EXTREMAL GRAPHS FOR HOMOMORPHISMS

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ABSTRACT. The study of graph homomorphisms has a long and distinguished history, with applications in many areas of graph theory. There has been recent interest in counting homomorphisms, and in particular on the question of finding upper bounds for the number of homomorphisms from a graph G into a fixed image graph H. We introduce our techniques by proving that the lex graph has the largest number of homomorphisms into K_2 with one looped vertex (or equivalently, the largest number of independent sets) among graphs with fixed number of vertices and edges. Our main result is the solution to the extremal problem for the number of homomorphisms into P_2°, the completely looped path of length 2 (known as the Widom-Rowlinson model in statistical physics). We show that there are extremal graphs that are threshold, give explicitly a list of five threshold graphs from which any threshold extremal graph must come, and show that each of these "potentially extremal" threshold graphs is in fact extremal for some number of edges.

1. Introduction

The study of graph homomorphisms has a long and distinguished history, with applications in many areas of graph theory (see for instance [10]). A *homomorphism* from a multigraph G to a multigraph H is a map $f : V(G) \to V(H)$ satisfying $v \sim_G w \implies f(v) \sim_H f(w)$. It is natural to allow loops in H, but redundant to allow multiple edges. In what follows we will always assume that G is a simple graph, with no loops or multiple edges. We shall write H° for the "fully looped" version of H, i.e., the multigraph with edges $E(H) \cup \{xx : x \in V(H)\}$. We denote the set of homomorphisms from G to H by $\mathrm{Hom}(G, H)$ and let $\hom(G, H) = |\mathrm{Hom}(G, H)|$.

There has been recent interest (see, for instance, [3], [7]) in counting homomorphisms. In particular, some of these investigations have focused on the question of finding upper bounds for the number of homomorphisms from a graph G into a fixed image graph H. A crucial paper was that of Galvin and Tetali [8] in which they prove that for G r-regular and bipartite with n vertices one has, for all H,

$$\hom(G, H) \le \hom(K_{r,r}, H)^{\frac{n}{2r}}.$$

The Galvin and Tetali paper builds on Kahn's papers [11, 12], which used entropy methods to bound the number of independent sets in an r-regular bipartite graph. In this paper we consider the following problem, which has a markedly different flavor than the Galvin-Tetali results. If $G = (V, E)$ is a graph, we let $n(G) = |V|$ and $e(G) = |E|$. Given a graph parameter p, we say that a graph G is *p-extremal* if

$$p(G) = \max \left\{ p(G') : n(G') = n(G), e(G') = e(G) \right\}.$$

Problem 1. Given integers n, e and a multigraph H, what is the maximum, over all graphs G having n vertices and e edges, of $\hom(G, H)$? Furthermore, which graphs are $\hom(\cdot, H)$-extremal?

If H is a fully looped complete graph with m vertices and G is *any* graph with n vertices then $\hom(G, H) = m^n$, since any function from $V(G)$ to $V(H)$ is a homomorphism. Therefore for this H the problem is trivial. The first non-trivial case of the problem occurs when H is K_2 with exactly one looped vertex. Then the only condition on a homomorphism $f : V(G) \to V(H)$ is that the inverse image of the unlooped vertex be an independent set. Giving an upper bound on $\hom(G,H)$ is then equivalent to giving an upper bound on the number of independent sets in G.

Another vein of much research is the case when H is a complete graph on q vertices with no loops. Since a homomorphism from a graph G to K_q is simply a proper q-coloring of G, Problem 1 becomes a question about which graph on n vertices and e edges has the maximum number of proper q-colorings. This question was first posed, independently, by Linial [16] and Wilf [20]. Lazebnik [15] was able to completely resolve the case $q = 2$ and much work has gone into other cases (see [17] for a more comprehensive history). Recently, Loh, Pikhurko, and Sudakov [17] provided an asymptotic answer for general q using a clever application of Szemerédi's Regularity Lemma.

If we insist that H is fully looped then the first interesting case is a fully looped path of length 2, a graph we denote P_2°.

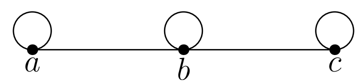

Figure 1. The graph P_2°

Our main result is a tight upper bound on $\hom(G, P_2^\circ)$. In the language of statistical physics a homomorphism $f \in \mathrm{Hom}(G, P_2^\circ)$ is called a *state of the Widom-Rowlinson model* on G. For this reason we write $\mathrm{wr}(G)$ for $\hom(G, P_2^\circ)$. This model has been extensively studied (see, e.g., [4], [9]), but as far as we know our extremal problem has not been discussed before now.

Somewhat surprisingly there are a variety of graphs which are wr-extremal, although they can be broadly categorized as either "lex-like" or "colex-like". The lexicographic and colexocographic orders are defined on (among other places) the set of subsets of $[n] = \{1, 2, \ldots, n\}$. The lex order is defined by $A <_L B$ if $\min(A \triangle B) \in A$, whereas the colex order is defined by $A <_C B$ if $\max(A \triangle B) \in B$. If we restrict to subsets of size 2 then we have orderings on the edges of K_n. The first few edges in the lex order are $\{1,2\}, \{1,3\}, \{1,4\}, \{1,5\}, \ldots, \{2,3\}, \{2,4\}, \ldots$. The first few edges in the colex order are $\{1,2\}, \{1,3\}, \{2,3\}, \{1,4\}, \{2,4\}, \{3,4\}, \{1,5\}, \ldots$. We define the *lex graph* $\mathcal{L}(n,e)$ (respectively the colex graph $\mathcal{C}(n,e)$) to be the graph having vertex set $[n]$ and edge set consisting of the initial segment in the lex ordering (respectively the colex ordering) of size e. The extremal examples are, in a natural sense, very close either to $\mathcal{C}(n,e)$ or $\mathcal{L}(n,e)$. We give the exact extremal graphs in Section 5.

Our proof involves first showing that we may assume that an extremal graph is a *threshold graph*. We discuss the definition and properties of threshold graphs in Section 2. We use a compression argument, and we discuss the relevant compression in the same section.

Before we give the proof of our main theorem we use the techniques of our proof to show that $\mathcal{L}(n,e)$ has the largest number of independent sets among all graphs on n vertices with e edges. This is the content of Section 3. While this result is a corollary of the Kruskal-Katona theorem [14, 13], we believe that seeing this example first will help in understanding the main proof. The remainder of the paper is devoted to a proof that the maximum value of $\mathrm{wr}(G)$ among graphs on n vertices having e edges is achieved by some graph coming from one of five families. These families have at most one member for a given n and e. In Section 4 we show that again we can use the compression from Section 3, and that we may assume our extremal graph is threshold. In Section 5 we introduce and discuss the five families. In Section 6 we state some lemmas, and use them to prove the main theorem, and the last section consists of proofs of these, rather technical, lemmas.

There are a variety of natural questions arising from this work that it seems interesting to resolve. For instance it is also very natural to consider the extremal problem for weighted homomorphisms. Even in the case of the easier result about independent sets, the extension to counting weighted independent sets does not seem to be known. It also seems likely the the techniques of Loh, Pikhurko, and Sudakov [17] might answer the question of when the wr-extremal graph switches from being "lex-like" to being a colex graph.

We refer the reader to [1] and [2] for any terminology not defined herein.

2. Threshold and Quasi-Threshold Graphs

In analyzing the structure of wr-extremal graphs it turns out that it is helpful to think about threshold graphs and quasi-threshold graphs. We define both of these classes in this section and prove some elementary facts about them. Both classes have been extensively studied—see, for instance, [18].

Definition. A simple graph G is a *threshold graph* if there exists a function $w : V(G) \to \mathbb{R}$ and a threshold $t \in \mathbb{R}$ such that $x \sim_G y$ if and only if $w(x) + w(y) \geq t$.

There are many ways to characterize threshold graphs; we include here a statement only of what we will need. A vertex x in a graph G is called *dominating* if $\{x\} \cup N(x) = V(G)$.

Lemma 2.1. *If G is a threshold graph then it can be formed from K_1 by successively adding either an isolated vertex or a dominating vertex. Thus for all threshold graphs G there exists a total ordering $<$ on $V(G)$ and a function $c : V(G) \to \{0, 1\}$ such that*

$$x \sim_G y \qquad \text{if and only if} \qquad c(\min(x, y)) = 1.$$

We call $c(v)$ the code of v. This code is unique up to changing the code of the first vertex.

Proof. See [5]. □

Notice that the codes of vertices from the beginning of the sequence are the most relevant. If our code is $(c_1, c_2, \ldots, c_n)$, then whether vertex v_i is adjacent to v_j is determined, if $i < j$, by c_i. In particular, the value c_n has no effect on the graph. One can think of constructing the graph from right to left: first we put down v_n, then we put down v_{n-1}, joined to v_n or not according to the value of c_{n-1}. We continue in this way, adding vertices and joining them to all or none of the vertices added so far.

We will often need to exhibit threshold graphs concisely. For this purpose we will use a diagram such as the one below, in which $+$ stands for vertices with code 1 and $-$ for vertices with code 0. The last vertex we denote by $\bullet$ since its code is irrelevant.

$$- - + + + - - - + + - - \bullet$$

Thus minuses are only adjacent to plusses to their left, while plusses are adjacent to every vertex to their right and also plusses on their left. We give a precise definition of threshold graphs with a given code below. First, for completeness we introduce our notation for the join and union of graphs.

Definition. The *join* of graphs G and H, denoted $G \vee H$, is the graph with vertex set $V(G) \cup V(H)$ and edge set $E(G) \cup E(H) \cup \{xy : x \in V(G) \text{ and } y \in V(H)\}$. The *disjoint union* of G and H, denoted $G \cup H$, has vertex set $V(G) \cup V(H)$ and edge set $E(G) \cup E(H)$.

For instance $+ + + + - - - - - - \bullet$ is $K_4 \vee E_6$, whereas $- - - - - - + + + \bullet$ is $K_4 \cup E_6$. In general we can define, as follows, a threshold graph based on any finite sequence of 0s and 1s.

Definition. Given a sequence $\sigma = (\sigma_i)_{i=1}^n$ with $\sigma_i \in \{0, 1\}$, we inductively define the *threshold graph with code σ* by setting $T()$ to be the null graph, and, for σ of length at least 1,

$$T(\sigma) = \begin{cases} v_1 \vee T(\sigma_2, \sigma_3, \ldots, \sigma_n) & \text{if } \sigma_1 = 1 \\ v_1 \cup T(\sigma_2, \sigma_3, \ldots, \sigma_n) & \text{if } \sigma_1 = 0 \end{cases}$$

We will write expressions such as $1^a0^b1^c\dots$ for the sequence consisting of a sequence of a 1s, b 0s, c 1s, etc. Also, given sequences σ and τ, we write $\sigma.\tau$ for their concatenation.

Example. The graph $T(1^n)$ is K_n, $T(0^n) = E_n$, and $T(1^a0^b)$ is the join of K_a and E_b. This last graph is called a *split graph.* Note also that $T(0) = T(1)$ is the unique one vertex graph, and in general $T(\sigma.0) = T(\sigma.1)$ for all sequences σ. It is easy to check that the lex graph $\mathcal{L}(n, e)$ is a threshold graph with code

$$++++++++++------(+)----\bullet$$

where the optional parenthetical plus can be located anywhere amongst the minuses. Likewise, the colex graph $\mathcal{C}(n, e)$ is a threshold graph with code:

$$----------+++++(-)++++\bullet$$

where again the optional parenthetical minus can be located anywhere amongst the plusses. The correspondence between the code above and the vertices $\{1, 2, 3, \dots, n\}$ of $\mathcal{C}(n, e)$ requires a little explanation. The vertices having code 0 (the minus signs above) are vertices $k, k+1, \dots, n$ for some k, and those with code 1 are $1, 2, \dots, k-1$. Exactly the same correspondence holds for $\mathcal{L}(n, e)$.

The second class of graphs we consider is the broader class of quasi-threshold graphs.

Definition. A graph G is *quasi-threshold* if for all $x, y \in V(G)$ with $x \sim y$ either

$$N[x] \subseteq N[y] \qquad \text{or} \qquad N[y] \subseteq N[x],$$

where we write $N[x]$ for the closed neighborhood of x, i.e., $N[x] = N(x) \cup \{x\}$.

We note that the set of threshold graphs is a proper subset of the set of quasi-threshold graphs since, for example, $K_2 \cup K_2$ is quasi-threshold but not threshold. As with threshold graphs, quasi-threshold graphs have many names and many characterizations. Most relevantly here they have an inductive description similar to that in Lemma 2.1. For completeness we give the proof here, though the result is standard.

Lemma 2.2. *A graph G is quasi-threshold if and only if it is either K_1, a non-trivial disjoint union of two quasi-threshold graphs, or a join of the form $K_1 \vee G'$ where G' is a quasi-threshold graph.*

Proof. If the graph is constructed as above, it is easy to check that it is quasi-threshold. We prove the other implication by induction on the number of vertices in a quasi-threshold graph $G = G(n)$. If G has one vertex, the claim is trivial. If G has more than one component then clearly each component is quasi-threshold, and we are done. Otherwise we may assume that G is connected. It suffices to prove that G has a dominating vertex, i.e., a vertex adjacent to all other vertices in G, since then it is of the form $K_1 \vee G'$, and G' is quasi-threshold since it is an induced subgraph of G. Suppose then that G does not have a dominating vertex and let x be a vertex of maximum degree in G. Since x is not a dominating vertex, there must be some vertex y such that $x \not\sim y$. Since G is connected, there is an x, y-path in H. Let P be an x, y-path of minimum length, and note that this length must be at least two since $x \not\sim y$. Let x_1 be the P-neighbor of x and x_2 the P-neighbor of x_1 that is not x. Since G is quasi-threshold and $x \sim x_1$, either $N[x] \subseteq N[x_1]$ or $N[x_1] \subseteq N[x]$, but $d(x)$ was chosen to be maximum, so $|N[x]| \geq |N[x_1]|$ and we cannot have $N[x] \subsetneq N[x_1]$. Therefore $N[x_1] \subseteq N[x]$. Since $x_1 \sim x_2$, x must be adjacent to x_2, contradicting the minimality of the path P. Thus x must be a dominating vertex. $\square$

We finish this section by introducing a compression which we will use later. Let G be any non-complete graph, and let x and y be adjacent vertices in G. The choice of x and y defines a natural partition of $V(G \setminus \{x, y\})$ into four parts: vertices which are adjacent only to x, vertices adjacent only to y, vertices adjacent to both and vertices adjacent to neither. We write

$$\begin{aligned} A_{x\bar{y}} &= \{v \in V(G \setminus \{x,y\}) \,:\, v \sim x, v \not\sim y\}\,, \\ A_{xy} &= \{v \in V(G \setminus \{x,y\}) \,:\, v \sim x, v \sim y\}\,, \text{ and} \\ A_{\bar{x}y} &= \{v \in V(G \setminus \{x,y\}) \,:\, v \not\sim x, v \sim y\}\,. \end{aligned}$$

Definition. The *compression of G from x to y*, denoted $G_{x\to y}$, is the graph obtained from G by deleting all edges between x and $A_{x\bar{y}}$ and adding all edges from y to $A_{x\bar{y}}$.

We will use this compression to make our graphs "more threshold". It is relatively straightforward to prove that a graph with the property that no compression changes its isomorphism type is quasi-threshold. Rather than prove this explicitly, we find it more convenient in the next lemmas to use the degree variance, or equivalently

$$d_2(G) = \sum_{x \in V(G)} d^2(x),$$

as a measure of how close we are to being threshold[1].

Lemma 2.3. *For any vertices $x, y \in V(G)$ the graph $G_{x\to y}$ satisfies $e(G_{x\to y}) = e(G)$ and $d_2(G_{x\to y}) \geq d_2(G)$. Moreover if x, y are such that $N[x] \nsubseteq N[y]$ and $N[y] \nsubseteq N[x]$ then $d_2(G_{x\to y}) > d_2(G)$.*

Proof. In changing G into $G_{x\to y}$ we have deleted $|A_{x\bar{y}}|$ edges and added $|A_{x\bar{y}}|$ edges, so $e(G_{x\to y}) = e(G)$. For the rest, we let $A_{x\bar{y}}$, A_{xy}, and $A_{\bar{x}y}$ be as defined as above, with $|A_{x\bar{y}}| = a$, $|A_{xy}| = b$ and $|A_{\bar{x}y}| = c$. If $x \sim y$ then

$$d_2(G_{x\to y}) - d_2(G) = (a+b+c+1)^2 + (b+1)^2 - (a+b+1)^2 - (b+c+1)^2 = 2ac \geq 0;$$

and if $x \not\sim y$ then

$$d_2(G_{x\to y}) - d_2(G) = (a+b+c)^2 + b^2 - (a+b)^2 - (b+c)^2 = 2ac \geq 0.$$

If $N[x]$ and $N[y]$ are incomparable then $a, c > 0$ so $d_2(G_{x\to y}) > d_2(G)$. □

Corollary 2.4. *Suppose that $\mathcal{G}$ is a family of graphs on a fixed vertex set V such that for any $G' \in \mathcal{G}$ and any $x, y \in V$ with $x \sim y$ we also have $G'_{x\to y} \in \mathcal{G}$. Suppose further that G satisfies*

$$d_2(G) = \max\left\{d_2(G') \,:\, G' \in \mathcal{G}\right\}.$$

Then G is quasi-threshold.

Proof. Suppose that there are $x, y \in V$ with $x \sim y$ and $N[x], N[y]$ incomparable. Then, by hypothesis, $G_{x\to y} \in \mathcal{G}$, and, by the previous lemma, $d_2(G_{x\to y}) > d_2(G)$, contradicting the maximality of G with respect to d_2. □

A very similar result is true if $\mathcal{G}$ is closed under all compressions $G \mapsto G_{x\to y}$ (rather than only those for which $x \sim y$). First we need a lemma which expresses the property of being threshold in terms of neighborhood inclusions.

Lemma 2.5. *A graph is threshold if and only if for every two distinct vertices x, y of G, either $N[x] \subseteq N[y]$ or $N[y] \subseteq N[x]$.*

Proof. See, for instance, [5]. □

[1]It was shown by Peled, Petreschi, and Sterbini in [19] that every d_2-extremal graph is of the form $T(0^a 1^b 0^c 1^d)$ or $T(1^a 0^b 1^c 0^d)$ with $\min\{b, c, d\} \leq 1$.

Lemma 2.6. *Suppose that $\mathcal{G}$ is a family of graphs on a fixed vertex set V such that for any $G' \in \mathcal{G}$ and any $x, y \in V$ we also have $G'_{x\to y} \in \mathcal{G}$. Suppose further that G satisfies*

$$d_2(G) = \max\left\{d_2(G') : G' \in \mathcal{G}\right\}.$$

Then G is threshold.

Proof. The proof of Lemma 2.3 shows that for all $x, y \in V$ we have either $N[x] \subseteq N[y]$ or $N[y] \subseteq N[x]$. The result follows by Lemma 2.5. □

3. Estimating the number of Independent Sets

In this section we consider Problem 1 in the case where H is K_2 with a loop on exactly one of the vertices. If 1 is the vertex with the loop, and 2 is the vertex without, then the only condition on a homomorphism $f : V(G) \to V(H)$ is that $f^{-1}(2)$ be an independent set in G. Thus we are trying to solve the following problem.

Problem 2. Given integers n, e, what is the maximum, over all graphs G having n vertices and e edges, of the number of independent set in G? (We denote this number by $i(G)$.)

The answer to this problem is a corollary to the Kruskal-Katona theorem [14, 13] involving minimizing the shadow of a set system. This section provides an introduction to our techniques that will be employed in the case of the Widom-Rowlinson model.

We begin by proving that compressing, as per the previous section, does not decrease the number of independent sets in G.

Lemma 3.1. *If G is a graph and x, y are distinct vertices of G then $i(G) \le i(G_{x\to y})$.*

Proof. Let us write $I(G)$ for the collection of all independent sets in G. We will show that $I \mapsto I \vartriangle \{x, y\}$ is an injection from $I(G) \setminus I(G_{x\to y})$ to $I(G_{x\to y}) \setminus I(G)$, and therefore $|I(G)| \le |I(G_{x\to y})|$. So, let I be a set that is independent in G, but not in $G_{x\to y}$. Then I must contain y and a vertex in $A_{x\bar{y}}$, say z, since the only edges in $G_{x\to y}$ that are not in G are between y and $A_{x\bar{y}}$. Further, note that $x \notin I$ since $xz \in E(G)$. We want to show that $I' = I \vartriangle \{x, y\}$ is independent in $G_{x\to y}$. It is certainly true that $I' \setminus \{x\} = I \setminus \{y\}$ is independent in $G_{x\to y}$, and x is not adjacent in $G_{x\to y}$ to any vertex outside of A_{xy}. Thus, if I' contained an edge, it would be between x and A_{xy}, which would imply that I contained an edge between y and A_{xy}, a contradiction. Finally, we note that I' is not independent in G since it contains both x and z, and $xz \in E(G)$. □

We now apply the compression technique of Section 2 to show that we may assume that the extremal graph for $i(G)$ is a threshold graph.

Lemma 3.2. *Let n, e be non-negative integers and suppose that G_1 is a graph having n vertices and e edges such that*

$$i(G_1) = \max\left\{i(G') : n(G') = n \text{ and } e(G') = e\right\}.$$

Then there exists a threshold graph G having the same number of vertices, edges, and independent sets as G_1.

Proof. Define $\mathcal{G}$ to be the set of all i-extremal graphs with the same vertex set as G_1, and the same number of edges as G_1. I.e.,

$$\mathcal{G} = \left\{G' : V(G') = V(G_1),\ e(G') = e, \text{ and } i(G') = i(G_1)\right\}.$$

By Lemma 3.1, if $G' \in \mathcal{G}$ and $x, y \in V(G')$ then $i(G'_{x\to y}) \ge i(G')$. Since, however, G' is i-extremal we also have $i(G'_{x\to y}) \le i(G')$. Thus $G'_{x\to y} \in \mathcal{G}$. We have shown that $\mathcal{G}$ satisfies the hypotheses of Lemma 2.6, and therefore any $G \in \mathcal{G}$ with $d_2(G) = \max\{d_2(G') : G' \in \mathcal{G}\}$ is threshold, and hence satisfies the conclusion of the lemma. □

One nice characteristic of threshold graphs is that the number of independent sets is relatively easy to count. The following definition allows us to talk easily about how to calculate $i(G)$ where G is threshold.

Definition. We define, for σ a finite $\{0,1\}$-sequence, a function $F_\sigma : \mathbb{N} \to \mathbb{N}$ inductively as follows. We let $F_0(k) = 2k$ and $F_1(k) = k+1$ for all $k \in \mathbb{N}$. For $|\sigma| >$ we define

$$F_{s_1 s_2 \dots s_k} = F_{s_1} \circ F_{s_2} \circ \dots \circ F_{s_k}.$$

If σ is the empty sequence then we define F_σ to be the identity function.

Lemma 3.3. *For all σ the function F_σ is a strictly increasing affine function with integer coefficients. If $G = T(\sigma)$ is a threshold graph, we have $i(G) = F_\sigma(1)$.*

Proof. The first statement is easy to prove by induction on $|\sigma|$. The claim about $i(G)$ is certainly true if G has 1 vertex; G in that case has 2 independent sets while $F_0(1) = F_1(1) = 2$. If $\sigma = 0.\sigma'$ then, letting $G' = T(\sigma')$, we have $i(G) = 2i(G')$. [We have added an isolated vertex to G'.] Thus

$$i(G) = 2i(G') = 2F_{\sigma'}(1) = F_0 \circ F_{\sigma'}(1) = F_\sigma(1).$$

Similarly, if $\sigma = 1.\sigma'$ then $i(G) = i(G') + 1$. [We have added a dominating vertex to G' and the only independent set containing this vertex has size 1.] So

$$i(G) = i(G') + 1 = F_{\sigma'}(1) + 1 = F_1 \circ F_{\sigma'}(1) = F_\sigma(1).$$

□

Now we are ready to show that $\mathcal{L}(n,e)$ has at least as many independent sets as any graph on n vertices and e edges.

Theorem 3.4. *If G is a graph on n vertices and e edges, then*

$$i(G) \le i(\mathcal{L}(n,e)).$$

Proof. We clearly may assume that G has

$$i(G) = \max\left\{ i(G') \,:\, n(G') = n \text{ and } e(G') = e \right\},$$

and therefore, by Lemma 3.2, we may assume that G is threshold. Say $G = T(\sigma)$. We will show that σ cannot be of the form $\phi.01.\psi.10.\rho$ (even if one or all of ϕ, ψ, or ρ are empty). If so we will compare G to $G' = T(\sigma')$ where $\sigma' = \phi.10.\psi.01.\rho$. It is easy to check that $e(G') = e(G)$, and we will show that $i(G') > i(G)$, contradicting the i-maximality of G. We will then show that the only threshold graphs whose codes do not contain this pattern are lex graphs.

Suppose then that σ has this form. By Lemma 3.3 we have

$$i(G) = F_\sigma(1) = F_\phi \circ F_{01} \circ F_\psi \circ F_{10} \circ F_\rho(1)$$
$$i(G') = F_{\sigma'}(1) = F_\phi \circ F_{10} \circ F_\psi \circ F_{01} \circ F_\rho(1).$$

Now every F_σ is strictly increasing, so $i(G') > i(G)$ if and only if

$$F_{10} \circ F_\psi \circ F_{01} \circ F_\rho(1) > F_{01} \circ F_\psi \circ F_{10} \circ F_\rho(1).$$

Let us denote $F_\rho(1)$ by s. By Lemma 3.3 the function F_ψ is a strictly increasing affine function, say $F_\psi(k) = ak + b$ for some constants a, b with $a > 0$. Thus

$$\begin{aligned} F_{10} \circ F_\psi \circ F_{01}(s) - F_{01} \circ F_\psi \circ F_{10}(s) &= F_{10} \circ F_\psi(2s+2) - F_{01} \circ F_\psi(2s+1) \\ &= F_{10}(a(2s+2)+b) - F_{01}(a(2s+1)+b) \\ &= 2a(2s+2) + 2b + 1 - \big(2a(2s+1) + 2b + 2\big) \\ &= 2a - 1 > 0. \end{aligned}$$

Hence under this hypothesis $i(G') > i(G)$, and G is not i-maximal.

We will call a 01 substring a *rise*, and a 10 substring a *fall*. We have shown that σ does not have a rise followed by a (disjoint) fall. We wish to show that σ is the code of a lex graph. Without loss of generality we may suppose that $\sigma_n = 0$, since the value of σ_n doesn't change the graph. Suppose first that σ has no rises; in that case σ is of the form 1^a0^b for some non-negative a, b and hence G is a lex graph. Otherwise we look for the first rise, and split σ there: $\sigma = \phi'.01.\psi' = \phi.\psi$, where $\phi = \phi'.0$ and $\psi = 1.\psi'$. Since ϕ does not contain a rise it is of the form 1^a0^b with $a \geq 0, b \geq 1$. Also, by the condition on σ we know that ψ' does not contain a fall; since $\sigma_n = 0$ this implies that $\psi = 0^c$ for some $c \geq 0$. Hence $\sigma = 1^a0^b10^c$ is the code for a lex graph. □

4. Estimating $\mathrm{wr}(G)$

Let us now consider the case of our problem where the image graph H is P_2°. A homomorphism $\phi \in \mathrm{Hom}(G, P_2^\circ)$ is determined by the two sets $A = \phi^{-1}(\{a\})$ and $C = \phi^{-1}(\{c\})$. The condition on these sets is simply that $E[A, C] = \emptyset$. Equivalently, there is a complete bipartite subgraph in $\bar{G}$ with bipartition (A, C). [There are a few subtleties to this correspondence, which we address in the proof of Lemma 6.7.]

We will show that the same compression $G \mapsto G_{x\to y}$ does not decrease the number of homomorphisms to P_2°, provided that $x \sim y$. It may well be that the restriction to $x \sim y$ is unnecessary, but we don't know a simple proof covering the other case. This lemma will show that we may take our wr-extremal graphs to be quasi-threshold. We later give an argument proving that we may take them to be threshold. As a reminder, we write $\mathrm{wr}(G)$ for $\hom(G, P_2^\circ)$.

Lemma 4.1. *If $x \sim y$, then* $\mathrm{wr}(G_{x\to y}) \geq \mathrm{wr}(G)$.

Proof. Suppose that $\phi \in \mathrm{Hom}(G, P_2^\circ) \setminus \mathrm{Hom}(G_{x\to y}, P_2^\circ)$. Since the only edges that are in $G_{x\to y}$ and not in G are between y and $A_{x\bar{y}}$, it must be the case that there exists a $z \in A_{x\bar{y}}$ such that either $\phi(y) = a$ and $\phi(z) = c$, or $\phi(y) = c$ and $\phi(z) = a$. Without loss of generality, assume that the former case holds. Since xz and xy are both edges in G, $\phi(x)$ must be b. Consider the map ϕ' defined by $\phi'(y) = \phi(x)$, $\phi'(x) = \phi(y)$ and $\phi' = \phi$ on all other vertices. Note that $\phi' \in \mathrm{Hom}(G_{x\to y}, P_2^\circ) \setminus \mathrm{Hom}(G, P_2^\circ)$ and thus the claim holds. Since the map $\phi \mapsto \phi'$ is an injection we are done. □

Lemma 4.2. *Let n, e be non-negative integers. There exists a quasi-threshold graph G with n vertices and e edges that is* wr*-extremal.*

The proof of Lemma 4.2 is exactly the same as that of Corollary 2.4, except we know now (by Lemma 4.1) that compressing from x to y does not decrease the number of homomorphisms to P_2° when $x \sim y$.

We now wish to boost up from quasi-threshold to threshold. We first calculate how the two constructions for threshold graphs affect $\mathrm{wr}(G)$.

Lemma 4.3.

(1) *If $v \in V(G)$ is an isolated vertex, then* $\mathrm{wr}(G) = 3\,\mathrm{wr}(G \setminus \{v\})$, *and*
(2) *If $v \in V(G)$ is dominating vertex, then* $\mathrm{wr}(G) = \mathrm{wr}(G \setminus \{v\}) + 2^{n(G)}$.

Proof. For (1), we simply note that the v can be mapped to any of the 3 vertices of P_2° and this does not affect where any other vertex of G is mapped. For (2), we consider cases according to where v is mapped to under a homomorphism, $\phi \in \mathrm{wr}(G)$. Let a, b and c be the vertices of P_2° as in Figure 1. If $\phi(v) = b$, then any other vertex in G is not restricted by its adjacency to v. Thus, the number of homomorphisms from G to P_2° such that $\phi(v) = b$ is simply $\mathrm{wr}(G \setminus \{v\})$. On the other hand, if $\phi(v) = a$, then every other vertex, since it is adjacent to v, must be mapped to either

a or b, and any such mapping is a homomorphism. Thus, the number of such homomorphisms is 2^{n-1}. The same argument applies when $\phi(v) = c$. Thus, adding these terms together, we get $\mathrm{wr}(G) = \mathrm{wr}(G \setminus \{v\}) + 2^n$. □

We are now ready to prove that there exist extremal graphs for $\mathrm{wr}(G)$ that are threshold graphs.

Lemma 4.4. *Let n, e be non-negative integers with $0 \le e \le \binom{n}{2}$. There exists a threshold graph G with n vertices and e edges that is* wr*-extremal.*

Proof. Let G be a wr-extremal graph with n vertices and e edges. By Lemma 4.2, we may assume that G is quasi-threshold. We prove the lemma by induction on n, the number of vertices in G. If $n = 1$, then G is obviously threshold, so we assume that $n > 1$ and the lemma is true for $n' < n$. If G contains an isolated vertex w then let $G_0 = G \setminus \{w\}$. Since $\mathrm{wr}(G) = 3\,\mathrm{wr}(G_0)$ it must be the case that G_0 is also wr-extremal. By induction, there is a threshold wr-extremal graph T with the same size and order as G_0, and adding an isolated vertex to T gives an extremal threshold graph. If G is connected, then by Lemma 2.2 G must have a dominating vertex, say v. Again set $G_0 = G \setminus \{v\}$. Since $\mathrm{wr}(G) = \mathrm{wr}(G_0) + 2^n$, G_0 is wr-extremal. By induction, there is again a threshold wr-extremal graph T with the same size and order as G_0, and adding a dominating vertex to T gives an extremal threshold graph.

If G is not connected, then, since $\mathrm{wr}(G)$ is the product of $\mathrm{wr}(C)$ for each component C, each component is wr-extremal, and hence, we may assume, threshold. Thus we may write

$$G = \bigcup_{i=1}^{k} (v_i \vee G_i),$$

where each $v_i \vee G_i$ is threshold. We will prove that $k = 1$, and hence that G is threshold.

Suppose then that $k \ge 2$. Set $H = (v_1 \vee G_1) \cup (v_2 \vee G_2)$, $R = G \setminus V(H)$, $\tilde{H} = (v_1 \vee (G_1 \cup G_2)) \cup \{v_2\} = G_{v_2 \to v_1}$, and $\tilde{G} = R \cup \tilde{H}$. Clearly $\tilde{G}$ has the same number of vertices and edges as does G. We will show that $\mathrm{wr}(\tilde{G}) > \mathrm{wr}(G)$, contradicting the wr-extremality of G. Let $h_i = \mathrm{wr}(G_i)$, $n_i = n(G_i)$ and $t_i = 2^{n_i}$. We have, by Lemma 4.3,

$$\mathrm{wr}(H) = (h_1 + 2t_1)(h_2 + 2t_2)$$

and

$$\mathrm{wr}(\tilde{H}) = 2(h_1 h_2 + 2t_1 t_2).$$

Thus,

$$\begin{aligned} \mathrm{wr}(\tilde{H}) - \mathrm{wr}(H) &= 2(h_1 h_2 + t_1 t_2 - t_1 h_2 - h_1 t_2) \\ &= 2(h_1 - t_1)(h_2 - t_2) > 0. \end{aligned}$$

(For the last inequality note that $\mathrm{wr}(G) > 2^{n(G)}$ for any graph with $n(G) \ge 1$.) Now

$$\mathrm{wr}(G) = \mathrm{wr}(H)\,\mathrm{wr}(R) < \mathrm{wr}(\tilde{H})\,\mathrm{wr}(R) = \mathrm{wr}(\tilde{G}),$$

contradicting the wr-extremality of G. □

We are now ready to state our main theorem, albeit in a somewhat simplified form. By applying the lemmas above, we know that there exists a wr-extremal graph that is a threshold graph. In fact, we are able to prove that any wr-extremal threshold graph has one of five forms.

Theorem 4.5. *Let G be a graph on n vertices and e edges. Then $\mathrm{wr}(G) \le \mathrm{wr}(H)$, where H is a threshold graph having n vertices, e edges, and of one of the following forms:*

$$
\begin{array}{cccccccccccccccccccccc}
- & - & - & - & - & - & - & - & - & - & + & + & + & + & + & (-) & + & + & + & + & + & \bullet \\
+ & + & + & + & + & + & + & + & + & + & - & - & - & - & - & (+) & - & - & - & - & - & \bullet \\
+ & + & + & + & + & + & + & + & + & + & - & - & - & - & - & - & - & - & - & + & + & \bullet \\
+ & + & + & + & + & + & + & (-) & + & + & - & - & - & - & - & - & - & - & - & - & - & \bullet \\
- & + & + & + & + & + & + & (-) & + & + & - & - & - & - & - & - & - & - & - & - & - & \bullet
\end{array}
$$

We will delay our proof of Theorem 4.5 until we have made the definitions of these potentially extremal graphs precise. Having done so, we will restate this theorem as Theorem 6.1.

5. The Potentially Extremal Graphs

Our theorem will prove that any graph G on n vertices and e edges has $\mathrm{wr}(G) \leq \mathrm{wr}(G')$ for some threshold graph G' chosen from a small collection of possibilities. We introduce those potentially extremal graphs here.

The first four examples are all very close to being split graphs, i.e., joins of a complete graph and an empty graph. We will call these graphs collectively *almost split graphs*. Writing $K(A)$ for the complete graph with vertex set A and similarly $E(A)$ for the empty graph on A, we define $\mathcal{S}(n,k)$ to be the split graph $K(\{1,\dots,k\}) \vee E(\{k+1,\dots,n\})$. The first almost split graph is the lex graph as defined in Section 1. Lex graphs interpolate between $\mathcal{S}(n,k-1)$ and $\mathcal{S}(n,k)$. If

$$(k-1)(n-k+1) < (k-1)(n-k+1) + w < k(n-k),$$

i.e., $0 \leq w \leq n-k-1$, then the lex graph with $e = (k-1)(n-k+1)+w$ edges is

$$\mathcal{L}(n,k,w) := \mathcal{L}(n,e) = \mathcal{S}(n,k) - \{kx \,:\, k+w+1 \leq x \leq n\}\,.$$

Our next almost split graph is also $\mathcal{S}(n,k)$ with some missing edges, but they are missing from the other side. For $1 \leq d < k \leq n$, we define the *deficient split graph of type* 1 *missing* d *edges* to be

$$\mathcal{D}_1(n,k,d) = \mathcal{S}(n,k) - \{(k+1)x \,:\, k-d+1 \leq x \leq k\}\,.$$

The *deficient split graph of type* 2 occurs when we remove at least k edges from the split graph, so for $k \leq n$ and $k \leq d < 2k$, we have

$$\mathcal{D}_2(n,k,d) = \mathcal{S}(n,k) - \{(k+1)x \,:\, 1 \leq x \leq k\} - \{(k+2)y \,:\, 2k-d+1 \leq y \leq k\}\,.$$

Our final almost split graph is the *buried triangle graph*. This is a split graph with a triangle inside the empty part. Formally,

$$\Delta(n,k) = \mathcal{S}(n,k) + \{(k+1)(k+2), (k+2)(k+3), (k+1)(k+3)\}$$

The other potentially extremal examples are the colex graphs, also defined in Section 1. These graphs interpolate between graphs

$$\mathcal{U}(n,q) = E(\{1,\dots,n-q\}) \cup K(\{n-q+1,\dots,n\}),$$

with consecutive values of q. [Our terminology arises from their structure as unions of an empty graph and a complete graph.] To be precise, for $0 \leq w \leq q \leq n-1$,

$$\mathcal{C}(n,q,w) := \mathcal{C}(n,e) = \mathcal{U}(n,q) + \{x(n-q) \,:\, n-w+1 \leq x \leq n\}\,,$$

with $e = \binom{q}{2} + w$. Thus, $\mathcal{C}(n,q,w)$ is a complete graph on q vertices, together with one vertex joined to w of these, and $n-q-1$ isolates. See Figure 2 for drawings of the potentially extremal graphs.

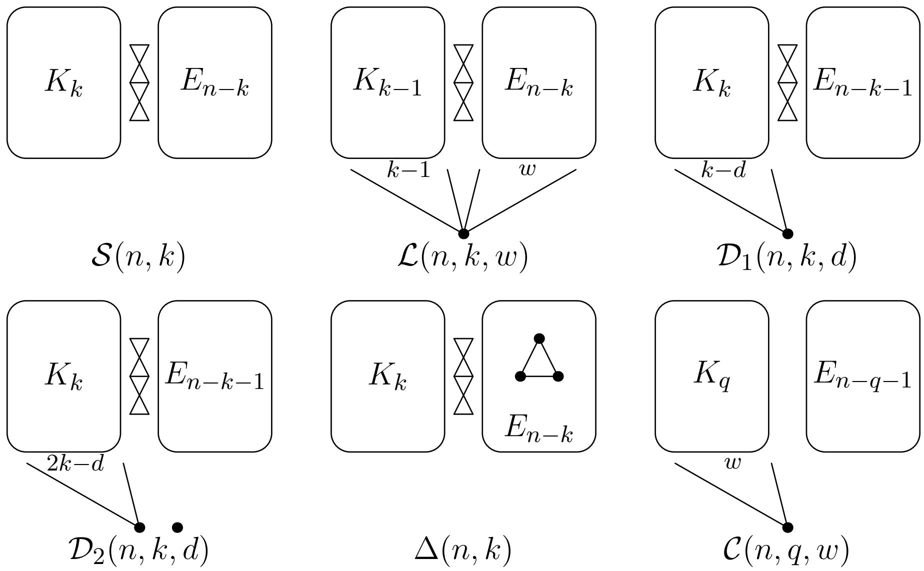

FIGURE 2. The potentially extremal graphs.

Lemma 5.1. *Colex graphs and almost split graphs are threshold, and, making the definitions in the left column, we have the identities in the right column:*

$$\begin{aligned} c(n,q,w) &:= 0^{n-q-1}1^w01^{q-w} & \mathcal{C}(n,q,w)) &= T(c(n,q,w)) \\ \ell(n,k,w) &:= 1^{k-1}0^{n-k-w}10^w & \mathcal{L}(n,k,w)) &= T(\ell(n,k,w)) \\ d_1(n,k,d) &:= 1^{k-d}01^d0^{n-k-1} & \mathcal{D}_1(n,k,d)) &= T(d_1(n,k,d)) \\ d_2(n,k,d) &:= 01^{2k-d}01^{d-k}0^{n-k-2} & \mathcal{D}_2(n,k,d)) &= T(d_2(n,k,d)) \\ b(n,k) &:= 1^k0^{n-k-3}1^3 & \Delta(n,k)) &= T(b(n,k)). \end{aligned}$$

Proof. Routine calculation. Note that vertices coded as 0 are on the empty side of the almost split graph, whereas those coded as 1 are on the complete side. The only exception to this statement are the three vertices of the triangle in $\Delta(n,k)$. □

We end this section with a lemma which giving the number of edges and homomorphisms to P_2° for each of the potentially extremal graphs. For convenience we also include these parameters for the split graph $\mathcal{S}(n,k)$ and the graph $\mathcal{U}(n,q)$. These will be helpful in the proof of the main theorem.

Lemma 5.2. *The potentially extremal graphs have the numbers of edges and homomorphisms to P_2° as in Table 1.*

Proof. Routine calculation. □

6. PROOF OF MAIN THEOREM

We are now in a position to state our main theorem precisely.

Theorem 6.1. *Let G be a graph on n vertices and e edges. Then there is some*

$$H \in \{\mathcal{L}(n,k,w), \mathcal{C}(n,q,w), \Delta(n,k), \mathcal{D}_1(n,k,d), \mathcal{D}_2(n,k,d)\},$$

such that $\mathrm{wr}(G) \le \mathrm{wr}(H)$ and H has e edges (and, of course, n vertices). Moreover, if G is wr*-extremal and threshold, then it is isomorphic to one of the graphs above.*

G	$e(G)$	$\mathrm{wr}(G)$
$\mathcal{S}(n,k)$	$\binom{k}{2}+k(n-k)$	$3^{n-k}+2^{n+1}-2^{n-k+1}$
$\mathcal{L}(n,k,w)$	$\binom{k}{2}+k(n-k)-(n-k-w)$	$2^{n+1}-2^{n-k+1}+3^{n-k}+2^{w+1}3^{n-w-k}$
$\Delta(n,k)$	$\binom{k}{2}+k(n-k)+3$	$2^{n+1}-2^{n-k+1}+5\cdot 3^{n-k-2}$
$\mathcal{D}_1(n,k,d)$	$\binom{k}{2}+k(n-k)-d$	$2^{n+1}-3\cdot 2^{n-k}+2^{n+d-k}+3^{n-k}$
$\mathcal{D}_2(n,k,d)$	$\binom{k}{2}+k(n-k)-d$	$3\cdot 2^{n}+3\cdot 2^{n+d-2k-1}-9\cdot 2^{n-k-1}+3^{n-k}$
$\mathcal{U}(n,q)$	$\binom{q}{2}$	$3^{n-q}(2^{q+1}-1)$
$\mathcal{C}(n,q,w)$	$\binom{q}{2}+w$	$2^{-w}3^{n-q-1}\left(2^{q+1}-3\cdot 2^{w}+2^{q+w+2}\right)$

Table 1. The number of edges and homomorphisms to P_2° for each of the classes of potentially extremal graphs.

Remark. For a given n and e, each of the potentially extremal families has at most one member with n vertices and e edges. Thus, the set of candidates in the theorem has at most five members. There are guaranteed to be at least two potentially extremal graphs, as the lex and colex graphs exist for any n and e.

When e is small, the optimal graph is "lex-like", and all four of the lex-like possibilities occur as the extremal graph for some value of e. For large values of e, the optimal graph is the colex graph. The lemmas below include crude estimates about when this change takes place, but we have no detailed theorem concerning the phase transition. We also do not know whether there are non-threshold wr-extremal graphs.

Before the proof of Theorem 6.1, we state several technical lemmas. Their proofs are in Section 7.

Lemma 6.2. *The threshold graph $G = T(1.c(n,q,w))$ is not* wr*-extremal unless $q \le (n-3)/2$.*

Lemma 6.3. *The threshold graph $G = T(0.\ell(n,k,w))$ with $w \ge 1$ is not* wr*-extremal unless one of the following conditions holds:*

(1) $k < \min\left\{\left(\dfrac{\ln(3/2)}{\ln(3)}\right)n-2, n-3\right\}$,
(2) $k = 1$, *in which case $G = T(0.\ell(n,k,w)) = \mathcal{L}(n+1,1,w)$ is potentially extremal, or*
(3) $w = n-k-1$, *in which case $G = T(0.\ell(n,k,w)) = \mathcal{D}_2(n+1,k,k+1)$ is potentially extremal.*

Lemma 6.4. *The threshold graph $G = T(0.b(n,k))$ is not* wr*-extremal unless*

$$3 \le k \le \frac{\ln(3/2)}{\ln(3)}(n-1).$$

Lemma 6.5. *Neither $G_0 = T(0.d_2(n,k,d))$ nor $G_1 = T(1.d_2(n,k,d))$ is* wr*-extremal, unless $k = d = 1$, in which case $G_0 = \mathcal{L}(n+1,1,n-2)$ is potentially extremal.*

Lemma 6.6. *If $n \ge 200$ and $k > 0.35n$, then neither $G = \mathcal{L}(n,k,w)$ nor $G = \Delta(n,k)$ is* wr*-extremal.*

Lemma 6.7. *If $k \ge n-4$, then $G = \mathcal{L}(n,k,w)$ is not* wr*-extremal, unless $e(G) \ge \binom{n}{2}-2$.*

Lemma 6.8. *If $n \ge 200$ and $0.04n < q < 0.6n$, then $G = \mathcal{C}(n,q,w)$ is not* wr*-extremal.*

Lemma 6.9. *If $n \ge 240$ and $21 \le q < .25n$, then $G = \mathcal{C}(n,q,w)$ is not* wr*-extremal.*

Proof of Theorem 6.1. We prove the result by induction on n. All the cases with $n \leq 240$ have been verified by computer search. The search is tremendously simplified by the fact that any suffix of a wr-extremal code must itself be extremal. Our program uses this observation to generate a list of all extremal codes on n vertices from the corresponding list for $n-1$ vertices (see [6]). Therefore, we may assume $n > 240$.

Without loss of generality, we may assume G is wr-extremal. By Lemma 4.4, we may assume that $G = T(\sigma_1, \sigma_2, \ldots, \sigma_n)$ is threshold. By Lemma 4.3, $G' = T(\sigma_2, \ldots, \sigma_n)$ is also wr-extremal. Thus, we may assume, by induction,

$$G' \in \{\mathcal{L}(n-1,k,w), \mathcal{C}(n-1,q,w), \Delta(n-1,k), \mathcal{D}_1(n-1,k,d), \mathcal{D}_2(n-1,k,d)\}$$

for some suitable values of k, w, q, d. The structure of the proof is outlined in Table 2. We deal with the cases $s_1 = 0, 1$, coupled with the five possibilities for the structure of G'.

	Choices for σ_1	
	0	1
$\mathcal{L}(n-1,k,w)$	Not extremal by Lemma 6.3 unless k is large or $k = 1, n-w-1$.	$G = \mathcal{L}(n,k+1,w)$
$\mathcal{C}(n-1,q,w)$	$G = \mathcal{C}(n,q,w)$	Not extremal by Lemma 6.2 unless q is small.
$\Delta(n-1,k)$	Not extremal by Lemma 6.4 unless k is large.	$G = \Delta(n,k)$
$\mathcal{D}_1(n-1,k,d)$	$G = \mathcal{D}_1(n,k,d+k)$	$G = \mathcal{D}_2(n,k+1,d)$
$\mathcal{D}_2(n-1,k,d)$	Not extremal by Lemma 6.5 unless $k = d = 1$.	Not extremal by Lemma 6.5.

TABLE 2. Structure of the proof of Theorem 6.1

To complete the proof, we need only address each "unless" in the table above. We deal with each one in turn, going down Table 2.

$G = T(0.\ell(n-1,k,w))$: Lemma 6.3 does not apply if $k \geq n-3$, $k \geq (\ln(3/2)/\ln(3))n - 2$, $k = 1$, or $k = n-w-1$. If $k \geq n-3$, by Lemma 6.7, either G' is not extremal, or $G' = \mathcal{C}(n,e)$. If $k \geq (\ln(3/2)/\ln(3))n - 2$, then by Lemma 6.6, since $k > 0.35(n-1)$, $\mathcal{L}(n-1,k,w)$ is not wr-extremal. If $k = 1$, then $G = \mathcal{L}(n,1,w)$. If $k = n-w-1$, then $G = \mathcal{D}_2(n,k,k+1)$.

$G = T(1.c(n-1,q,w))$: Lemma 6.2 does not apply if $q \leq (n-3)/2$. If $21 \leq q < 0.6(n-1)$ then, either by Lemma 6.8 or Lemma 6.9, G' is not extremal. If $q < 21$, then G consists of some graph on at most $\binom{21}{2} - 1$ vertices, together with a collection of isolated vertices. Therefore, our computer analysis of graphs on at most 240 vertices has already established that no such graph is wr-extremal, except $\mathcal{C}(n-1,0,w)$ for $w \leq 3$. Each of these three graphs is either isomorphic to a lex graph or a triangle.

$G = T(0.b(n-1,k))$: Lemma 6.4 does not apply if $k < (\ln(3/2)/\ln(3))(n-1)$ in which case Lemma 6.6 implies that, since $k > 0.35(n-1)$, $\Delta(n-1,k)$ is not wr-extremal.

$G = T(0.d_2(n-1,1,1))$: As we observe in Lemma 6.5, we have $G = \mathcal{L}(n,1,n-3)$.

We have established that G falls into one of the five cases described in the Theorem, and so we are done. □

7. Proofs of Lemmas

Lemma 6.2. *The threshold graph* $G = T(1.c(n,q,w))$ *is not* wr*-extremal unless* $q \le (n-3)/2$.

Proof. We will show that $G = T(1.c(n,q,w))$ is beaten by the colex graph with the same number of edges, i.e.,

$$\mathrm{wr}(1.c(n,q,w)) < \mathrm{wr}(\mathcal{C}(n+1, e(T(1.c(n,q,w))))).$$

There are two possibilities for $C = \mathcal{C}(n+1, e(T(1.c(n,q,w))))$; either

$$C = \begin{cases} \mathcal{C}(n+1, q+1, n+w-q) & \text{if } w \le 2q+1-n, \\ \mathcal{C}(n+1, q+2, n+w-2q-1) & \text{if } 2q+1-n < w \le 3q+3-n. \end{cases}$$

In the latter case, we have $q+2 \le n$. We cannot have $C = \mathcal{C}(n+1, q', w')$ with $q' = q+2$ since if that were the case, we'd have

$$\binom{q}{2} + 3q + 3 \le \binom{q'}{2} + w' = \binom{q}{2} + n + w \le \binom{q}{2} + n + q,$$

hence $n \ge 2q+3$, contradicting our hypothesis that $q > (n-3)/2$.

Suppose firstly that $C = \mathcal{C}(n+1, q+1, n+w-q)$. By Lemma 5.2, we have

$$\mathrm{wr}(C) - \mathrm{wr}(G) = 2 \cdot 3^{-q-1} \left(-2^n 3^{q+1} + 2^{q+1} 3^n - 2^{q-w} 3^n + 2^{2q+1-n-w} 3^n\right).$$

We are left with showing that this is at least zero. We can ignore the $2 \cdot 3^{-q-1}$ factor and note that, inside the parentheses, the term $2^{q+1}3^n$ beats both negative terms, the first by a factor of $(2/3)^{n-q-1}$ and the second by a factor of 2^{-w-1}. It therefore beats their sum unless either $q = n-1$, or $q = n-2$ and $w = 0$. When $q = n-1$ (and so $w = 1$), G and C are the same graph, namely, $\mathcal{C}(n+1, n, 2)$. On the other hand, when $q = n-2$ and $w = 0$, then the difference in the number of homomorphisms becomes 2^{n-2} and so we are done.

On the other hand, if $C = \mathcal{C}(n+1, q+2, n+w-2q-1)$, then

$$\mathrm{wr}(C) - \mathrm{wr}(G) = 2 \cdot 3^{-q-2} \left(3^{n+1} + 2^{q+1}3^n + 2^{3q-n-w+3}3^n - 2^n 3^{q+2} - 2^{q-w}3^{n+1}\right). \qquad (1)$$

Since $w \ge 2q+2-n$, we have $3^{n+1} > 2^{q-w}3^{n+1}$. Since $2^{q+1}3^n$ beats $2^n 3^{q+2}$ by a factor of $\frac{1}{3}\left(\frac{3}{2}\right)^{n-q-1}$, the above is certainly positive unless $q = n-1$ or $q = n-2$. The case $q = n-1$ does not occur since $q \le n-2$. In the case $q = n-2$, (1) reduces to

$$2^{-w-2}\left(2^n - 6\right)\left(2^n - 2^{w+2}\right).$$

This is positive as long as $n \ge 3$. ☐

Lemma 6.3. *The threshold graph* $G = T(0.\ell(n,k,w))$ *with* $w \ge 1$ *is not* wr*-extremal unless one of the following conditions holds:*

1. $k < \min\left\{\left(\dfrac{\ln(3/2)}{\ln(3)}\right)n - 2, n-3\right\}$,
2. $k = 1$ *in which case* $G = T(0.\ell(n,k,w)) = \mathcal{L}(n+1, 1, w)$ *is extremal, or*
3. $w = n-k-1$ *in which case* $G = T(0.\ell(n,k,w)) = \mathcal{D}_2(n+1, k, k+1)$ *is potentially extremal.*

Proof. We will show that $G = T(0.\ell(n,k,w))$ is beaten by either a lex graph with the same number of edges or a deficient split graph of type 2. There are in fact three possibilities for this alternative graph;

$$G' = \begin{cases} \mathcal{L}(n+1, k-1, n+w-2k+3) & \text{if } 0 \le w < k-1 \\ \mathcal{L}(n+1, k, w-k+1) & \text{if } k-1 \le w \le n-2k \\ \mathcal{D}_2(n+1, k, n-w) & \text{if } n-2k < w \le n-k. \end{cases}$$

In each case, we have $e(G) = e(G') = \binom{k}{2} + k(n-k) - (n-k-w)$.

In the first case, we have

$$\mathrm{wr}(G') - \mathrm{wr}(G) = 2 \cdot 3^{n-k+1} + 2^{n+w-2k+4}3^{k-w-1} - 2^{n+1} - 2^{n-k+2} - 2^{w+1}3^{n-k-w+1}.$$

We bound the ratios between each of the negative terms and the dominant positive term, 3^{n-k+2}.

$$\begin{aligned}
\frac{2^{w+1}3^{n-k-w+1}}{2 \cdot 3^{n-k+1}} &= \left(\frac{2}{3}\right)^{w} \leq \frac{2}{3} && \text{(since } w \geq 1\text{)} \\
\frac{2^{n-k+2}}{2 \cdot 3^{n-k+1}} &= \left(\frac{2}{3}\right)^{n-k+1} < \left(\frac{2}{3}\right)^{3} && \text{(since } k < n-3\text{)} \\
\frac{2^{n+1}}{2 \cdot 3^{n-k+1}} &= \left(\frac{2}{3}\right)^{n} \cdot 3^{k-1}.
\end{aligned}$$

We will show that $(2/3)^n 3^{k-1} < 1/27$ and therefore

$$\frac{\mathrm{wr}(G') - \mathrm{wr}(G)}{2 \cdot 3^{n-k+1}} > 1 - \frac{2}{3} - \left(\frac{2}{3}\right)^3 - \frac{1}{27} = 0.$$

The condition $(2/3)^n 3^{k-1} < 1/27$ reduces to

$$k < \left(\frac{\ln(3/2)}{\ln(3)}\right) n - 2,$$

which is true by hypothesis.

In the second case, by Lemma 5.2, we have

$$\begin{aligned}
\mathrm{wr}(G') - \mathrm{wr}(G) &= 2\left(2^{n-k+1} + 2^{w-k+1}3^{n-w} - 2^n - 2^w 3^{n-w-k+1}\right) \\
&= 2^{w-k+2}3^{n-2}\left(1 - \frac{2^n - 2^{n-k+1}}{3^{n-w}2^{w-k+1}} - \left(\frac{2}{3}\right)^{k-1}\right)
\end{aligned}$$

We need only consider the case $k \geq 2$, since $k = 1$ is one of the exceptional cases in the Lemma. If $k = 2$, the quantity in parentheses above reduces to $1 - (2/3)^{n-w} - 2/3 > 1 - (2/3)^4 - 2/3 > 0$, since $n - w \geq 2k = 4$. If $k \geq 3$, then

$$\begin{aligned}
\mathrm{wr}(G') - \mathrm{wr}(G) &= 2^{w-k+2}3^{n-2}\left(1 - \frac{2^n - 2^{n-k+1}}{3^{n-w}2^{w-k+1}} - \left(\frac{2}{3}\right)^{k-1}\right) \\
&> 2^{w-k+2}3^{n-2}\left(1 - \frac{2^n}{3^{n-w}2^{w-k+1}} - \left(\frac{2}{3}\right)^{k-1}\right) \\
&= 2^{w-k+2}3^{n-2}\left(1 - \left(\frac{2}{3}\right)^{n-w}2^{k-1} - \left(\frac{2}{3}\right)^{k-1}\right) \\
&\geq 2^{w-k+2}3^{n-2}\left(1 - \left(\frac{2}{3}\right)^{2k}2^{k-1} - \left(\frac{2}{3}\right)^{k-1}\right) \\
&> 2^{w-k+2}3^{n-2}\left(1 - \frac{1}{2}\left(\frac{8}{9}\right)^{k} - \left(\frac{2}{3}\right)^{k-1}\right) \\
&> 0,
\end{aligned}$$

where the final inequality follows from $k \geq 3$.

Now, for the last case, we have $G' = \mathcal{D}_2(n+1,k,n-w)$ and $n-2k < w \leq n-k$. In this case,

$$\begin{aligned}\mathrm{wr}(G') - \mathrm{wr}(G) &= 3\cdot 2^{-2k-w}\left(2^{n+k+w} - 2^{2k+2w+1}3^{n-w-k} + 4^n\right)\\ &> 3\cdot 2^{-2k-w}\left(4^n - 2\cdot 3^{n-(w+k)}4^{w+k}\right)\\ &= 4^n\cdot 3\cdot 2^{-2k-w}\left(1 - 2\left(\frac{3}{4}\right)^{n-(w+k)}\right)\end{aligned}$$

This is clearly positive unless $n-(w+k) \leq 2$, which implies that $w = n-k-1$ or $w = n-k-2$. The first case is one of the exceptional cases in the statement of the Lemma. In the second case,

$$\mathrm{wr}(G') - \mathrm{wr}(G) = 3\cdot 2^{n-k-1}.$$

□

Lemma 6.4. *The threshold graph $G = T(0.b(n,k))$ is not* wr*-extremal unless*

$$3 \leq k \leq \frac{\ln(3/2)}{\ln(3)}(n-1).$$

Proof. Let $L = \mathcal{L}(n+1,k,n-2k+4)$. Both G and L have $\binom{k}{2} + k(n-k) + 3$ edges. Note that $0 \leq n-2k+4 \leq n+1-k$. We have

$$\begin{aligned}\mathrm{wr}(L) - \mathrm{wr}(G) &= 4\cdot 3^{n-k-1} + 3^{k-3}2^{n-2k+5} - 2^{n+1} - 2^{n-k-1}\\ &> 4\cdot 3^{n-k-1} - 2^{n+1}\\ &> 0.\end{aligned}$$

The final inequality follows from the hypothesis on k. □

Lemma 6.5. *Neither $G_0 = T(0.d_2(n,k,d))$ nor $G_1 = T(1.d_2(n,k,d))$ is* wr*-extremal, unless $k = d = 1$, in which case $G_0 = \mathcal{L}(n+1,1,n-2)$ is extremal.*

Proof. Note that $\mathcal{D}_2(n,k,d)$ only exists when $k \leq d \leq 2k-1$. We first consider the case of G_0. Let $L_0 = \mathcal{L}(n+1,k,n-2k-d+1)$. Note that

$$e(G_0) = e(L_0) = \binom{k}{2} + k(n-k) - d.$$

The case $k = 1$ (and hence $d = 1$) is easy to check; both G_0 and L_0 consist of $K_{1,n-2} \cup E_2$, a potentially extremal graph. In the cases $k = 2, 3$, an explicit numerical computation establishes that $\mathrm{wr}(L_0) > \mathrm{wr}(G_0)$. Henceforth, we assume $k \geq 4$. We have

$$\begin{aligned}\mathrm{wr}(L_0) - \mathrm{wr}(G_0) &= 2^{n-2k-d-1}\left(11\cdot 2^{d+k} - 10\cdot 2^{d+2k} + 8\cdot 3^{d+k} - 9\cdot 4^d\right)\\ &> 2^{n-2k-d-1}\left(8\cdot 3^{d+k} - 10\cdot 2^{d+2k} - 9\cdot 4^d\right)\\ &> 2^{n-2k-d-1}\left(8\cdot 3^{d+k} - 10\cdot 2^{d+2k} - 10\cdot 2^{d+2k}2^{d-2k}\right)\\ &= 2^{n-2k-d-1}\left(8\cdot 3^{d+k} - \left(1 + 2^{d-2k}\right)10\cdot 2^{d+2k}\right)\end{aligned}$$

Thus, to prove $\mathrm{wr}(L_0) > \mathrm{wr}(G_0)$, it suffices to show

$$\left(\frac{3}{2}\right)^d\left(\frac{3}{4}\right)^k > \left(1 + 2^{d-2k}\right)\frac{5}{4}.$$

We consider two cases. If $d = 2k-1$, it reduces to

$$\left(\frac{27}{16}\right)^k > \frac{45}{16},$$

which is true for $k \geq 2$. On the other hand, if $d < 2k-1$, then we have

$$\left(\frac{3}{2}\right)^d \left(\frac{3}{4}\right)^k \geq \left(\frac{9}{8}\right)^k \geq \left(\frac{9}{8}\right)^4 > \left(\frac{5}{4}\right)^2 \geq \left(1+2^{d-2k}\right)\frac{5}{4}.$$

Proving that G_1 is not extremal is more straightforward. Define $G_1' = \mathcal{D}_2(n+1, k+1, d)$. We have

$$e(G_1) = e(G_1') = n + \binom{k}{2} + k(n-k) - d,$$

and

$$\mathrm{wr}(G_1') - \mathrm{wr}(G_1) = 2^n - 3 \cdot 2^{n+d-2k-2} > 2^n - 3 \cdot 2^{n-2} > 0,$$

since $d < 2k$. □

Lemma 6.6. *If $n \geq 200$ and $k > 0.35n$, then neither $G = \mathcal{L}(n,k,w)$ nor $G = \Delta(n,k)$ is* wr-*extremal.*

Proof. We will show that G is beaten by a colex graph. Then $\mathrm{wr}(G) < \mathrm{wr}(\mathcal{S}(n,k-1))$ since $\mathcal{S}(n,k-1)$ is a subgraph of G. We will choose m in such a way that $C = K_m \cup E_{n-m}$ has $e(C) \geq e(\mathcal{S}(n,k-1))$ and $\mathrm{wr}(C) > \mathrm{wr}(\mathcal{S}(n,k-1))$. If

$$e(K_m) = (m^2-m)/2 \geq e(\mathcal{S}(n,k-1)) = \binom{k-1}{2} + (k-1)(n-k+1),$$

then

$$m^2 - m - (k-1)(k-2) - 2(k-1)(n-k+1) \geq 0.$$

This will be true if

$$m \geq \frac{1+\sqrt{1+4(k-1)(2n-k)}}{2}.$$

Therefore, we define $m = \left\lceil \sqrt{k(2n-k)} + 1/2 \right\rceil$ which is sufficiently large since

$$\sqrt{k(2n-k)} = \frac{1}{2}\sqrt{4k(2n-k)} \geq \frac{1}{2}\sqrt{1+4(k-1)(2n-k)}.$$

Computing the number of homomorphisms, we have

$$\mathrm{wr}(C) \geq 3^{n-m}2^m = 3^n\left(\frac{2}{3}\right)^m$$

$$\mathrm{wr}(S(n,k-1)) \leq 3^{n-k+1} + 2^{n+1} = 3^n\left[\left(\frac{1}{3}\right)^{k-1} + 2\left(\frac{2}{3}\right)^n\right].$$

Note that, for $m \leq n-4$,

$$\frac{1}{2}\,\mathrm{wr}(C) \geq \frac{1}{2}3^n\left(\frac{2}{3}\right)^m \geq 3^n \cdot 2\left(\frac{2}{3}\right)^n = 2^{n+1}.$$

Now, we compare $\mathrm{wr}(C)/2$ with the other term, namely, 3^{n-k+1}. Writing $\alpha = k/n$,

$$\left(\frac{\mathrm{wr}(K_m)}{2\cdot 3^{n-k+1}}\right)^{1/n} \geq \frac{(2/3)^{\sqrt{2\alpha-\alpha^2}+2/n}}{(1/3)^\alpha 6^{1/n}} = \frac{(2/3)^{\sqrt{2\alpha-\alpha^2}}}{(1/3)^\alpha}\left(\frac{1}{14}\right)^{1/n}.$$

By hypothesis, $n \geq 200$, so $(1/14)^{1/n} \geq 0.95$ and

$$\geq 0.95 \frac{(2/3)^{\sqrt{2\alpha-\alpha^2}}}{(1/3)^{\alpha}}.$$

Routine analysis of this function of α establishes that it is strictly bigger than 1 for $\alpha > 0.35$.

Now, let $C' = \mathcal{C}(n, e)$, where $e = e(G)$. We know that C' is a subgraph of C since $e \leq e(C)$. Therefore,

$$\text{wr}(C') \leq \text{wr}(C) < \text{wr}(G),$$

establishing that G is not wr-extremal. □

Lemma 6.7. *If $k \geq n - 4$, then $G = \mathcal{L}(n, k, w)$ is not* wr*-extremal, unless $e(G) \geq \binom{n}{2} - 2$.*

Proof. Note that $\text{wr}(G) = 2^{n+1} - 1 + 2\,\text{cb}(\overline{G})$, where $\text{cb}(H)$ is the number of complete bipartite subgraphs of H. A homomorphism can either have range $\{a, b\}$, range $\{b, c\}$, or map to both a and c (where vertices of P_2° are labelled as in Figure 1). The first two cases account for $2^{n+1} - 1$ homomorphisms, while the remaining homomorphisms are in 2-to-1 correspondence with complete bipartite subgraphs of $\overline{G}$. Thus, maximizing $\text{wr}(G)$ is the same problem as maximizing $\text{cb}(\overline{G})$. Under the hypotheses of the Lemma, $\overline{G}$ is supported on vertices $\{n-3, n-2, n-1, n\}$. A simple case analysis proves that $\overline{G}$ is not cb-extremal unless $e(\overline{G}) \leq 2$. □

Lemma 6.8. *If $n \geq 200$ and $0.04n < q < 0.6n$, then $G = \mathcal{C}(n, q, w)$ is not* wr*-extremal.*

Proof. We will show that G is beaten by a lex graph. We know $\text{wr}(G) < \text{wr}(K_q \cup E_{n-q})$ since $K_q \cup E_{n-q}$ is a subgraph of G. We will choose k in such a way that $S = \mathcal{S}(n, k)$ has $e(S) \geq e(K_q \cup E_{n-q})$ and $\text{wr}(S) > \text{wr}(K_q \cup E_{n-q})$. We will choose k such that $k^2 + 2k(n-k) \geq q^2 + n$, for then

$$e(\mathcal{S}(n,k)) = \binom{k}{2} + k(n-k) \geq \binom{q}{2} = e(K_q \cup E(n-q)).$$

To be precise, we define

$$k = \left\lceil n - \sqrt{n^2 - q^2} + \frac{n}{2\sqrt{n^2 - q^2}} \right\rceil \leq n - \sqrt{n^2 - q^2} + 2.$$

Computing the number of homomorphisms, we have

$$\text{wr}(K_q \cup E_{n-q}) \leq 2 \cdot 3^n \left(\frac{2}{3}\right)^q$$

$$\text{wr}(S) \geq 3^{n-k}.$$

Therefore, writing $\beta = q/n$,

$$\left(\frac{H(S)}{H(K_q \cup E_{n-q})}\right)^{1/n} \geq \frac{(1/3)^{1-\sqrt{1-\beta^2}}}{(2/3)^{\beta}} \cdot \left(\frac{1}{18}\right)^{1/n}$$

For $n \geq 200$ and $0.04 < \beta < 0.6$, it is a routine calculation to check that

$$(1 - \sqrt{1-\beta^2}) \ln(1/3) - \beta \ln(2/3) \geq 0.015 \geq \frac{\ln(18)}{n},$$

and hence the Lemma is proved. □

Lemma 6.9. *If $n \geq 240$ and $21 \leq q < .25n$, then $G = \mathcal{C}(n, q, w)$ is not* wr*-extremal.*

Proof. We will show that G is beaten by a lex graph. First, we consider the case $q > 10\sqrt{n}$. We know $\mathrm{wr}(G) \le 3^{n-q}2^{q+1}$. We write $e = e(G)$ and define $\varepsilon = e/n^2$. We note that $\varepsilon n^2 \le q^2/2 \le (0.25)^2 n^2/2$, and thus $\varepsilon \le 0.05$. We define

$$k = \left\lceil \frac{\varepsilon n}{0.85} \right\rceil,$$

and $S = \mathcal{S}(n,k)$. We will show $e(S) \ge e(G)$ and $\mathrm{wr}(S) > \mathrm{wr}(G)$. First note that

$$k \le \frac{\varepsilon n}{0.82} - 1,$$

since otherwise we would have $\varepsilon n \le 46$ and hence $q \le 10\sqrt{n}$, contrary to our assumption on q. We have

$$\begin{aligned}\frac{\mathrm{wr}(S)}{\mathrm{wr}(G)} &\ge \frac{3^{n-k}}{3^{n-q}2^{q+1}} \\ &= \frac{(1/3)^k}{2(2/3)^q} \\ &\ge \frac{(1/3)^{\varepsilon n/0.82-1}}{2(2/3)^{\sqrt{\varepsilon}n}} \\ &\ge \frac{(1/3)^{\varepsilon n/0.82}}{(2/3)^{\sqrt{\varepsilon}n}}.\end{aligned}$$

So,

$$\left(\frac{\mathrm{wr}(S)}{\mathrm{wr}(G)}\right)^{1/n} \ge \frac{(1/3)^{\varepsilon/0.82}}{(2/3)^{\sqrt{\varepsilon}}}.$$

Routine calculation shows that this function of ε is at least 1 for all $\varepsilon \le 0.08$.

Now we will do the case $q \le 10\sqrt{n}$. Let $L = \mathcal{L}(n,k,w)$ be the lex graph on n vertices with e edges. Note that $e \ge kn$, and so

$$k \le \frac{e}{n} \le \frac{(10\sqrt{n}+1)(10\sqrt{n})}{2n} \le 51.$$

We have, for $q \ge 21$,

$$0.64(q-2)^2 \ge \binom{q+1}{2} \ge e \ge kn,$$

hence $q \ge \sqrt{kn/0.64} + 2$. We have

$$\begin{aligned}\frac{\mathrm{wr}(L)}{\mathrm{wr}(G)} &> \frac{3^{n-k}}{2 \cdot 3^n (2/3)^q} \\ &\ge \frac{(3/2)^{\sqrt{kn/0.64}}}{3^k}.\end{aligned}$$

Hence,

$$\left(\frac{\mathrm{wr}(L)}{\mathrm{wr}(G)}\right)^{1/k} \ge \frac{(3/2)^{\sqrt{\frac{n}{0.64k}}}}{3}.$$

This last expression is at least 1 for $\sqrt{n/0.64k} \ge \ln(3)/\ln(3/2)$, i.e., for $n \ge 0.64k(\ln(3)/\ln(3/2))^2$, which is true for $n \ge 4.7k$. Thus, since $k \le 51$, the Lemma is proved. ☐

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