{othewise} \end{cases} .$$

When endpoints of $[a,b]$ and $[c,d]$ include $-\infty$ or $+\infty$, the definitions above must be modified slightly.

We use interval arithmetic to prove the strict upper bound $< 2/\sqrt{3}$, the maximum graphon spread claimed in Theorem 3.5.1, for any solutions to 15 of the 17 constrained optimization problems SPR_S stated in Lemma 3.5.3. The constraints in each SPR_S allow us to derive equations for the variables $(\alpha_i, f_i, g_i)_{i\in S}$ in terms of each other, and μ and ν. For the reader's convenience, we relocate these formulas and their derivations to Appendix 3.7.1. In the programs corresponding to each set $S \in \mathcal{S}_{17}$, we find we find two indices $i \in S \cap \{1,2,3,4\}$ and $j \in S \cap \{5,6,7\}$ such that for all $k \in S$, α_k, f_k, and g_k may be calculated, step-by-step, from α_i, α_j, μ, and ν. See Table 3.2 for each set $S \in \mathcal{S}_{17}$, organized by the chosen values of i and j.

	1	2	3	4
5	1|57	24|57 1|24|57	1|234|57	4|57 1|4|57
6	1|567	24|567 1|24|567	234|567 1|234|567	4|567 1|4|57
7	1|7	1|24|7	1|234|7	1|4|7

Table 3.2 The indices i, j corresponding to the search space used for SPR_S.

In in program corresponding to a set $S \in \mathcal{S}_{17}$, we search a carefully chosen set $\Omega \subseteq [0,1]^3 \times [-1,0]$ for values of $(\alpha_i, \alpha_j, \mu, \nu)$ which satisfy SPR_S. We first divide Ω into a grid of "boxes". Starting at depth 0, we test each box B for feasibility by assuming that $(\alpha_i, \alpha_j, \mu, \nu) \in B$ and that $\mu - \nu \geq 2/\sqrt{3}$. Next, we calculate α_k, f_k, and g_k for all $k \in S$ in interval arithmetic using the formulas from Section 3.7. When the calculation detects that a constraint of SPR_S is not satisfied, e.g., by showing that some α_k, f_k, or g_k lies in an empty interval, or by constraining $\sum_{i\in S} \alpha_i$ to a union of intervals which does not contain 1, then the box is deemed infeasible. Otherwise, the box is split into two boxes of equal dimensions, with the dimension of the cut alternating cyclically.

For each $S \in \mathcal{S}_{17}$, the program SPR_S has 3 norm constraints, $2|S|$ linear eigenvector constraints, $|S|$ elliptical constraints, $\binom{|S|}{2}$ inequality constraints, and $3|S|$ interval membership constraints. By using interval arithmetic, we have a computer-assisted proof of the following result.

Lemma 3.5.4. *Suppose* $S \in \mathcal{S}_{17} \setminus \{\{1,7\},\{4,5,7\}\}$*. Then any solution to* SPR_S *attains a value strictly less than* $2/\sqrt{3}$*.*

To better understand the role of interval arithmetic in our proof, consider the following example.

Example 3.5.5. *Suppose* μ, ν*, and* (α_i, f_i, g_i) *is a solution to* $SPR_{\{1,\ldots,7\}}$*. We show that* $(\alpha_3, \mu, \nu) \notin [.7, .8] \times [.9, 1] \times [-.2, -.1]$*. By Proposition 3.7.1,* $g_3^2 = \dfrac{\nu(\alpha_3 + 2\mu)}{\alpha_3(\mu+\nu) + 2\mu\nu}$*. Using interval arithmetic,*

$$\begin{aligned}
\nu(\alpha_3 + 2\mu) &= [-.2, -.1] \times \big([.7, .8] + 2 \times [.9, 1]\big) \\
&= [-.2, -.1] \times [2.5, 2.8] = [-.56, -.25], \text{ and} \\
\alpha_3(\mu+\nu) + 2\mu\nu &= [.7, .8] \times \big([.9, 1] + [-.2, -.1]\big) + 2 \times [.9, 1] \times [-.2, -.1] \\
&= [.7, .8] \times [.7, .9] + [1.8, 2] \times [-.2, -.1] \\
&= [.49, .72] + [-.4, -.18] = [.09, .54].
\end{aligned}$$

Thus

$$g_3^2 = \frac{\nu(\alpha_3 + 2\mu)}{\alpha_3(\mu+\nu) + 2\mu\nu} = [-.56, -.25] \div [.09, .54] = [-6.\overline{2}, -.4\overline{629}].$$

Since $g_3^2 \geq 0$*, we have a contradiction.*

Example 3.5.5 illustrates a number of key elements. First, we note that through interval arithmetic, we are able to provably rule out the corresponding region. However, the resulting interval for the quantity g_3^2 is over fifty times bigger than any of the input intervals. This growth in the size of intervals is common, and so, in some regions, fairly small intervals for variables are needed to provably illustrate the absence of a solution. For this reason, using a computer to complete this procedure is ideal, as doing millions of calculations by hand would be untenable.

However, the use of a computer for interval arithmetic brings with it another issue. Computers have limited memory, and therefore cannot represent all numbers in $\mathbb{R}^*$. Instead, a computer can only store a finite subset of numbers, which we will denote by $F \subsetneq \mathbb{R}^*$. This set F is not closed under the basic arithmetic operations, and so when some operation is performed and the resulting answer is not in F, some rounding procedure must be performed to choose an element of F to approximate the exact answer. This issue is the cause of roundoff error in floating point arithmetic, and must be treated in order to use computer-based interval arithmetic as a proof.

PyInterval is one of many software packages designed to perform interval arithmetic in a manner which accounts for this crucial feature of floating point arithmetic. Given some $x \in \mathbb{R}^*$, let $fl_-(x)$ be the largest $y \in F$ satisfying $y \leq x$, and $fl_+(x)$ be the smallest $y \in F$ satisfying $y \geq x$. Then, in order to maintain a mathematically accurate system of interval arithmetic on a computer, once an operation is performed, the resulting real interval $[a, b]$ is replaced by some interval or union of intervals containing $[fl_-(a), fl_+(b)]$. The programs which prove Lemma 3.5.4 can be found at [12].

3.5.3 Solving $\mathbf{SPR}_{457}$ and $\mathbf{SPR}_{17}$

Finally, we complete the second main result of this paper. Trusting the output of computer programs, the proof is self-contained.

Proof of Theorem 3.5.1. Let W be a graphon such that $\operatorname{spr}(W) = \max_{U \in \mathcal{W}} \operatorname{spr}(W)$. By Lemma 3.5.4, the following claim holds.

Claim A: Suppose $\operatorname{spr}(W) \geq 2/\sqrt{3}$. Then there exists a solution to one of the problems $\text{SPR}_{\{4,5,7\}}, \text{SPR}_{\{1,7\}}$ equal to $\operatorname{spr}(W)$.

We proceed by proving the following claims. First, let $T := \{(\varepsilon_1, \varepsilon_2) \in (-1/3, 2/3) \times (-2/3, 1/3) : \varepsilon_1 + \varepsilon_2 \in (0, 1)\}$, and for all $\varepsilon = (\varepsilon_1, \varepsilon_2) \in T$, let

$$M(\varepsilon) := \begin{bmatrix} 2/3 - \varepsilon_1 & 0 & 1/3 - \varepsilon_2 \\ 0 & 0 & 1/3 - \varepsilon_2 \\ 2/3 - \varepsilon_1 & \varepsilon_1 + \varepsilon_2 & 0 \end{bmatrix}.$$

As a motivation, suppose μ, ν, and $(\alpha_4, \alpha_5, \alpha_7)$ are part of a solution to $\mathrm{SPR}_{\{4,5,7\}}$ such that $\alpha_7 = 0$. Then with $\varepsilon := (\varepsilon_1, \varepsilon_2) = (2/3 - \alpha_5, 1/3 - \alpha_4)$, $\varepsilon \in T$ and μ, ν are the maximum and minimum eigenvalues of $M(\varepsilon)$, respectively. By the end of the proof, we show that any solution of $\mathrm{SPR}_{\{4,5,7\}}$ has $\alpha_7 = 0$.

To proceed, we prove the following claims.

Claim B: For all $\varepsilon \in T$, $M(\varepsilon)$ has two distinct positive eigenvalues and one negative eigenvalue.

Since $M(\varepsilon)$ is diagonalizable, it has 3 real eigenvalues which we may order as $\mu \geq \delta \geq \nu$. Since $\mu\delta\nu = \det(M(\alpha)) = -\alpha_4\alpha_5\alpha_7 \neq 0 < 0$, $M(\alpha)$ has an odd number of negative eigenvalues. Since $0 < \alpha_5 = \mu + \delta + \nu$, it follows that $\mu \geq \delta > 0 > \nu$. Finally, note by the Perron-Frobenius Theorem that $\mu > \delta$. This completes the proof of Claim B.

Next, we define the following quantities, treated as functions of ε for all $\varepsilon \in T$. For convenience, we suppress the argument "α" in most places. Let $k(x) = ax^3 + bx^2 + cx + d$ be the characteristic polynomial of $M(\varepsilon)$. By inspection,

$$a = 1 \qquad b = \varepsilon_1 - \frac{2}{3}$$

$$c = \frac{(3\varepsilon_2 + 2)(3\varepsilon_2 - 1)}{9} \qquad d = \frac{(\varepsilon_1 + \varepsilon_2)(3\varepsilon_1 - 2)(3\varepsilon_2 - 1)}{9}$$

Continuing, let

$$p := \frac{3ac - b^2}{3a^2} \qquad q := \frac{2b^3 - 9abc + 27a^2 d}{27a^3}$$

$$A := 2\sqrt{\frac{-p}{3}} \qquad B := \frac{-b}{3a}$$

$$\phi := \arccos\left(\frac{3q}{Ap}\right).$$

Let $S(\varepsilon)$ be the difference between the maximum and minimum eigenvalues of $M(\varepsilon)$. We show the following claim.

Claim C: For all $\varepsilon \in T$,

$$S(\varepsilon) = \sqrt{3} \cdot A(\varepsilon) \cdot \cos\left(\frac{2\phi(\varepsilon) - \pi}{6}\right).$$

Moreover, S is analytic on T.

Indeed, by Viéte's Formula, using the fact that $k(x, y)$ has exactly 3 distinct real roots, the quantities $a(\varepsilon), \ldots, \phi(x, y)$ are analytic on T. Moreover, the eigenvalues of $M(\varepsilon)$ are x_0, x_1, x_2 where, for all $k \in \{0, 1, 2\}$,

$$x_k(\varepsilon) = A(\varepsilon) \cdot \cos\left(\frac{\phi + 2\pi \cdot k}{3}\right) + B(\varepsilon).$$

Moreover, $x_0(\varepsilon), x_1(\varepsilon), x_2(\varepsilon)$ are analytic on T. For all $k, \ell \in \{1, 2, 3\}$, let

$$D(k, \ell, x) := \cos\left(x + \frac{2\pi k}{3}\right) - \cos\left(x + \frac{2\pi \ell}{3}\right)$$

For all $(k, \ell) \in \{(0, 1), (0, 2), (2, 1)\}$, note the trigonometric identities

$$D(k, \ell, x) = \sqrt{3} \cdot \begin{cases} \cos\left(x - \frac{\pi}{6}\right), & (k, \ell) = (0, 1) \\ \cos\left(x + \frac{\pi}{6}\right), & (k, \ell) = (0, 2) \\ \sin(x), & (k, \ell) = (2, 1) \end{cases}.$$

By graphical inspection, for all $x \in (0, \pi/3)$,

$$D(0, 1) > \max\{D(0, 2), D(2, 1)\} \geq \min\{D(0, 2), D(2, 1)\} \geq 0.$$

Since $A > 0$ and $\phi \in (0, \pi/3)$, the claimed equality holds. Since $x_0(\varepsilon), x_1(\varepsilon)$ are analytic, $S(\varepsilon)$ is analytic on T. This completes the proof of Claim C.

Next, we compute the derivatives of $S(\varepsilon)$ on T. For convenience, denote by A_i, ϕ_i, and S_i for the partial derivatives of A and ϕ by ε_i, respectively, for $i \in \{1, 2\}$. Furthermore, let

$$\psi(\varepsilon) := \frac{2\phi(\varepsilon) - \pi}{6}.$$

The next claim follows directly from Claim C.

Claim D: Suppose ε_0 is a local maximum of S on T. Then

$$\tan(\psi(\varepsilon^*)) = \frac{3A_1(\varepsilon^*)}{A(\varepsilon^*) \cdot \psi_1(\varepsilon^*)} = \frac{3A_2(\varepsilon^*)}{A(\varepsilon^*) \cdot \psi_2(\varepsilon^*)}$$

Moreover, each expression is analytic on T.

In claims E and F, we solve $\mathrm{SPR}_{\{4,5,7\}}$.

Claim E: If $(\alpha_4, \alpha_5, \alpha_7)$ is a solution to $\mathrm{SPR}_{\{4,5,7\}}$, then $0 \in \{\alpha_4, \alpha_5, \alpha_7\}$.

Let $(\alpha_4, \alpha_5, \alpha_7) := (1/3 - \varepsilon_2, 2/3 - \varepsilon_1, \varepsilon_1 + \varepsilon_2)$. Since S is analytic on T, it is sufficient to show that S has no local maxima on T. Suppose $\varepsilon*$ is a local maximum. Then by Claim D,

$$A_1(\varepsilon^*) \cdot \psi_2(\varepsilon^*) - A_2(\varepsilon^*) \cdot \psi_1(\varepsilon^*) = 0.$$

With the help of a computer algebra system, we note that $(A_1(\varepsilon) \cdot \psi_2(\varepsilon) - A_2(\varepsilon) \cdot \psi_1(\varepsilon))^2$ is a rational polynomial whose numerator is a multiple of $P(\varepsilon_1, \varepsilon_2)$ where

$$P(\varepsilon_1, \varepsilon_2) = 9\varepsilon_1^3 + 18\varepsilon_1^2\varepsilon_2 + 54\varepsilon_1\varepsilon_2^2 + 18\varepsilon_2^3 - 15\varepsilon_1^2 - 33\varepsilon_1\varepsilon_2 - 27\varepsilon_2^2 + 5\varepsilon_1 + \varepsilon_2.$$

Additionally, Claim D implies that for some integer k,

$$\frac{2\phi(\varepsilon^*) - \pi}{6} + \pi \cdot k = \arctan\left(\frac{3A_1(\varepsilon^*)}{A(\varepsilon^*) \cdot \psi_1(\varepsilon^*)}\right).$$

Using the definition of $\psi(\varepsilon)$, we see that

$$\cos\left(\arccos\left(\frac{3q(\varepsilon^*)}{A(\varepsilon^*) \cdot p(\varepsilon^*)}\right) + (6k-1)\pi\right) = \cos\left(6\arctan\left(\frac{3A_1(\varepsilon^*)}{A(\varepsilon^*) \cdot \psi_1(\varepsilon^*)}\right)\right).$$

Using the trigonometric identity

$$\cos\left(6\arctan(x)\right) = \frac{-(x^2+4x+1)(x^2-4x+1)(x+1)(x-1)}{(x^2+1)^3},$$

we obtain an equation $F(\varepsilon^*) = 0$ where $F(\varepsilon)$ is a rational polynomial. In particular, the numerator of $F(\varepsilon)$ is a constant multiple of $(3\varepsilon_1 - 2)^3 \cdot (\varepsilon_1 + \varepsilon_2) \cdot (3\varepsilon_2 - 1) \cdot Q(\varepsilon)$ where $Q(\varepsilon) = 4782969\varepsilon_1^{16} + \cdots (-266240)$ is a polynomial of degree 16 in $\varepsilon_1, \varepsilon_2$. Since $3\varepsilon_1^* - 2, \varepsilon_1^* + \varepsilon_2^*, 3\varepsilon_2^* - 1 \neq 0$, it follows that $Q(\varepsilon^*) = 0$. For brevity, we do not express Q explicitly.

To complete the proof of Claim E, it is sufficient to show that T contains no common zeroes of $P(\varepsilon)$ and $Q(\varepsilon)$. Again using a computer algebra system, we first find all common zeroes of P and Q on $\mathbb{R}^2$. Included are the rational solutions $(2/3, -2/3), (-1/3, 1/3), (0, 0), (2/3, 1/3)$, and $(2/3, -1/6)$ which do not lie in T. Furthermore, the solution $(1.2047\ldots, 0.0707\ldots)$ may also be eliminated. For the remaining 4 zeroes, $S_1, S_2 \neq 0$. This completes the proof of Claim E.

Next, we complete the following claim.

Claim F: If μ, ν, and $\alpha = (\alpha_4, \alpha_5, \alpha_7)$ is part of a solution to $\mathrm{SPR}_{\{4,5,7\}}$ such that $\mu - \nu \geq 1$, then $\alpha_7 = 0$.

By definition of $\mathrm{SPR}_{\{4,5,7\}}$, μ and ν are eigenvalues of the matrix

$$N(\alpha) := \begin{bmatrix} \alpha_5 & 0 & \alpha_4 \\ 0 & 0 & \alpha_4 \\ \alpha_5 & \alpha_7 & 0 \end{bmatrix}$$

. Furthermore, $N(\alpha)$ has characteristic polynomial

$$p(x) = x^3 - \alpha_5 x^2 - \alpha_4 \cdot (\alpha_5 + \alpha_7) + \alpha_4\alpha_5\alpha_7.$$

Recall that $\alpha_4 + \alpha_5 + \alpha_7 = 1$. By Claim E, $0 \in \{4, 5, 7\}$, and it follows that $p \in \{p_4, p_5, p_7\}$ where

$$p_4(x) := x^2 \cdot (x - \alpha_5),$$
$$p_5(x) := x \cdot (x^2 - \alpha_4(1 - \alpha_4)), \text{ and}$$
$$p_7(x) := x \cdot (x^2 - (1 - \alpha_4)x - \alpha_4(1 - \alpha_4)).$$

If $p = p_4$, then $\mu - \nu = \alpha_5 \leq 1$, and if $p = p_5$, then $\mu - \nu = 2\sqrt{\alpha_4(1 - \alpha_4)} \leq 1$. So $P = P_7$, which completes the proof of Claim F.

Finally, we complete the proof of the desired claim. Note that the

$$\begin{bmatrix} \alpha_5 & 0 & 0 \\ 0 & 0 & 0 \\ \alpha_5 & 1 - \alpha_5 & 0 \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} \alpha_5 & 0 \\ \alpha_5 & 1 - \alpha_5 \end{bmatrix}$$

have the same multiset of nonzero eigenvalues. By Claim F and the definition of $\mathrm{SPR}_{\{4,5,7\}}$ and $\mathrm{SPR}_{\{4,5\}}$, we have the following. Ifμ, ν, and $(\alpha_4, \alpha_5, \alpha_7)$ are part of a solution to $\mathrm{SPR}_{\{4,5,7\}}$, then $\alpha_7 = 0$ and the quantities μ, ν, and $(\alpha_4, 1 - \alpha_4)$ are part of a solution to $\mathrm{SPR}_{\{4,5\}}$. By setting $(\alpha_1', \alpha_7') := (\alpha_5, 1 - \alpha_5)$, it follows by inspection of the definition of $\mathrm{SPR}_{\{4,5\}}$ and $\mathrm{SPR}_{\{1,7\}}$ that μ, ν, and (α_1', α_7') are part of a solution to $\mathrm{SPR}_{\{1,7\}}$.

By Claim A, it suffices to demonstrate the uniqueness of the desired solution μ, ν, and $(\alpha_i, f_i, g_i)_{i\in\{1,7\}}$ to $\mathrm{SPR}_{\{1,7\}}$. Indeed, we first note that with

$$N(\alpha) := \begin{bmatrix} \alpha_1 & 1 - \alpha_1 \\ \alpha_1 & 0 \end{bmatrix},$$

the quantities μ and ν are precisely the eigenvalues of the characteristic polynomial

$$p(x) = x^2 - \alpha_1 x - \alpha_1(1 - \alpha_1).$$

In particular,

$$\mu = \frac{\alpha_1 + \sqrt{\alpha_1(4 - 3\alpha_1)}}{2}, \quad \nu = \frac{\alpha_1 - \sqrt{\alpha_1(4 - 3\alpha_1)}}{2},$$

and

$$\mu - \nu = \sqrt{\alpha_1(4 - 3\alpha_1)}.$$

Optimizing, it follows that μ, ν, and (α_1, α_7) match those from the statement of Theorem 3.5.1. By considering the equations corresponding to μ and ν as eigenvalues of $N(2/3, 1/3)$ and the norm constrains on the functions f and g, this completes the proof. □

3.6 From graphons to graphs

In this section, we show that Theorem 3.5.1 implies Conjecture 1 for all n sufficiently large; that is, the solution to the problem of maximizing the spread of a graphon implies the solution to the problem of maximizing the spread of a graph for sufficiently large n.

Theorem 3.6.1. *There exists a constant N so that the following holds: Suppose G is a graph on $n \geq N$ vertices with maximum spread; then G is the join of a clique on $\lfloor 2n/3 \rfloor$ vertices and an independent set on $\lceil n/3 \rceil$ vertices.*

The outline for our argument is as follows. First, we define the spread-maximum graphon W as in Theorem 3.5.1. Let $\{G_n\}$ be any sequence where each G_n is a spread-maximum graph on n vertices and denote by $\{W_n\}$ the corresponding sequence of graphons. We show that, after applying measure-preserving transformations to each W_n, the extreme eigenvalues and eigenvectors of each W_n converge suitably to those of W. It follows for n sufficiently large that except for $o(n)$ vertices, G_n is a join of a clique of $2n/3$ vertices and an independent set of $n/3$ vertices. Using results from Section 3.2, we precisely estimate the extreme eigenvector entries on this $o(n)$ set. Finally, Proposition 3.6.4 completes the proof.

Before proceeding with the proof, we state the following version of the Davis-Kahan theorem [4], stated for graphons.

Corollary 3.6.2. *Suppose $W, W' : [0,1]^2 \to [0,1]$ are graphons Let μ be an eigenvalue of W with f a corresponding unit eigenfunction. Let $\{h_k\}$ be an orthonormal eigenbasis for W' with corresponding eigenvalues $\{\mu'_k\}$. Suppose that $|\mu'_k - \mu| > \delta$ for all $k \neq 1$. Then*

$$\sqrt{1 - \langle h_1, f\rangle^2} \leq \frac{\|A_{W'-W} f\|_2}{\delta}.$$

Before proving Theorem 3.6.1, we prove the following lemmas. For all nonnegative integers n_1, n_2, n_3, let $G(n_1, n_2, n_3) := (K_{n_1} \coprod K_{n_2}^c) \vee K_{n_3}^c$.

Lemma 3.6.3. *For all positive integers integers n, let G_n denote a graph on n vertices which maximizes spread. Then $G_n = G(n_1, n_2, n_3)$ for some nonnegative integers n_1, n_2, n_3 such that $n_1 = (2/3 + o(1))n$, $n_2 = o(n)$, and $n_3 = (1/3 + o(1))n$.*

Proof. Our argument outline is:

1. show that the eigenvectors for the spread-extremal graphs resemble the eigenfunctions of the spread-extremal graphon in an L_2 sense

2. show that with the exception of a small proportion of vertices, a spread-extremal graph is the join of a clique and an independent set

Let $\mathcal{P} := [0, 2/3]$ and $\mathcal{N} := [0,1] \setminus \mathcal{P}$. By Theorem 3.5.1, the graphon W which is the indicator function of the set $[0,1]^2 \setminus \mathcal{N}^2$ maximizes spread. Denote by μ and ν its maximum and minimum eigenvalues, respectively. For every positive integer n, let G_n denote a graph on n vertices which maximizes spread, let W_n be any stepgraphon corresponding to G_n, and let μ_n and ν_n denote the maximum and minimum eigenvalues of W_n, respectively. By Theorems 3.3.2 and 3.5.1, and compactness of $\hat{\mathcal{W}}$,

$$\max\{|\mu - \mu_n|, |\nu - \nu_n|, \delta_\square(W, W_n)\} \to 0.$$

Moreover, we may apply measure-preserving transformations to each W_n so that without loss of generality, $\|W - W_n\|_\square \to 0$. As in Theorem 3.5.1, let f and g be unit eigenfunctions which take values f_1, f_2, g_1, g_2. Furthermore, let φ_n be a nonnegative unit μ_n-eigenfunction for W_n and let ψ_n be a ν_n-eigenfunction for W_n.

We show that without loss of generality, $\varphi_n \to f$ and $\psi_n \to g$ in the L_2 sense. Since μ is the only positive eigenvalue of W and it has multiplicity 1, taking $\delta := \mu/2$, Corollary 3.6.2 implies that

$$\begin{aligned}
1 - \langle f, \varphi_n \rangle^2 &\leq \frac{4\|A_{W-W_n}\|_2^2}{\mu^2} \\
&= \frac{4}{\mu^2} \cdot \langle A_{W-W_n} f, A_{W-W_n} f \rangle \\
&\leq \frac{4}{\mu^2} \cdot \|A_{W-W_n} f\|_1 \cdot \|A_{W-W_n} f\|_\infty \\
&\leq \frac{4}{\mu^2} \cdot (\|A_{W-W_n}\|_{\infty \to 1} \|f\|_\infty) \cdot \|f\|_\infty \\
&= \frac{16\|W - W_n\|_\square \cdot \|f\|_\infty^2}{\mu^2}
\end{aligned}$$

Since $\|f\|_\infty \leq 1/\mu$, this proves the first claim. The second claim follows by replacing f with g, and μ with $|\nu|$.

Note: For the remainder of the proof, we will introduce quantities $\varepsilon_i > 0$ in lieu of writing complicated expressions explicitly. When we introduce a new ε_i, we will instead remark that as long as $\varepsilon_0, \ldots, \varepsilon_{i-1}$ are sufficiently small, then ε_i can be made sufficiently small enough to meet some other conditions.

Let $\varepsilon_0 > 0$ and for all $n \geq 1$, define

$$\begin{aligned}
\mathcal{P}_n &:= \{x \in [0,1] : |\varphi_n(x) - f_1| < \varepsilon_0 \text{ and } |\psi_n(x) - g_1| < \varepsilon_0\}, \\
\mathcal{N}_n &:= \{x \in [0,1] : |\varphi_n(x) - f_2| < \varepsilon_0 \text{ and } |\psi_n(x) - g_2| < \varepsilon_0\}, \text{ and} \\
\mathcal{E}_n &:= [0,1] \setminus (\mathcal{P}_n \cup \mathcal{N}_n).
\end{aligned}$$

Since

$$\begin{aligned}
\int_{|\varphi_n - f| \geq \varepsilon_0} |\varphi_n - f|^2 &\leq \int |\varphi_n - f|^2 \to 0, \text{ and} \\
\int_{|\psi_n - g| \geq \varepsilon_0} |\psi_n - g|^2 &\leq \int |\psi_n - g|^2 \to 0,
\end{aligned}$$

it follows that

$$\max\{m(\mathcal{P}_n\setminus\mathcal{P}), m(\mathcal{N}_n\setminus\mathcal{N}), m(\mathcal{E}_n)\}\to 0.$$

For all $u\in V(G_n)$, let S_u be the subinterval of $[0,1]$ corresponding to u in W_n, and denote by φ_u and ψ_u the constant values of φ_n on S_u. For convenience, we define the following discrete analogues of $\mathcal{P}_n,\mathcal{N}_n,\mathcal{E}_n$:

$$\begin{aligned}
P_n &:= \{u\in V(G_n) : |\varphi_u - f_1| < \varepsilon_0 \text{ and } |\psi_u - g_1| < \varepsilon_0\},\\
N_n &:= \{u\in V(G_n) : |\varphi_u - f_2| < \varepsilon_0 \text{ and } |\psi_u - g_2| < \varepsilon_0\}, \text{ and}\\
E_n &:= V(G_n)\setminus(P_n\cup N_n).
\end{aligned}$$

Let $\varepsilon_1>0$. By Lemma 3.2.6 and using the fact that $\mu_n\to\mu$ and $\nu_n\to\nu$,

$$\left|\mu\varphi_u^2-\nu\psi_u^2-(\mu-\nu)\right|<\varepsilon_1 \quad \text{for all } u\in V(G_n) \tag{3.10}$$

for all n sufficiently large.

Let $\varepsilon_0'>0$. For the remainder of the proof, we show the following claim.

Claim I. Suppose ε_0 is sufficiently small and n is sufficiently large in terms of ε_0'. Then for all $v\in E_n$,

$$\max\left\{\left|\varphi_v-\frac{f_2}{3\mu}\right|,\left|\psi_v-\frac{g_2}{3\nu}\right|\right\}<\varepsilon_0'. \tag{3.11}$$

Indeed, suppose $v\in E_n$ and let

$$U_n := \{w\in V(G_n) : vw\in E(G_n)\} \quad \text{and} \quad \mathcal{U}_n := \bigcup_{w\in U_n} S_w.$$

We take two cases, depending on the sign of ψ_v.

Case A: $\psi_v\geq 0$.

Recall that $f_2>0>g_2$. Furthermore, $\varphi_v\geq 0$ and by assumption, $\psi_v\geq 0$. It follows that for all n sufficiently large, $f_2\varphi_v-g_2\psi_v>0$, so by Proposition 3.2.3, $N_n\subseteq U_n$. Since φ_n is a μ_n-eigenfunction for K_n,

$$\begin{aligned}
\mu_n\varphi_v &= \int_{y\in[0,1]} K_n(x,y)\varphi_n(y)\\
&= \int_{y\in\mathcal{P}_n\cap\mathcal{U}_n}\varphi_n(y)+\int_{y\in\mathcal{N}_n}\varphi_n(y)+\int_{y\in\mathcal{E}_n\cap\mathcal{U}_n}\varphi_n(y).
\end{aligned}$$

Similarly,

$$\begin{aligned}\nu_n \psi_v &= \int_{y\in[0,1]} K_n(x,y)\psi_n(y)\\ &= \int_{y\in\mathcal{P}_n\cap\mathcal{U}_n} \psi_n(y) + \int_{y\in\mathcal{N}_n} \psi_n(y) + \int_{y\in\mathcal{E}_n\cap\mathcal{U}_n} \psi_n(y).\end{aligned}$$

Let $\rho_n := \lambda(\mathcal{P}_n \cap \mathcal{U}_n)$. Note that for all $\varepsilon_2 > 0$, as long as n is sufficiently large and ε_1 is sufficiently small, then

$$\max\left\{\left|\varphi_v - \frac{3\rho_n f_1 + f_2}{3\mu}\right|, \left|\psi_v - \frac{3\rho_n g_1 + g_2}{3\nu}\right|\right\} < \varepsilon_2. \tag{3.12}$$

Let $\varepsilon_3 > 0$. By Equations (3.10) and (3.12) and with $\varepsilon_1, \varepsilon_2$ sufficiently small,

$$\left|\mu \cdot \left(\frac{3\rho_n f_1 + f_2}{3\mu}\right)^2 - \nu \cdot \left(\frac{3\rho_n g_1 + g_2}{3\nu}\right)^2 - (\mu - \nu)\right| < \varepsilon_3.$$

Substituting the values of f_1, f_2, g_1, g_2 from Theorem 3.5.1 and simplifying, it follows that

$$\left|\frac{\sqrt{3}}{2} \cdot \rho_n(3\rho_n - 2)\right| < \varepsilon_3$$

Let $\varepsilon_4 > 0$. It follows that if n is sufficiently large and ε_3 is sufficiently small, then

$$\min\{\rho_n, |2/3 - \rho_n|\} < \varepsilon_4. \tag{3.13}$$

Combining Equations (3.12) and (3.13), it follows that with $\varepsilon_2, \varepsilon_4$ sufficiently small, then

$$\max\left\{\left|\varphi_v - \frac{f_2}{3\mu}\right|, \left|\psi_v - \frac{g_2}{3\mu}\right|\right\} < \varepsilon_0', \text{ or}$$
$$\max\left\{\left|\varphi_v - \frac{2f_1 + f_2}{3\mu}\right|, \left|\psi_v - \frac{2g_1 + g_2}{3\mu}\right|\right\} < \varepsilon_0'.$$

Note that

$$f_1 = \frac{2f_1 + f_2}{3\mu} \quad \text{and} \quad g_1 = \frac{2g_1 + g_2}{3\nu}.$$

Since $v \in E_n$, the second inequality does not hold. This completes the proof of Claim A.

Case B: $\psi_v < 0$.

Recall that $f_1 > g_1 > 0$. Furthermore, $\varphi_v \geq 0$ and by assumption, $\psi_v < 0$. It follows that for all n sufficiently large, $f_1\varphi_v - g_1\psi_v > 0$, so by Theorem 3.2.3, $P_n \subseteq U_n$. Since φ_n is a

μ_n-eigenfunction for K_n,

$$\begin{aligned}\mu_n\varphi_v &= \int_{y\in[0,1]} K_n(x,y)\varphi_n(y)\\ &= \int_{y\in\mathcal{N}_n\cap\mathcal{U}_n}\varphi_n(y) + \int_{y\in\mathcal{P}_n}\varphi_n(y) + \int_{y\in\mathcal{E}_n\cap\mathcal{U}_n}\varphi_n(y).\end{aligned}$$

Similarly,

$$\begin{aligned}\nu_n\psi_v &= \int_{y\in[0,1]} K_n(x,y)\psi_n(y)\\ &= \int_{y\in\mathcal{N}_n\cap\mathcal{U}_n}\psi_n(y) + \int_{y\in\mathcal{P}_n}\psi_n(y) + \int_{y\in\mathcal{E}_n\cap\mathcal{U}_n}\psi_n(y).\end{aligned}$$

Let $\rho_n := \lambda(\mathcal{N}_n\cap\mathcal{U}_n)$. Note that for all $\varepsilon_5 > 0$, as long as n is sufficiently large and ε_1 is sufficiently small, then

$$\max\left\{\left|\varphi_v - \frac{f_1+3\rho_n f_2}{3\mu}\right|, \left|\psi_v - \frac{g_1+3\rho_n g_2}{3\nu}\right|\right\} < \varepsilon_5. \tag{3.14}$$

Let $\varepsilon_6 > 0$. By Equations (3.10) and (3.14) and with $\varepsilon_1, \varepsilon_2$ sufficiently small,

$$\left|\mu\cdot\left(\frac{f_1+3\rho_n f_2}{3\mu}\right)^2 - \nu\cdot\left(\frac{g_1+3\rho_n g_2}{3\nu}\right)^2 - (\mu-\nu)\right| < \varepsilon_6.$$

Substituting the values of f_1, f_2, g_1, g_2 from Theorem 3.5.1 and simplifying, it follows that

$$\left|2\sqrt{3}\cdot\rho_n(3\rho_n - 1)\right| < \varepsilon_6$$

Let $\varepsilon_7 > 0$. It follows that if n is sufficiently large and ε_6 is sufficiently small, then

$$\min\left\{\rho_n, |1/3-\rho_n|\right\} < \varepsilon_7. \tag{3.15}$$

Combining Equations (3.12) and (3.15), it follows that with $\varepsilon_2, \varepsilon_4$ sufficiently small, then

$$\begin{gathered}\max\left\{\left|\varphi_v - \frac{2f_1}{3\mu}\right|, \left|\psi_v - \frac{2g_1}{3\mu}\right|\right\} < \varepsilon_0', \text{ or}\\ \max\left\{\left|\varphi_v - \frac{2f_1+f_2}{3\mu}\right|, \left|\psi_v - \frac{2g_1+g_2}{3\mu}\right|\right\} < \varepsilon_0'.\end{gathered}$$

Again, note that

$$f_1 = \frac{2f_1+f_2}{3\mu} \quad\text{and}\quad g_1 = \frac{2g_1+g_2}{3\nu}.$$

Since $v \in E_n$, the second inequality does not hold.

Similarly, note that

$$f_2 = \frac{2f_1}{3\mu} \quad \text{and} \quad g_2 = \frac{2g_1}{3\nu}.$$

Since $v \in E_n$, the first inequality does not hold, a contradiction. So Claim I holds.

Before completing the proof of the main result, we observe the following.

Claim II. For all n sufficiently large, G_n is the join of a an independent set N_n with a disjoint union of a clique P_n and an independent set E_n. As above, we let $\varepsilon_0, \varepsilon_0' > 0$ be arbitrary. By definition of P_n and N_n and by Equation (3.11) from Claim I, then for all n sufficiently large,

$$\begin{aligned} \max\{|\varphi_v - f_1|, |\psi_v - g_1|\} &< \varepsilon_0 && \text{for all } v \in P_n \\ \max\left\{\left|\varphi_v - \frac{f_2}{3\mu}\right|, \left|\psi_v - \frac{g_2}{3\nu}\right|\right\} &< \varepsilon_0' && \text{for all } v \in E_n \\ \max\{|\varphi_v - f_2|, |\psi_v - g_2|\} &< \varepsilon_0 && \text{for all } v \in P_n \end{aligned}$$

With rows and columns respectively corresponding to the vertex sets P_n, E_n, and N_n, we note the following inequalities: Indeed, note the following inequalities:

<table>
<tr><td>$f_1^2 > g_1^2$</td><td>$f_1 \cdot \frac{f_2}{3\mu} < g_1 \cdot \frac{g_2}{3\nu}$</td><td>$f_1 f_2 > g_1 g_2$</td></tr>
<tr><td></td><td>$\left(\frac{f_2}{3\mu}\right)^2 < \left(\frac{g_2}{3\nu}\right)^2$</td><td>$\frac{f_2}{3\mu} \cdot f_2 > \frac{g_2}{3\nu}$</td></tr>
<tr><td></td><td></td><td>$f_2^2 < g_2^2$</td></tr>
</table>

.

Let $\varepsilon_0, \varepsilon_0'$ be sufficiently small. Then for all n sufficiently large and for all $u, v \in V(G_n)$, then $\varphi_u \varphi_v - \psi_u \psi_v < 0$ if and only if $u, v \in E_n$, $u, v \in N_n$, or $(u, v) \in (P_n \times E_n) \cup (E_n \times P_n)$. By Lemma 3.2.1, Claim II holds. Altogether, this completes the proof. □

Lemma 3.6.4. *For all nonnegative integers r, s, t, let $G(n_1, n_2, n_3) := (K_{n_1} \cup K_{n_2}^c) \vee K_{n_3}^c$. Then for all n sufficiently large, the following holds. If $spr(G(n_1, n_2, n_3))$ is maximized subject to the constraint, then $n_1 + n_2 + n_3 = n$, then $n_2 = 0$.*

Proof. First, we make a general definition. For all $\varepsilon_1, \varepsilon_2, z \in \mathbb{R}$, let

$$M_z(\varepsilon_1, \varepsilon_2) := \begin{bmatrix} \frac{2}{3} - \varepsilon_1 - z & 0 & \frac{1}{3} - \varepsilon_2 \\ 0 & 0 & \frac{1}{3} - \varepsilon_2 \\ \frac{2}{3} - \varepsilon_1 & \varepsilon_1 + \varepsilon_2 & 0 \end{bmatrix}.$$

Since $M_z(\varepsilon_1, \varepsilon_2)$ is diagonalizable, we may let $S_z(\varepsilon_1, \varepsilon_2)$ be the difference between the maximum and minimum eigenvalues of $M_z(\varepsilon_1, \varepsilon_2)$.

Let $\mathbb{N}$ denote the set of nonnegative integers. In order, we consider the optimization problems $\mathcal{P}_{z,C}$ defined for all $z \geq 0$ and all $C > 0$ by

$$(\mathcal{P}_{z,C}) : \begin{cases} \max & S_z(\varepsilon_1, \varepsilon_2) \\ \text{s.t.} & \varepsilon_1, \varepsilon_2 \in [-C, C] \end{cases}$$

and $\mathcal{Q}_n$ defined for all $n \in \mathbb{N}$ by

$$(\mathcal{Q}_n) : \begin{cases} \max & S_z(2/3 - n_1/n, 1/3 - n_3/n) \\ \text{s.t.} & n_1, n_3 \in \mathbb{N} \\ & n_1 + n_3 \leq n \\ & 0 \leq (2/3 - n_1/n) + (1/3 - n_3/n) \end{cases}.$$

Note that $\mathcal{Q}_n$ is equivalent to the problem of maximizing $\text{spr}(G(n_1, n_2, n_3))$ subject to the constraint that $n_1 + n_2 + n_3 = n$. If $G = G(n_1, n_2, n_3)$ and

$$\left(\frac{n_1}{n}, \frac{n_2}{n}, \frac{n_3}{n}\right) = \left(\frac{2}{3} - \varepsilon_1, \varepsilon_1 + \varepsilon_2, \frac{1}{3} - \varepsilon_2\right),$$

then $n \cdot M_{n^{-1}}(\varepsilon_1, \varepsilon_2)$ is the "reduced" matrix for A_G and thus they same maximum and minimum eigenvalues and the same spread. To complete the proof, we solve $\mathcal{P}_{z,C}$ for some small constant C and all $z > 0$ sufficiently small. Appealing to concavity, we deduce that for all n sufficiently large, $\mathcal{Q}$ has a unique solution (n_1^*, n_3^*), and moreover, $n_1^* + n_3^* = n$.

First, we find $S_z(\varepsilon_1, \varepsilon_3)$ using Viète's Formula. In doing so, we define functions $k_z(\varepsilon_1, \varepsilon_2; x), \ldots, \delta_z(\varepsilon_1, \varepsilon_2)$. To ease the burden on the reader, we suppress the subscript z and the arguments $\varepsilon_1, \varepsilon_2$ when convenient and unambiguous. Let $k(x) = ax^3 + bx^2 + cx + d$ be the characteristic polynomial of $M_z(\varepsilon_1, \varepsilon_2)$. By inspection,

$$a = 1 \qquad b = \varepsilon_1 + z - \frac{2}{3}$$

$$c = \frac{(3\varepsilon_2 + 2)(3\varepsilon_2 - 1)}{9} \qquad d = \frac{(\varepsilon_1 + \varepsilon_2)(3\varepsilon_1 + 3z - 2)(3\varepsilon_2 - 1)}{9}$$

Continuing, let

$$p := \frac{3ac - b^2}{3a^2} \qquad q := \frac{2b^3 - 9abc + 27a^2 d}{27a^3}$$

$$A := 2\sqrt{\frac{-p}{3}} \qquad B := \frac{-b}{3a}$$

$$\phi := \arccos\left(\frac{3q}{Ap}\right).$$

By Viète's Formula, the roots of $k_z(\varepsilon_1, \varepsilon_2; x)$ are the suggestively defined quantities:

$$\mu := A\cos\left(\frac{\phi}{3}\right) + B \qquad \nu := A\cos\left(\frac{\phi + 2\pi}{3}\right) + B$$

$$\delta := A\cos\left(\frac{\phi + 4\pi}{3}\right) + B.$$

First, We prove the following claim.

Claim A: If $(\varepsilon_1, \varepsilon_2, z)$ is sufficiently close to $(0, 0, 0)$, then

$$S_z(\varepsilon_1, \varepsilon_2) = A_z(\varepsilon_1, \varepsilon_2)\sqrt{3} \cdot \cos\left(\frac{2\phi_z(\varepsilon_1, \varepsilon_2) - \pi}{6}\right). \tag{3.16}$$

Indeed, suppose $z > 0$ and $z \to 0$. Then for all $(\varepsilon_1, \varepsilon_2) \in (-3z, 3z)$, $\varepsilon_1, \varepsilon_2 \to 0$. With the help of a computer algebra system, we substitute in $z = 0$ and $\varepsilon_1, \varepsilon_2 = 0$ to find the limits:

$$(a, b, c, d) \to \left(1, \frac{-2}{3}, \frac{-2}{9}, 0\right)$$

$$(p, q) \to \left(\frac{-10}{27}, \frac{-52}{729}\right)$$

$$(A, B, \phi) \to \left(\frac{2\sqrt{10}}{9}, \frac{2}{9}, \arccos\left(\frac{13\sqrt{10}}{50}\right)\right).$$

Using a computer algebra system, these substitutions imply that

$$(\mu, \nu, \delta) \to (0.9107\ldots, -0.2440\ldots, 0.)$$

So for all z sufficiently small, $S = \mu - \nu$. After some trigonometric simplification,

$$\mu - \nu = A \cdot \left(\cos\left(\frac{\phi}{3}\right) - \cos\left(\frac{\phi + 2\phi}{3}\right) \right) = A\sqrt{3} \cdot \cos\left(\frac{2\phi - \pi}{6}\right)$$

and Equation (3.16). This completes the proof of Claim A.

Now we prove the following claim.

Claim B: There exists a constants $C_0' > 0$ such that the following holds. If $|z|$ is sufficiently small, then S_z is concave-down on $[-C_0, C_0]^2$ and strictly decreasing on $[-C_0, C_0]^2 \setminus [-C_0 z, C_0 z]^2$.

First, we define

$$D_z(\varepsilon_1, \varepsilon_2) := \left(\frac{\partial^2 S_z}{\partial \varepsilon_1^2} \cdot \frac{\partial^2 S_z}{\partial \varepsilon_2^2} - \left(\frac{\partial^2 S_z}{\partial \varepsilon_1 \partial \varepsilon_2} \right)^2 \right) \Bigg|_{(\varepsilon_1, \varepsilon_2, z)}.$$

As a function of $(\varepsilon_1, \varepsilon_2)$, D_z is the determinant of the Hessian matrix of S_z. Using a computer algebra system, we note that

$$D_0(0,0) = -22.5\ldots, \quad \text{and}$$
$$\left(\frac{\partial^2 S}{\partial \varepsilon_1^2}, \frac{\partial^2 S}{\partial \varepsilon_1 \partial \varepsilon_2}, \frac{\partial^2 S}{\partial \varepsilon_2^2} \right) \Bigg|_{(0,0,0)} = (-8.66\ldots, -8.66\ldots, -11.26\ldots).$$

Since S is analytic at $(0,0,0)$, there exist constants $C_1, C_2 > 0$ such that the following holds. For all $z \leq C_1$, all $(\varepsilon_1, \varepsilon_2) \in [-C_1, C_1]^2$, and any unit vectors $\mathbf{u}, \mathbf{v} \in \mathbb{R}$,

$$\frac{\partial^2 S}{\partial \mathbf{u} \partial \mathbf{v}} \Bigg|_{(\varepsilon_1, \varepsilon_2, z)} \leq -C_2.$$

In particular, S_z is concave-down on $[-C_1, C_1]^2$ for all $z > 0$ sufficiently small. So the first claim holds.

For the second claim, note the following. Since S is analytic at $(0,0,0)$, there exists a constant $0 < C_3 < C_1$ and another constant $C_4 > 0$ such for all $z < C_3$ and all $(\varepsilon_1, \varepsilon_2) \in [-C_3, C_3]^2$,

$$\frac{\partial^2 S}{\partial z \partial \varepsilon_i} \leq C_4.$$

Since $(0,0)$ is a local maximum of S_0,

$$\begin{aligned}\left.\frac{\partial S}{\partial \varepsilon_i}\right|_{(\varepsilon_1,\varepsilon_2,z)} &= \left.\frac{\partial S}{\partial \varepsilon_i}\right|_{(0,0,0)} + \int_{w=0}^{z} \left.\frac{\partial^2 S}{\partial z \partial \varepsilon_i}\right|_{(0,0,w)} dw \\ &\quad + \int_{\mathbf{u}=(0,0)}^{(\varepsilon_1,\varepsilon_2)} \left.\frac{\partial^2 S}{\partial \mathbf{u} \partial \varepsilon_i}\right|_{(\mathbf{u},z)} d\mathbf{u} \\ &\leq C_4 \cdot z - C_2 \cdot \|(\varepsilon_1,\varepsilon_2)\|_2.\end{aligned}$$

Since $C_2, C_4 > 0$, this completes the proof of Claim B.

Next, we prove the following claim.

Claim C: If z is sufficiently small, then $\mathcal{P}_{z,C_0}$ is solved by a unique point $(\varepsilon_1^*,\varepsilon_2^*) = (\varepsilon_1^*(z),\varepsilon_2^*(z))$. Moreover as $z \to 0$,

$$(\varepsilon_1^*,\varepsilon_2^*) = \left((1+o(z))\,\frac{7z}{30}, (1+o(z))\,\frac{-z}{3}\right). \tag{3.17}$$

Indeed, the existence of a unique maximum $(\varepsilon_1^*,\varepsilon_2^*)$ on $[-C_0,C_0]^2$ follows from the fact that S_z is strictly concave-down and bounded on $[-C_0,C_0]^2$ for all z sufficiently small. Since S_z is strictly decreasing on $[-C_0,C_0]^2 \setminus (-C_0z, C_0z)^2$, it follows that $(\varepsilon_1^*,\varepsilon_2^*) \in (-C_0z, C_0z)$. For the second claim, note that since S is analytic at $(0,0,0)$,

$$\left.\frac{\partial S}{\partial \varepsilon_1}\right|_{(\varepsilon_1^*,\varepsilon_2^*,z)} = \left.\frac{\partial S}{\partial \varepsilon_2}\right|_{(\varepsilon_1^*,\varepsilon_2^*,z)} = 0.$$

Let

$$\tau_i := \frac{3 \cdot \dfrac{\partial A}{\partial \varepsilon_i}}{A \cdot \dfrac{\partial \phi}{\partial \varepsilon_i}}$$

for both $i = 1$ and $i = 2$ Then by Equation (3.16),

$$\arctan(\tau_i)\big|_{(\varepsilon_1^*,\varepsilon_2^*,z)} = \left.\frac{2\phi - \pi}{6}\right|_{(\varepsilon_1^*,\varepsilon_2^*,z)}$$

for both $i = 1$ and $i = 2$. We first consider linear approximation of the above quantities under the limit $(\varepsilon_1,\varepsilon_2,z) \to (0,0,0)$. Here, we write $f(\varepsilon_1,\varepsilon_2,z) \sim g(\varepsilon_1,\varepsilon_2,z)$ to mean that

$$f(\varepsilon_1,\varepsilon_2,z) = (1 + o(\max\{|\varepsilon_1|,|\varepsilon_2|,|z|\})) \cdot g(\varepsilon_1,\varepsilon_2,z).$$

With the help of a computer algebra system, we note that

$$\arctan(\tau_1) \sim \frac{-78\varepsilon_1 - 96\varepsilon_2 - 3z - 40\arctan\left(\frac{1}{3}\right)}{40}$$
$$\arctan(\tau_2) \sim \frac{-64\varepsilon_1 - 103\varepsilon_2 - 14z - 20\arctan\left(\frac{1}{3}\right)}{20}$$
$$\frac{2\phi - \pi}{6} \sim \frac{108\varepsilon_1 + 81\varepsilon_2 + 18z + 20\arccos\left(\frac{13\sqrt{10}}{50}\right) - 10\pi}{60}.$$

By inspection, the constant terms match due to the identity

$$-\arctan\left(\frac{1}{3}\right) = \frac{1}{3}\arccos\left(\frac{13\sqrt{10}}{50}\right) - \frac{\pi}{6}.$$

Since $\max\{|\varepsilon_1^*|, |\varepsilon_2^*|\} \leq C_0 z$, replacing $(\varepsilon_1, \varepsilon_2)$ with $(\varepsilon_1^*, \varepsilon_2^*)$ implies that

$$\frac{-78\varepsilon_1^* - 96\varepsilon_2^* - 3z}{2} = (1 + o(z)) \cdot (36\varepsilon_1^* + 27\varepsilon_2^* + 6z), \quad \text{and}$$
$$-64\varepsilon_1^* - 103\varepsilon_2^* - 14z = (1 + o(z)) \cdot (36\varepsilon_1^* + 27\varepsilon_2^* + 6z)$$

as $z \to 0$. After applying Gaussian Elimination to this 3-variable system of 2 equations, it follows that

$$(\varepsilon_1^*, \varepsilon_2^*) = \left((1 + o(z)) \cdot \frac{7z}{30}, (1 + o(z)) \cdot \frac{-z}{3}\right).$$

This completes the proof of Claim C.

For the next step, we prove the following claim.

Claim D: For all n sufficiently large, $\mathcal{Q}_n$ is solved by a unique point (n_1^*, n_3^*). Moreover, $n_1^* + n_3^* = n$.

Note by Lemma 3.6.3 that for all n sufficiently large,

$$\max\left\{\left|\frac{n_1}{n} - \frac{2}{3}\right|, \left|\frac{n_3}{n} - \frac{1}{3}\right|\right\} \leq C_0.$$

Moreover, by Claim C, $\mathcal{P}_{n^{-1}}$ is solved uniquely by

$$(\varepsilon_1^*, \varepsilon_2^*) = \left((1 + o(z)) \cdot \frac{7}{30n}, (1 + o(z)) \cdot \frac{-1}{3n}\right).$$

Since

$$\frac{2n}{3} - n \cdot \varepsilon_1^* = \frac{2n}{3} - (1 + o(1)) \cdot \frac{7}{30}$$

and $7/30 < 1/3$, it follows for n sufficiently large that $2n/3 - n \cdot \varepsilon_1^* \in S_1$ where

$$I_1 = \begin{cases} \left(\frac{2n}{3} - 1, \frac{2n}{3}\right), & 3 \mid n \\ \left(\left\lfloor \frac{2n}{3} \right\rfloor, \left\lceil \frac{2n}{3} \right\rceil\right), & 3 \nmid n \end{cases}.$$

Similarly since

$$n \cdot (\varepsilon_1^* + \varepsilon_2^*) = (1 + o(1)) \cdot \left(\frac{7}{30} - \frac{1}{3}\right) = (1 + o(1)) \cdot \frac{-1}{10}$$

and $1/10 < 1/3$, it follows that $n \cdot (\varepsilon_1^* + \varepsilon_2^*) \in (-1, 0)$. Altogether,

$$\left(\frac{2n}{3} - n \cdot \varepsilon_1, n \cdot (\varepsilon_1^* + \varepsilon_2^*)\right) \in I_1 \times (-1, 0).$$

Note that to solve $\mathcal{Q}_n$, it is sufficient to maximize $S_{n^{-1}}$ on the set

$$[-C_0, C_0]^2 \cap \{(n_1/n, n_3/n)\}_{u,v \in \mathbb{N}}$$

. Since $S_{n^{-1}}$ is concave-down on $I_1 \times (-1, 0)$, $(n_1^*, n - n_1^* - n_3^*)$ is a corner of the square $I_1 \times (-1, 0)$. So $n_1^* + n_2^* = n$, which implies Claim D. This completes the proof of the main result. □

Finally, we find the unique graph on n vertices which maximizes spread, where n is sufficiently large.

Proof of Theorem 3.6.1. Suppose G is a graph on n vertices which maximizes spread. By Lemma 3.6.3, $G = (K_{n_1} \coprod K_{n_2}^c) \vee K_{n_3}^c$ for some nonnegative integers n_1, n_2, n_3 such that $n_1 + n_2 + n_3 = n$ where

$$(n_1, n_2, n_3) = \left(\left(\frac{2}{3} + o(1)\right), o(n), \left(\frac{1}{3} + o(1)\right) \cdot n\right).$$

By Lemma 3.6.4, if n is sufficiently large, then $n_2 = 0$. To complete the proof the the main result, it is sufficient to find the unique maximum of $\text{spr}(K_{n_1} \vee K_{n_2}^c)$, subject to the constraint that $n_1 + n_2 = n$. For completeness, we prove this result directly. Let $G = K_{n_1} \vee K_{n_2}^c$. Then A_G has the same spread as the "reduced matrix" defined as

$$A(n_1, n_2) = \begin{bmatrix} n_1 - 1 & n_2 \\ n_1 & 0 \end{bmatrix}.$$

By inspection, $A(n_1, n_2)$ has characteristic polynomial $x^2 - (n_1 - 1)x + -n_1 n_2$ and thus its eigenvalues are

$$\frac{n_1 - 1 \pm \sqrt{n_1^2 + 4n_1 n_2 - 2n_1 + 1}}{2}$$

and

$$\operatorname{spr}(G) = \sqrt{n_1^2 + 4n_1 n_2 - 2n_1 + 1}.$$

Making the substitution $(n_1, n_2) = (rn, (1-r)n)$ and simplifying, we see that

$$\begin{aligned} \operatorname{spr}(G)^2 &= -3n^2 r^2 + 2n(2n-1)a + 1 \\ &= -3n^2 \cdot \left(\left(r - \frac{2n-1}{3n} \right)^2 - \frac{2(2n^2 - 2n - 1)}{9n^2} \right), \end{aligned}$$

which is maximized when $r = n_1/n$ is nearest $2/3 - 1/(3n)$, or equivalently, when n_1 is nearest $(2n-1)/3$. Since

$$\left\lfloor \frac{2n}{3} \right\rfloor - \frac{2n-1}{3} = \begin{cases} 1/3, & n \equiv 0 \pmod 3 \\ -1/3, & n \equiv 1 \pmod 3 \\ 0, & n \equiv 2 \pmod 3 \end{cases},$$

this completes the proof. □

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3.7 Appendix

In this appendix, we derive the formulas that a stepgraphon corresponding to some set $S \subset \{1,2,3,4,5,6,7\}$ in Lemma 3.5.3 satisfies, and detail the algorithm used to conclude that any stepgraphon corresponding to a given S cannot be spread-extremal.

3.7.1 Formulas

In this subsection, we derive the formulas used by our algorithm, from the equations described in Section 3.5.1. First, we define a number of functions which will ease the notational burden in the results that follow. Let

$$\begin{aligned}
F_1(x) &:= (\mu+\nu)x + 2\mu\nu, \\
F_2(x) &:= 2(\mu\nu + (\mu+\nu)x)^2 + (\mu+\nu)x^3, \\
F_3(x) &:= 4\mu^2\nu^2 \cdot (\mu\nu + (\mu+\nu)x)^2 \\
&\quad - 2(\mu+\nu)x^3 \cdot ((\mu+\nu)x + \mu\nu)((\mu+\nu)x + 3\mu\nu) \\
&\quad - (\mu+\nu)x^5 \cdot (2\mu\nu + (\mu+\nu)x), \\
F_4(x) &:= 4\mu^2\nu^2 x \cdot ((3(\mu+\nu)x + \mu\nu) \cdot (2(\mu+\nu)x + \mu\nu) - \mu\nu(\mu+\nu)x) \\
&\quad + 4(\mu+\nu)x^4 \cdot (((\mu+\nu)x + \mu\nu)^2 + (\mu+\nu)^2 \cdot ((\mu+\nu)x + 4\mu\nu)) \\
&\quad + (\mu+\nu)^2 x^7.
\end{aligned}$$

Letting $S := \{i \in \{1,\dots,7\} : \alpha_i > 0\}$, we prove the following six formulas.

Proposition 3.7.1. *Let $i \in \{1,2,5\} \cap S$ and $j \in \{3,4,6,7\} \cap S$ be such that $N_i \cap S = (N_j \cap S) \coprod \{j\}$. Then*

$$f_j^2 = \frac{(\alpha_j + 2\nu)\mu}{F_1(\alpha_j)}, \qquad g_j^2 = \frac{(\alpha_j + 2\mu)\nu}{F_1(\alpha_j)}$$

and

$$f_i = \left(1 + \frac{\alpha_j}{\mu}\right) f_j, \qquad g_i = \left(1 + \frac{\alpha_j}{\nu}\right) g_j.$$

Moreover, $F_1(\alpha_j)$ and $\alpha_j + 2\nu$ are negative.

Proof. By Lemma 3.3.6,

$$\mu f_i^2 - \nu g_i^2 = \mu - \nu$$
$$\mu f_j^2 - \nu g_j^2 = \mu - \nu.$$

By taking the difference of the eigenvector equations for f_i and f_j (and also g_i and g_j), we obtain

$$\alpha_j f_j = \mu(f_i - f_j)$$
$$\alpha_j g_j = \nu(g_i - g_j),$$

or, equivalently,

$$f_i = \left(1 + \frac{\alpha_j}{\mu}\right) f_j$$
$$g_i = \left(1 + \frac{\alpha_j}{\nu}\right) g_j.$$

This leads to the system of equations

$$\begin{bmatrix} \mu & -\nu \\ \mu \cdot \left(1 + \frac{\alpha_j}{\mu}\right)^2 & -\nu \cdot \left(1 + \frac{\alpha_j}{\nu}\right)^2 \end{bmatrix} \cdot \begin{bmatrix} f_j^2 \\ g_j^2 \end{bmatrix} = \begin{bmatrix} \mu - \nu \\ \mu - \nu \end{bmatrix}.$$

If the corresponding matrix is invertible, then after substituting the claimed formulas for f_j^2, g_j^2 and simplifying, it follows that they are the unique solutions. To verify that $F_1(\alpha_j)$ and $\alpha_j + 2\nu$ are negative, it is sufficient to inspect the formulas for f_j and g_j, noting that ν is negative and both μ and $\alpha_j + 2\mu$ are positive.

Suppose the matrix is not invertible. By assumption $\mu, \nu \neq 0$, and so

$$\left(1 + \frac{\alpha_j}{\mu}\right)^2 = \left(1 + \frac{\alpha_j}{\nu}\right)^2.$$

But, since $i \in \{1,2,5\}$ and $j \in \{3,4,6,7\}$,

$$1 > f_j^2 g_i^2 = f_i^2 g_i^2 \cdot \left(1 + \frac{\alpha_j}{\mu}\right)^2 = f_i^2 g_i^2 \cdot \left(1 + \frac{\alpha_j}{\nu}\right)^2 = f_i^2 g_j^2 > 1,$$

a contradiction. □

Proposition 3.7.2. *Let $i \in \{1,2,5\} \cap S$ and $j \in \{3,4,6,7\} \cap S$ be such that $N_i \cap S = (N_j \cap S) \coprod \{i\}$. Then*

$$f_i^2 = \frac{(\alpha_i - 2\nu)\mu}{-F_1(-\alpha_i)}, \qquad g_i^2 = \frac{(\alpha_i - 2\mu)\nu}{-F_1(-\alpha_i)},$$

and

$$f_j = \left(1 - \frac{\alpha_i}{\mu}\right) f_i, \qquad g_j = \left(1 - \frac{\alpha_i}{\nu}\right) g_i.$$

Moreover, $-F_1(-\alpha_i)$ is positive and $\alpha_i - 2\mu$ is negative.

Proof. The proof of Proposition 3.7.1, slightly modified, gives the desired result. □

Proposition 3.7.3. *Suppose $i, j, k \in S$ where (i,j,k) is either $(2,3,4)$ or $(5,6,7)$. Then*

$$f_k = \frac{\mu f_j - \alpha_i f_i}{\mu}, \qquad g_k = \frac{\nu g_j - \alpha_i g_i}{\nu},$$

and

$$\alpha_i = \frac{2\mu^2\nu^2\alpha_j}{F_2(\alpha_j)}.$$

Proof. Using the eigenfunction equations for f_j, f_k and for g_j, g_k, it follows that

$$f_k = \frac{\mu f_j - \alpha_i f_i}{\mu}, \qquad g_k = \frac{\nu g_j - \alpha_i g_i}{\nu}.$$

Combined with Lemma 3.3.6, it follows that

$$\begin{aligned} 0 &= \mu f_k^2 - \nu g_k^2 - (\mu - \nu) \\ &= \mu \left(\frac{\mu f_j - \alpha_i f_i}{\mu}\right)^2 - \nu \left(\frac{\nu g_j - \alpha_i g_i}{\nu}\right)^2 - (\mu - \nu). \end{aligned}$$

After expanding, we note that the right-hand side can be expressed purely in terms of the quantities $\mu, \nu, \alpha_i, f_i^2, f_i f_j, f_j^2, g_i^2, g_i g_j$, and g_j^2. Note that Proposition 3.7.1 gives explicit formulas for $f_i^2, f_i f_j$, and f_j^2, as well as $g_i^2, g_i g_j$, and g_j^2, purely in terms of μ, ν, and α_j. With the help of a computer algebra system, we make these substitutions and factor the right-hand side as:

$$0 = (\mu - \nu) \cdot \alpha_i \cdot \frac{2\mu^2\nu^2 \cdot \alpha_j - F_2(\alpha_j) \cdot \alpha_i}{\mu^2\nu^2 \cdot F_1(\alpha_i)}.$$

Since $\alpha_i, (\mu - \nu) \neq 0$, the desired claim holds. □

Proposition 3.7.4. *Suppose* $1, i, j, k \in S$ *where* (i, j, k) *is either* $(2, 3, 4)$ *or* $(5, 6, 7)$. *Then*

$$f_1 = \frac{\mu f_i + \alpha_k f_k}{\mu}, \qquad g_1 = \frac{\nu g_i + \alpha_k g_k}{\nu},$$

and

$$\alpha_k = \frac{\alpha_j \cdot F_2(\alpha_j)^2}{F_3(\alpha_j)}.$$

Proof. Using the eigenfunction equations for f_1, f_i, f_j, f_k and for g_1, g_i, g_j, g_k, it follows that

$$f_1 = \frac{\mu f_i + \alpha_k f_k}{\mu}, \qquad g_1 = \frac{\nu g_i + \alpha_k g_k}{\nu},$$

and

$$f_k = \frac{\mu f_j - \alpha_i f_i}{\mu}, \qquad g_k = \frac{\nu g_j - \alpha_i g_i}{\nu}.$$

Altogether,

$$f_1 = \frac{\mu^2 f_i + \alpha_k(\mu f_j - \alpha_i f_i)}{\mu^2}, \qquad g_1 \qquad = \frac{\nu^2 g_i + \alpha_k(\nu g_j - \alpha_i g_i)}{\nu^2}$$

Combined with Lemma 3.6, it follows that

$$\begin{aligned} 0 &= \mu f_1^2 - \nu g_1^2 - (\mu - \nu) \\ &= \mu \left(\frac{\mu^2 f_i + \alpha_k(\mu f_j - \alpha_i f_i)}{\mu^2} \right)^2 - \nu \left(\frac{\nu^2 g_i + \alpha_k(\nu g_j - \alpha_i g_i)}{\nu^2} \right)^2 - (\mu - \nu). \end{aligned}$$

After expanding, we note that the right-hand side can be expressed purely in terms of the quantities $\mu, \nu, f_i^2, f_i f_j, f_j^2, g_i^2, g_i g_j$, and α_i. Not that Proposition 3.7.1 give explicit formulas for $f_i^2, f_if_j, f_j^2, g_i^2, g_ig_j$, and g_j^2 purely in terms of μ, ν, and α_j. With the help of a computer algebra system, we make these substitutions and factor the right-hand side as:

$$0 = 2\alpha_k \cdot (\mu - \nu) \cdot \frac{\alpha_j \cdot F_2(\alpha_j)^2 - \alpha_k \cdot F_3(\alpha_j)}{F_1(\alpha_j) \cdot F_2(\alpha_j)^2}.$$

So the desired claim holds. □

Proposition 3.7.5. *Suppose* $1, i, k \in S$ *and* $j \notin S$ *where* (i, j, k) *is either* $(2, 3, 4)$ *or* $(5, 6, 7)$. *Then,*

$$f_1 = \frac{\mu f_i + \alpha_k f_k}{\mu}, \qquad g_1 = \frac{\nu g_i + \alpha_k g_k}{\nu},$$

and

$$\alpha_k = \frac{2\alpha_i \mu^2 \nu^2}{F_2(-\alpha_i)}$$

Proof. Using the eigenfunction equations for f_1, f_i, f_j, f_k and for g_1, g_i, g_j, g_k, it follows that

$$f_1 = \frac{\mu f_i + \alpha_k f_k}{\mu}, \qquad g_1 = \frac{\nu g_i + \alpha_k g_k}{\nu},$$

and

$$f_k = \frac{\mu f_i - \alpha_i f_i}{\mu}, \qquad g_k = \frac{\nu g_i - \alpha_i g_i}{\nu}.$$

Altogether,

$$f_1 = \frac{\mu^2 f_i + \alpha_k(\mu f_i - \alpha_i f_i)}{\mu^2}, \qquad g_1 \qquad = \frac{\nu^2 g_i + \alpha_k(\nu g_i - \alpha_i g_i)}{\nu^2}$$

Combined with Lemma 3.6, it follows that

$$\begin{aligned} 0 &= \mu f_1^2 - \nu g_1^2 - (\mu - \nu) \\ &= \mu \left(\frac{\mu^2 f_i + \alpha_k(\mu f_i - \alpha_i f_i)}{\mu^2} \right)^2 - \nu \left(\frac{\nu^2 g_i + \alpha_k(\nu g_i - \alpha_i f_i)}{\nu^2} \right)^2 - (\mu - \nu). \end{aligned}$$

After expanding, we note that the right-hand side can be expressed purely in terms of the quantities $\mu, \nu, f_i^2, f_if_j, f_j^2, g_i^2, g_ig_j$, and α_i. Not that Proposition 3.7.1 give explicit formulas for $f_i^2, f_if_j, f_j^2, g_i^2, g_ig_j$, and g_j^2 purely in terms of μ, ν, and α_j. With the help of a computer algebra system, we make these substitutions and factor the right-hand side as:

$$0 = 2\alpha_k \cdot (\mu - \nu) \cdot \frac{\alpha_j \cdot F_2(\alpha_j)^2 - \alpha_k \cdot F_3(\alpha_j)}{F_1(\alpha_j) \cdot F_2(\alpha_j)^2}.$$

So the desired claim holds. □

Proposition 3.7.6. *Suppose* $1 \notin S$ *and* $i, j, k, \ell \in S$ *where* (i, j, k, ℓ) *is either* $(2, 3, 4, 7)$ *or* $(5, 6, 7, 4)$. *Then*

$$\alpha_k = \frac{F_4(x)}{F_3(x)}.$$

Proof. Using the eigenfunction equations for f_ℓ, f_i, f_j, f_k and for g_ℓ, g_i, g_j, g_k, it follows that

$$f_\ell = \frac{\alpha_i f_i + \alpha_j f_j + \alpha_k f_k}{\mu}, \qquad g_1 = \frac{\alpha_i g_i + \alpha_j g_j + \alpha_k g_k}{\nu},$$

and

$$f_k = \frac{\mu f_j - \alpha_i f_i}{\mu}, \qquad g_k = \frac{\nu g_j - \alpha_i g_i}{\nu}.$$

Altogether,

$$f_\ell = \frac{\mu \alpha_i f_i + \alpha_j f_j + \alpha_k(\mu f_j - \alpha_i f_i)}{\mu^2}, \qquad g_\ell \qquad = \frac{\nu \alpha_i g_i + \alpha_j g_j + \alpha_k(\nu g_j - \alpha_i g_i)}{\nu^2}$$

Combined with Lemma 3.3.6, it follows that

$$\begin{aligned} 0 &= \mu f_\ell^2 - \nu g_\ell^2 - (\mu - \nu) \\ &= \mu \left(\frac{\mu \alpha_i f_i + \alpha_j f_j + \alpha_k(\mu f_j - \alpha_i f_i)}{\mu^2} \right)^2 - \nu \left(\frac{\nu \alpha_i g_i + \alpha_j g_j + \alpha_k(\nu g_j - \alpha_i g_i)}{\nu^2} \right)^2 \\ &\quad - (\mu - \nu) \end{aligned}$$

After expanding, we note that the right-hand side can be expressed purely in terms of $\mu, \nu, f_i^2, f_i f_j, f_j^2, g_i^2, g_i g_j$, and α_i. Not that Proposition 3.7.1 give explicit formulas for each of the quantities $f_i^2, f_i f_j, f_j^2, g_i^2, g_i g_j, g_j^2, \alpha_i, \alpha_j, \alpha_k$ purely in terms of μ, ν, and α_j. With the help of a computer algebra system, we make these substitutions and factor the right-hand side as:

$$0 = 2(\mu - \nu) \cdot \alpha_k \cdot \frac{F_4(\alpha_j) - \alpha_k \cdot F_3(\alpha_j)}{F_1(\alpha_j) \cdot F_2(\alpha_j)^2}$$

□

3.7.2 Algorithm

In this subsection, we rigorously detail the algorithm used in the computer-assisted proof of Theorem 3.5.1. This algorithm is implemented in Python using the PyInterval package. In

Appendix 3.8 we provide the program containing the formulas for different variables, and the subroutines used to check that certain equalities and inequalities are satisfied. In Appendix 3.9, we provide the program that, once run to completion, provably shows that the optimal step-graphon is not of the form $S = \{1, 2, 3, 4, 5, 6, 7\}$.

We begin by reviewing the definitions contained in Appendix 3.8. In this program, for simplicity, we make use of three functions of μ and ν, given by

$$u = \mu - \nu, \qquad v = \mu + \nu, \qquad mn = \mu\nu.$$

In addition, we refer to the conjectured optimal spread of $2/\sqrt{3}$ as SPR_MAX, $\emptyset$ as NULL_INT, $[0, 1]$ as UNIT_INT, $[1, \infty)$ as GEQ_ONE, and $[0, \infty)$ as POS.

This program contains formulas for

- α_2, assuming $\{2, 3, 4\} \subset S$ (using Proposition 3.7.3)
- α_4, assuming $\{1, 2, 3, 4\} \subset S$ (using Proposition 3.7.4)
- α_4, assuming $\{2, 3, 4, 7\} \subset S$, $1 \notin S$ (using Proposition 3.7.6)
- α_4, assuming $\{1, 2, 4\} \subset S$, $3 \notin S$ (using Proposition 3.7.5)
- f_3 and g_3, assuming $\{2, 3\} \subset S$ (using Proposition 3.7.1)
- f_2 and g_2, assuming $\{2, 3\} \subset S$ (using Proposition 3.7.1)
- f_4 and g_4, assuming $\{2, 3, 4\} \subset S$ (using Proposition 3.7.3)
- f_1 and g_1, assuming $\{1, 2, 4\} \subset S$ (using Propositions 3.7.4 and 3.7.5)
- f_2 and g_2, assuming $\{2, 4\} \subset S$, $3 \notin S$ (using Proposition 3.7.2)
- f_4 and g_4, assuming $\{2, 4\} \subset S$, $3 \notin S$ (using Proposition 3.7.2)

as a function of α_3, μ, and ν (and α_2 and α_4, which can be computed as functions of α_3, μ, and ν). Some of the formulas are slightly modified compared to their counterparts in this section, for the purpose of minimizing accumulated error.

Each formula is performed using interval arithmetic, while restricting the resulting interval solution to the correct range. In particular, we recall that we have the inequalities

- $\alpha_i \in [0,1]$, for $i \in S$
- $|g_2|, |f_3| \leq 1$, $|f_2|, |g_3| \geq 1$, for $\{2,3\} \subset S$
- $|f_4| \leq 1$, $|g_4| \geq 1$, for $4 \in S$
- $|f_1| \geq 1$, $|g_1| \leq 1$, for $\{1,2,4\} \in S$
- $|f_4|, |g_2| \leq 1$, $|f_2|, |g_4| \geq 1$, for $\{2,4\} \in S$, $3 \notin S$
- $\alpha_3 + 2\nu \leq 0$, for $\{2,3\} \in S$ (using Proposition 3.7.1)
- $\alpha_2 - 2\mu \leq 0$, for $\{2,4\} \in S$, $3 \notin S$ (using Proposition 3.7.2).

This completes the analysis of the formulas in Appendix 3.8. Next, we detail the different functions which determine feasibility. There are a number of different properties which can be checked, including eigenvector equations, bounds on edge density, norm equations for the eigenvectors, and the ellipse equations. Each of these properties has an associated function which returns FALSE, if the property cannot be satisfied, given the intervals for each variable, and returns TRUE otherwise. The implementation of each of these properties is rather intuitive, and we refer the reader to Appendix 3.8 for more details.

Next, we examine the program in Appendix 3.9, that rules out $S = \{1,2,3,4,5,6,7\}$ as the structure of an optimal step-graphon. The programs for the other choices of S are very similar in nature, and can be found on github.

This program is made up of two parts. The first part is a function is_feasible(mu,nu,a3,a6) that computes the intervals for all variables and checks feasibility using the functions defined in Appendix 3.8 and detailed above. The second part is a divide and conquer algorithm that breaks the hypercube

$$(\mu, \nu, \alpha_3, \alpha_6) \in [.65, 1] \times [-.5, -.15] \times [0,1] \times [0,1]$$

into sub-boxes of size 1/20 by 1/20 by 1/10 by 1/10, checks feasibility in each box, and subdivides any box that does not rule out feasibility (i.e., subdivides any box that returns TRUE). This subdivision breaks a single box into two boxes of equal size, by subdividing along one of the four variables. The variable used for this subdivision is chosen iteratively, in the order $\alpha_3, \alpha_6, \mu, \nu, \alpha_3, \ldots$. The entire divide and conquer algorithm terminates after all sub-boxes, and therefore, the entire domain

$$(\mu, \nu, \alpha_3, \alpha_6) \in [.65, 1] \times [-.5, -.15] \times [0, 1] \times [0, 1],$$

has been shown to be infeasible, at which point the algorithm prints 'infeasible'.

3.8 Formula and Casework Code

```
from interval import interval, inf, imath, fpu

SPR_MAX = imath.sqrt(interval[4]/3)

NULL_INT = interval()
UNIT_INT = interval[0,1]
GEQ_ONE = interval[1, inf]
POS = interval[0,inf]


# these are helper methods meant to be used when
# handling cases that share formulas

# every method begins with the variable to be returned
# and ends with a string indicating assumptions made
# most often, the string is a list of indices w/ weight
# assumed to be positive
# when weights are assumed 0, the string corresponds to
# an interval in increasing order; in the interval:
    # any number in {1, ..., 7} indicates a positive weight
```

```
    # N indicates the weight is assumed 0
    # X (wildcard) indicates no assumption on the weight



# always, we assume that:
    # u = mu - nu,
    # v = mu + nu, and
    # mn = mu*nu

# all other variables are self-evident
# formulas are written to minimize FLOPs and accumulated
# error when possible

def a2_assume234(a3, mn, v):

    a2num = 2*a3*(mn)**2
    a2denom = 2*( mn + a3*v )**2 + a3**3*v

    return (a2num / a2denom) & UNIT_INT



def a4_assume1234(a3, mn, v):

    a4num = a3*(2*(mn + a3*v)**2 + a3**3*v)**2
    a4denom = 4*mn**2*(mn + a3*v)**2
    a4denom -= 2*a3**3 * (a3*v + mn)*(a3*v + 3*mn)*v
    a4denom -= a3**5*v*( 2*mn + a3*v )
```

```
    return (a4num / a4denom) & UNIT_INT


def a4_assumeN2347(a3, mn, v):
    a4num = 4*((3*a3*v + mn)*(2*a3*v + mn) - a3*mn*v)*mn**2*a3
    a4num += 4*v*a3**4*((mn + a3*v)**2 + v**2*(4*mn + a3*v))
    a4num += v**2*a3**7

    a4denom = 4*mn**2*(mn + a3*v)**2
    a4denom -= 2*a3**3 * (a3*v + mn)*(a3*v + 3*mn)*v
    a4denom -= a3**5*v*( 2*mn + a3*v )

    return (a4num / a4denom) & UNIT_INT


def a4_assume12N4(a2, mn, v):

    a4num = 2*a2*mn**2
    a4denom = 2*(a2*v - mn)**2 - a2**3*v

    return (a4num / a4denom) & UNIT_INT


def fg3_assume23(mu, nu, a3, mn, v, g_pos = True):

    f3num = ((a3+2*nu)*mu) & (-POS)
    g3num = ((a3+2*mu)*nu) & (-POS)
    denom = (a3*v + 2*mn) & (-POS)
```

```
    f3 = imath.sqrt((f3num / denom) & UNIT_INT) & UNIT_INT
    g3 = imath.sqrt((g3num / denom) & GEQ_ONE) & GEQ_ONE

    if g_pos:
        return f3, g3
    return f3, -g3


def fg2_assume23(mu, nu, a3, f3, g3, g_pos = True):

    f2 = ((1+a3/mu)*f3) & GEQ_ONE
    g2 = ((1+a3/nu)*g3)

    if g_pos:
        return f2, g2 & UNIT_INT
    return f2, g2 & (-UNIT_INT)


def fg4_assume234(mu, nu, a2, f2, f3, g2, g3, g_pos = True):

    f4 = (f3-a2*f2/mu) & UNIT_INT
    g4 = (g3-a2*g2/nu)

    if g_pos:
        return f4, g4 & GEQ_ONE
    return f4, g4 & (-GEQ_ONE)
```

```python
def fg1_assume124(mu, nu, a4, f2, f4, g2, g4):

    f1 = (f2+a4*f4/mu) & GEQ_ONE
    g1 = (g2+a4*g4/nu) & UNIT_INT

    return f1, g1


def fg2_assume2N4(mu, nu, a2, mn, v, g_pos = True):

    f2num = ((a2-2*nu)*mu) & POS
    g2num = ((a2-2*mu)*nu) & POS
    denom = (a2*v - 2*mn) & POS

    f2 = imath.sqrt((f2num / denom) & GEQ_ONE) & GEQ_ONE
    g2 = imath.sqrt((g2num / denom) & UNIT_INT) & UNIT_INT

    if g_pos:
        return f2, g2
    return f2, -g2


def fg4_assume2N4(mu, nu, a2, f2, g2, g_pos = True):

    f4 = ((1-a2/mu)*f2) & UNIT_INT
    g4 = ((1-a2/nu)*g2)

    if g_pos:
```

```
        return f4, g4 & GEQ_ONE
    return f4, g4 & (-GEQ_ONE)



# below are methods to directly determine feasibility
# as a convention:
    # avec is filled with the ai's, including 0's for the
    # missing vertices
    # for fvec and gvec, a missing vertex is indicated by None



# checks that fvec and gvec can satisfy the eigen-equations

def fg_row_feasible(mu, nu, fvec, gvec, avec):

    if not fvec[0] == None:
        fsum = interval(0)
        gsum = interval(0)
        for j in range(7):
            if not fvec[j] == None:
                fsum += avec[j]*fvec[j]
                gsum += avec[j]*gvec[j]
        if fsum & (mu*fvec[0]) == NULL_INT:
            return False
        if gsum & (nu*gvec[0]) == NULL_INT:
            return False
```

```
if not fvec[1] == None:
    fsum = interval(0)
    gsum = interval(0)
    for j in [0,1,2,4,5,6]:
        if not fvec[j] == None:
            fsum += avec[j]*fvec[j]
            gsum += avec[j]*gvec[j]
    if fsum & (mu*fvec[1]) == NULL_INT:
        return False
    if gsum & (nu*gvec[1]) == NULL_INT:
        return False


if not fvec[2] == None:
    fsum = interval(0)
    gsum = interval(0)
    for j in [0,1,4,5,6]:
        if not fvec[j] == None:
            fsum += avec[j]*fvec[j]
            gsum += avec[j]*gvec[j]
    if fsum & (mu*fvec[2]) == NULL_INT:
        return False
    if gsum & (nu*gvec[2]) == NULL_INT:
        return False


if not fvec[3] == None:
    fsum = interval(0)
```

```
        gsum = interval(0)
        for j in [0,4,5,6]:
            if not fvec[j] == None:
                fsum += avec[j]*fvec[j]
                gsum += avec[j]*gvec[j]
        if fsum & (mu*fvec[3]) == NULL_INT:
            return False
        if gsum & (nu*gvec[3]) == NULL_INT:
            return False

    if not fvec[4] == None:
        fsum = interval(0)
        gsum = interval(0)
        for j in [0,1,2,3,4,5]:
            if not fvec[j] == None:
                fsum += avec[j]*fvec[j]
                gsum += avec[j]*gvec[j]
        if fsum & (mu*fvec[4]) == NULL_INT:
            return False
        if gsum & (nu*gvec[4]) == NULL_INT:
            return False

    if not fvec[5] == None:
        fsum = interval(0)
        gsum = interval(0)
        for j in [0,1,2,3,4]:
```

```
            if not fvec[j] == None:
                fsum += avec[j]*fvec[j]
                gsum += avec[j]*gvec[j]
        if fsum & (mu*fvec[5]) == NULL_INT:
            return False
        if gsum & (nu*gvec[5]) == NULL_INT:
            return False



    if not fvec[6] == None:
        fsum = interval(0)
        gsum = interval(0)
        for j in [0,1,2,3]:
            if not fvec[j] == None:
                fsum += avec[j]*fvec[j]
                gsum += avec[j]*gvec[j]
        if fsum & (mu*fvec[6]) == NULL_INT:
            return False
        if gsum & (nu*gvec[6]) == NULL_INT:
            return False

    return True



# checks that the edge density is not less than
# the sum of the squares of the two known eigenvalues

def density_feasible(mu, nu, avec):
```

```
    d = 1-(avec[2]+avec[3])**2-(avec[5]+avec[6])**2
           - 2*(avec[1]*avec[3]+avec[4]*avec[6])

    if (d-mu**2-nu**2) & POS == NULL_INT:
        return False
    return True



# checks that fvec and gvec can have norm 1

def norm_feasible(fvec, gvec, avec):

    fnorm = interval(0)
    gnorm = interval(0)

    for i in range(7):
        if not fvec[i] == None:
            fnorm += avec[i]*fvec[i]**2
            gnorm += avec[i]*gvec[i]**2

    if fnorm & interval(1) == NULL_INT:
        return False

    if gnorm & interval(1) == NULL_INT:
        return False

    return True
```

```
# checks the ellipse equations can be satisfied

def ellipse_feasible(mu, nu, fvec, gvec, u):

    for i in range(len(fvec)):
        if not fvec[i] == None:
            if (mu*fvec[i]**2-nu*gvec[i]**2) & u == NULL_INT:
                return False

    return True
```

3.9 Interval Arithmetic for $S = \{1, 2, 3, 4, 5, 6, 7\}$

```
\begin{singlespace}
# case 1|234|567

from interval import interval, inf, imath, fpu
from casework_helper import *

import queue



# numerically attempts to rule out solutions to
# the constraints, falling into the given intervals

def is_feasible(mu, nu, a3, a6):
```

```
# first, we ignore cases that cannot exceed
# the conjectured optimum of 2/sqrt(3)
# some helper variables are also used

u = mu-nu
if ((u - SPR_MAX) & POS) == NULL_INT:
    return False

v = mu+nu
mn = mu*nu



# ignore cases where weight sum exceeds 1

asum = (a3+a6) & UNIT_INT

if asum == NULL_INT:
    return False



# again, weight sum cannot exceed 1;
# formulas for ai's, fi's, and gi's...

a2 = a2_assume234(a3, mn, v)
asum = (asum + a2) & UNIT_INT
if asum == NULL_INT:
    return False
```

```
a4 = a4_assume1234(a3, mn, v)
asum = (asum + a4) & UNIT_INT
if asum == NULL_INT:
    return False

a5 = a2_assume234(a6, mn, v)
asum = (asum + a5) & UNIT_INT
if asum == NULL_INT:
    return False

a7 = a4_assume1234(a6, mn, v)
asum = (asum + a7) & UNIT_INT
if asum == NULL_INT:
    return False

a1 = (1-asum) & UNIT_INT
avec = [a1, a2, a3, a4, a5, a6, a7]


# the sum of squares of eigenvalues equals
# the graph edge density

if not density_feasible(mu, nu, avec):
    return False



# formulas for f1, g1, ..., f7, g7 must hold
```

```
f3, g3 = fg3_assume23(mu, nu, a3, mn, v)
f2, g2 = fg2_assume23(mu, nu, a3, f3, g3)
f4, g4 = fg4_assume234(mu, nu, a2, f2, f3, g2, g3)
f1, g1 = fg1_assume124(mu, nu, a4, f2, f4, g2, g4)

if f1 == NULL_INT:
    return False
if g1 == NULL_INT:
    return False

f6, g6 = fg3_assume23(mu, nu, a6, mn, v, g_pos = False)
f5, g5 = fg2_assume23(mu, nu, a6, f6, g6, g_pos = False)
f7, g7 = fg4_assume234(mu, nu, a5, f5, f6, g5, g6, g_pos = False)

f1bot, g1bot = fg1_assume124(mu, nu, a7, f5, f7, g5, g7)
f1 = f1 & f1bot
g1 = g1 & g1bot

if f1 == NULL_INT:
    return False
if g1 == NULL_INT:
    return False


# check eigenvector equations

fvec = [f1, f2, f3, f4, f5, f6, f7]
gvec = [g1, g2, g3, g4, g5, g6, g7]
```

```
    if not fg_row_feasible(mu, nu, fvec, gvec, avec):
        return False

    # might as well also check the norms and ellipse equations

    if not norm_feasible(fvec, gvec, avec):
        return False

    if not ellipse_feasible(mu, nu, fvec, gvec, u):
        return False

    return True


# divide-and-conquer!  begin with a grid over (mu, nu, a3, a6)
# in the box [.65, 1] x [-.5, -.15] x [0, 1] x [0, 1]
# subdivide by the stepsizes .05, .05, .1, .1, respective
# queue up each box as a separate case, stored with depth term
# if a case cannot be ruled infeasible, split it in half along
# one dimension, queueing each half of the box
# the halved dimension is chosen according to the
# congruence mod 4 of the depth

case_queue = queue.Queue()

Mdenom = 20
```

```
Ndenom = 20
A3denom = 10
A6denom = 10

for M in range(7, 20):
    for N in range(-10, -3):
        for A3 in range(0, 10):
            for A6 in range(0, 10-A3):
                case_queue.put( (M,Mdenom, N,Ndenom, A3,
                                              A3denom, A6,A6denom, 0) )

curr_depth = -1
curr_size = 0
next_size = case_queue.qsize()

ctr = 0

print 'trying case 1|234|567 ...'

while not case_queue.empty():
    (M,Mdenom, N,Ndenom, A3,A3denom, A6,A6denom, depth) = case_queue.get()
    if depth != curr_depth:
        curr_depth = depth
        curr_size = next_size
        ctr += curr_size
        next_size = 0
        print '\ton depth =', curr_depth, '...', 'size =', curr_size,
              '...', 'so far', ctr, '...'
```

```
mu = interval[M, M+1] / interval(Mdenom)
nu = interval[N, N+1] / interval(Ndenom)
a3 = interval[A3, A3+1] / interval(A3denom)
a6 = interval[A6, A6+1] / interval(A6denom)


if is_feasible(mu, nu, a3, a6):
    next_size += 2

    if depth % 4 == 0:
        case_queue.put( (M,Mdenom, N,Ndenom, 2*A3,
                        2*A3denom, A6, A6denom, depth+1) )
        case_queue.put( (M,Mdenom, N,Ndenom, 2*A3+1,
                        2*A3denom, A6, A6denom, depth+1) )

    if depth % 4 == 1:
        case_queue.put( (M,Mdenom, N,Ndenom, A3,
                        A3denom, 2*A6, 2*A6denom, depth+1) )
        case_queue.put( (M,Mdenom, N,Ndenom, A3,
                        A3denom, 2*A6+1, 2*A6denom, depth+1) )

    if depth % 4 == 2:
        case_queue.put( (2*M,2*Mdenom, N,Ndenom, A3,
                        A3denom, A6, A6denom, depth+1) )
        case_queue.put( (2*M+1,2*Mdenom, N,Ndenom, A3,
                        A3denom, A6, A6denom, depth+1) )
```

```
        if depth % 4 == 3:
            case_queue.put( (M,Mdenom, 2*N,2*Ndenom, A3,
                            A3denom, A6, A6denom, depth+1) )
            case_queue.put( (M,Mdenom, 2*N+1,2*Ndenom, A3,
                            A3denom, A6, A6denom, depth+1) )

print 'infeasible\n'
\end{singlespace}
```

CHAPTER 4. GENERAL CONCLUSIONS

In extremal graph theory, we search for graphs which optimize some parameter subject to some constraint. Oftentimes, the optimal graph is highly structured. For example, there may exist a partition of the vertex into a small number of parts such that vertices within a part behave identically. Other times, the optimal graph has random or random-like structure.

In Chapter 2, we consider the edit distance problem which asks, for some graph F, how many edges-additions and edge-deletions are must be applied to a host graph G to ensure the resulting graph G' contains no induced copy of F. More generally, the edit distance function $\mathrm{ed}_{\mathcal{H}}(p)$ is defined to be this maximum number of edits, subject to the constraint that G has edge density p. While it is known that an Erdős-Rényi random graph asymptotically attains this maximum number of edits, we consider the case when F itself is an Erdős-Rényi random graph. Here, we find a precise asymptotically almost sure formula for the edit distance function for F in this as long as F has edge density lying in $[1-1/\phi, 1/\phi]$, where ϕ is the Golden Ratio. While random graphs solve the general edit distance problem, we find several structural features of the colored colored regularity graphs (CRGs) used to compute edit distance functions. In particular, we show that the spectra of the weighted adjacency of a CRG K can be used to eliminate K from the computation of an edit distance function.

In extremal spectral graph theory, we tell a similar story. Rather than consider a quantity defined on graphs, we first identify graphs with matrices and then ask which graphs optimize a quantity defined on matrices. As previous, the optimal graphs are frequently some combination of highly-structured and random-like.

In Chapter 3, we prove the Spread Conjecture which concerns the the spread $s(G)$ of a graph G, defined to be the maximum difference between any two eigenvalues of the adjacency matrix of G, for all n sufficiently large. In doing so, we demonstrate the utility of translating a discrete problem to an analytic setting. To begin, we solve the analogous problem for graphons (symmetric functions $W : [0,1]^2 \to [0,1]$) in several steps. We show that if W is optimal, then it has a step-graphon with 7 steps and fixed behavior between them.

We then use interval arithmetic, a systematic technique for bounding error in computation, to reduce the 7 steps to only 3. We then reduce the 3 steps to 2 with calculus and a computer algebra system. To return to the Spread Conjecture, we first show that the graphs resemble the optimal stepgraphon with possibly a small exceptional set of vertices. Again using calculus and a computer algebra system, we eliminate the exceptional vertices.