Generating p-extremal graphs

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Abstract

Let $f(n,p)$ be the maximum number of edges in a graph on n vertices with p perfect matchings. Dudek and Schmitt proved that there exist constants n_p and c_p so that for even $n \geq n_p$, $f(n,p) = \frac{n^2}{4} + c_p$; we call a graph *$p$-extremal* if it has p perfect matchings and $\frac{n^2}{4} + c_p$ edges. In this paper, we develop structural theorems in matching theory to study p-extremal graphs and use them in a new computational method. This method extends the known sizes of p-extremal graphs from $p \leq 10$ to $p \leq 27$ while providing a complete characterization. This information provides further evidence towards a conjectured upper bound for all values of p and shows the sequence c_p is not monotonic.

1 Introduction

A *perfect matching* is a set of disjoint edges that cover all vertices. Let $\Phi(G)$ be the number of perfect matchings in a graph G, and for even n and positive p let $f(n,p)$ be the maximum number of edges in a graph G on n vertices with $\Phi(G) = p$. The exact behavior of $f(n,p)$ is not completely understood. In this work, we determine $f(n,p)$ for all $p \leq 27$ as well as characterize the graphs meeting these extremal values. We achieve these results by developing an extremal adaptation of structural results in matching theory and then applying these results in an isomorph-free generation algorithm. In the development, we use Lovász's Two Ear Theorem [4], structure theorems of Hartke, Stolee, West, and Yancey [3], and an isomorph-free generation scheme for 2-connected graphs [9].

Hetyei first characterized the extremal graphs with a single perfect matching and n vertices (unpublished; see [5, Corollary 5.3.14]) giving $f(n,1) = \frac{n^2}{4}$ for all even n. Dudek and Schmitt [1] generalized the problem for an arbitrary constant p and found the general form of $f(n,p)$ for sufficiently large n.

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Theorem 1.1 (Dudek, Schmitt [1]). *For every $p \geq 1$, there exist constants c_p, n_p so that for all even $n \geq n_p$, $f(n,p) = \frac{n^2}{4} + c_p$.*

From this theorem, understanding the behavior of $f(n,p)$ relies on understanding the sequences n_p and c_p. An important step to proving Theorem 1.1 is that if a graph exists with p perfect matchings, n vertices, and $\frac{n^2}{4} + c$ edges, then $f(m,p) \geq \frac{m^2}{4} + c$ for all even $m \geq n$ [1, Lemma 2.1]). This motivates defining the *excess* of G to be $c(G) = e(G) - \frac{1}{4}n(G)^2$, since any graph G with p perfect matchings gives a lower bound $c(G) \leq c_p$. A graph G with $\Phi(G) = p$ is *p-extremal* if it has $\frac{n^2}{4} + c_p$ edges. In other words, p-extremal graphs have the largest excess out of all graphs with p perfect matchings.

Dudek and Schmitt [1] computed c_p for $2 \leq p \leq 6$ and provided the exact structure of p-extremal graphs for $p \in \{2,3\}$. Hartke, Stolee, West, and Yancey [3] analyzed the structure of p-extremal graphs and found that for a fixed p, the infinite family is constructable from a finite set of fundamental graphs. Using McKay's graph generation program `geng` [7], they discovered these fundamental graphs, computed c_p for $7 \leq p \leq 10$, and described the structure of p-extremal graphs for $4 \leq p \leq 10$. These values of c_p are given in Table 1. The best previously known upper bound[1] is $c_p \leq p - 6$ for $p \geq 11$, while the best known lower bound is $c_p \geq 1$ for all $p \geq 2$ [3, Theorem 2.3].

p	1	2	3	4	5	6	7	8	9	10
n_p	2	4	4	6	6	6	6	6	6	6
c_p	0	1	2	2	2	3	3	3	4	4
	[1]						[3]			

Table 1: Known values of n_p and c_p.

For an integer n, the *double factorial* $n!!$ is the product of all numbers at most n with the same parity. The values of c_p are conjectured to be on order $O\left(\left(\frac{\ln p}{\ln \ln p}\right)^2\right)$, given below.

Conjecture 1.2 (Hartke, Stolee, West, Yancey [3]). *Let p, k, t be integers so that $k \in \{1, \dots, 2t\}$ and $k(2t-1)!! \leq p < (k+1)(2t-1)!!$ and set $C_p = t^2 - t + k - 1$. Always $c_p \leq C_p$.*

When $p = k(2t-1)!!$, a construction shows that $c_p \geq t^2 - t + k - 1$ [3].

We first extend structural theorems which form the core of the generation algorithm. After the algorithm framework is developed, we develop additional structure theorems to make the computation more efficient as well as significantly prune the search space. These theorems are motivated by algorithmic necessity, but may be of independent interest to the theory of perfect matchings. From this search, we obtain the sequence c_p and the structure of p-extremal graphs for all $p \leq 27$.

We begin by discussing the structure of p-extremal graphs in Section 2. Sections 3 through 7 contain the description of the computational technique and optimization strategies. A brief outline of these sections is given at the end of Section 2. In Section 8, we discuss the results of executing the search.

[1] This upper bound is given by $c_p \leq \max_{q<p} c_q + 1$ [1, Lemma 2.4] and that $c_p \leq 4$ for all $p \leq 10$ [3].

Notation

In this work, H and G are graphs, all of which will are simple: there are no loops or multi-edges. For a graph G, $V(G)$ is the vertex set and $E(G)$ is the edge set. The number of vertices is denoted $n(G)$ while $e(G)$ is the number of edges.

2 Structure of p-Extremal Graphs

In this section, we describe the structure of p-extremal graphs as demonstrated by Hartke, Stolee, West, and Yancey [3].

A graph is *matchable* if it has a perfect matching. An edge $e \in E(G)$ is *extendable* if there exists a perfect matching of G which contains e. Otherwise, e is *free*. The *extendable subgraph* (*free subgraph*) of G is the spanning subgraph containing all extendable (free) edges of G.

If the extendable subgraph of a matchable graph G is connected, then G is *elementary*. A set $S \subset V(G)$ is a *barrier*[2] if the number of connected components with an odd number of vertices in $G - S$ (denoted $\text{odd}(G - S)$) is equal to $|S|$. Recall Tutte's Theorem [11] states G is matchable if and only if $|S| \geq \text{odd}(G - S)$ for all subsets $S \subseteq V(G)$, so barriers are the sets which make this condition sharp. Note that the singletons $\{v\}$ for each $v \in V(G)$ is a barrier.

Elementary graphs and their barriers share important structure, which will be investigated thoroughly in Section 5. If G is both elementary and p-extremal, then $n(G)$ is bounded by a function of p and c_p.

Theorem 2.1 (Corollary 5.8 [3]). *Let $p \geq 2$. If G is a p-extremal elementary graph, then G has at most N_p vertices, where N_p is the largest even integer at most $3 + \sqrt{16p - 8c_p - 23}$.*

Any excess $c(G)$ for a graph G with $\Phi(G) = p$ can replace c_p in Theorem 2.1 to give an upper bound on the order of a p-extremal elementary graph.

Let G be a graph with $\Phi(G) > 0$. A *chamber* is a subgraph of G induced by a connected component of the extendable subgraph of G. Chambers are the maximal elementary subgraphs of G. Let $G_1, \ldots, G_k$ be elementary graphs and for each i let $X_i \subseteq V(G_i)$ be a barrier in G_i. The *spire* generated by $G_1, \ldots, G_k$ on $X_1, \ldots, X_k$ is the graph given by disjoint union of $G_1, \ldots, G_k$ and edges $x_i v_j$ for all $x_i \in X_i$ and $v_j \in V(G_j)$, whenever $i < j$. The following theorem states that all p-extremal graphs are spires with very specific conditions on $G_1, \ldots, G_k$ and $X_1, \ldots, X_k$.

Theorem 2.2 (Theorem 5.9 [3]). *Consider $p \geq 1$. For each p-extremal graph G in $\mathcal{F}_p$:*

1. *G is a spire generated by elementary graphs $G_1, \ldots, G_k$ on barriers $X_1, \ldots, X_k$.*
2. *The chambers of G are $G_1, \ldots, G_k$.*
3. *For each $i < k$, X_i is a barrier of maximum size in G_i.*
4. *For all $i < j$, $\frac{|X_i|}{n(G_i)} \geq \frac{|X_j|}{n(G_j)}$ and if equality holds, G_i and G_j can be swapped to form another p-extremal graph.*

[2] We adopt the convention that the empty set is a barrier.

5. $c(G) \leq \sum_{i=1}^{k} c(G_i)$. *Equality holds if and only if* $\frac{|X_i|}{n(G_i)} = \frac{1}{2}$ *for all* $i < k$.
6. *Let* $p_i = \Phi(G_i)$. $p = \prod_{i=1}^{k} p_i$.
7. *For all* i, $n(G_i) \leq N_{p_i}$.
8. *If* $p_i = 1$, *then* $G_i \cong K_2$, $|X_i| = 1$.

Theorem 2.2 provides an automated procedure for describing all p-extremal graphs. Begin by determining all q-extremal elementary graphs for each factor q of p. Then, compute the maximum-size barriers for these graphs. For all factorizations $p = \prod_{i=1}^{k} p_i$ and combinations of p_i-extremal elementary graphs G_i with maximum-size barrier X_i, compute $c(G)$ for the spire generated by $G_1, \dots, G_k$ on $X_1, \dots, X_k$. The maximum excess of these graphs is the value c_p. Larger graphs are built by adding elementary graphs isomorphic to K_2 and ordering the list of elementary graphs by the relative barrier size $\frac{|X_i|}{n(G_i)}$.

The most difficult part of this procedure is determining all q-extremal elementary graphs, which is the focus of the remainder of this work. In [3], the authors found the q-extremal elementary graphs by enumerating all graphs of order N_q using McKay's `geng` program [7] until $N_q \geq 14$ for $q \geq 11$, where this technique became infeasible. Our method greatly extends the range of computable values. We split elementary graphs into extendable and free subgraphs, which are generated in two stages of a computer search. We begin by investigating the structure of extendable subgraphs in Section 3. In Section 4, we utilize this structure to design an algorithm for generating all possible extendable subgraphs of q-extremal elementary graphs which focuses the search to a very sparse family of graphs. In Section 5, we investigate the structure of free subgraphs and design an algorithm to generate maximal graphs with a given extendable subgraph. This algorithm requires the full list of barriers for an extendable subgraph, so we describe in Section 6 an on-line algorithm for computing this list. In Section 7, we combine these techniques to bound the possible excess reachable from a given graph in order to significantly prune the search space. These algorithms are combined to a final implementation and the results of the computation are summarized in Section 8.

3 Structure of Extendable Subgraphs

A connected graph is *1-extendable* if every edge is extendable[3]. By the definition of elementary graph, the extendable subgraph of an elementary graph is 1-extendable.

A graph H with $n(H) \geq 3$ is *2-connected* if there is no vertex $x \in V(G)$ so that $H - x$ is disconnected.

Proposition 3.1. *If H is 1-extendable with $\Phi(H) \geq 2$, then H is 2-connected.*

Proof. Since $\Phi(H) \geq 2$, there are at least four vertices in H. Suppose H was not 2-connected. Then, there exists a vertex $x \in V(H)$ so that $H - x$ has multiple components. Since H has an even number of vertices, at least one component of $H - x$ must have an odd number of vertices. Since H has perfect matchings, Tutte's Theorem implies exactly one such component C has an odd number

[3] This term comes from k-extendable graphs, where every matching of size k extends to a perfect matching.

of vertices. Moreover, in every perfect matching of H, x is matched to some vertex in C. Hence, the edges from x to the other components never appear in perfect matchings, contradicting that H was 1-extendable. ∎

2-connected graphs are characterized by *ear decompositions*. An *ear* is a path given by vertices $x_0, x_1, \dots, x_k$ so that x_0 and x_k have degree at least three and x_i has degree exactly two for all $i \in \{1, \dots, k-1\}$. The vertices x_0 and x_k are *branch vertices* while $x_1, \dots, x_{k-1}$ are *internal vertices*. In the case of a cycle, the entire graph is considered to be an ear. For an ear ε, the *length* of ε is the number of edges between the endpoints and its *order* is the number of internal vertices between the endpoints. We will focus on the order of an ear. An ear of order 0 (length 1) is a single edge, called a *trivial* ear.

An *ear augmentation* is the addition of a path between two vertices of the graph. This process is invertible: an *ear deletion* takes an ear $x_0, x_1, \dots, x_k$ in a graph and deletes all vertices $x_1, \dots, x_{k-1}$ (or the edge x_0x_1 if $k = 1$). For a graph H, an ear augmentation is denoted $H + \varepsilon$ while an ear deletion is denoted $H - \varepsilon$. Every 2-connected graph H has a sequence of graphs $H^{(1)} \subset \cdots \subset H^{(k)} = H$ so that $H^{(1)}$ is a cycle and for all $i < k$, $H^{(i+1)} = H^{(i)} + \varepsilon_i$ for some ear ε_i [13].

Lovász's Two Ear Theorem gives the vital structural decomposition of 1-extendable graphs using a very restricted type of ear decomposition. A sequence $H^{(1)} \subset H^{(2)} \subset \cdots \subset H^{(k)}$ of ear augmentations is a *graded ear decomposition* if each $H^{(i)}$ is 1-extendable. The decomposition is *non-refinable* if for all $i < k$, there is no 1-extendable graph H' so that $H^{(i)} \subset H' \subset H^{(i+1)}$ is a graded ear decomposition.

Theorem 3.2 (Two Ear Theorem [4]; See also [5, 10]). *If H is 1-extendable, then there is a non-refinable graded ear decomposition $H^{(1)} \subset \cdots \subset H^{(k)}$ so that $H^{(1)} \cong C_{2\ell}$ for some ℓ and each ear augmentation $H^{(i)} \subset H^{(i+1)}$ uses one or two new ears, each with an even number of internal vertices.*

We will consider making single-ear augmentations to build 1-extendable graphs, so we classify the graphs which appear after the first ear of a two-ear augmentation. A graph H is *almost 1-extendable* if the free edges of H appear in a single ear of H. The following corollary is a restatement of the Two Ear Theorem using almost 1-extendable graphs.

Corollary 3.3. *If H is 1-extendable, then there is an ear decomposition $H^{(1)} \subset \cdots \subset H^{(k)}$ so that $H^{(1)} \cong C_{2\ell}$ for some ℓ, each ear augmentation $H^{(i)} \subset H^{(i+1)}$ uses a single ear of even order, each $H^{(i)}$ is either 1-extendable or almost 1-extendable, and if $H^{(i)}$ is almost 1-extendable then $H^{(i-1)}$ and $H^{(i+1)}$ are 1-extendable.*

An important property of graded ear decompositions is that $\Phi(H^{(i)}) < \Phi(H^{(i+1)})$, since the perfect matchings in $H^{(i)}$ extend to perfect matchings of $H^{(i+1)}$ using alternating paths within the augmented ear(s) and the other edges must appear in a previously uncounted perfect matching.

We use this theorem to develop our search space for the canonical deletion technique, forming the first stage of the search. The second stage adds free edges to a 1-extendable graph with p

perfect matchings. The structure of free edges is even more restricted, as shown in the following proposition.

Proposition 3.4 (Theorems 5.2.2 & 5.3.4 [5])**.** *Let G be an elementary graph. An edge e is free if and only if the endpoints are in the same barrier. If adding any missing edge to G increases the number of perfect matchings, then every barrier in G of size at least two is a clique of free edges.*

In Section 5, we describe a technique for adding free edges to a 1-extendable graph, providing the second stage of the search. In order to better understand the first stage, we investigate what types of ear augmentations are allowed in a non-refinable graded ear decomposition.

Lemma 3.5. *Let $H \subset H+\varepsilon$ be a one-ear augmentation between 1-extendable graphs H and $H+\varepsilon$. The endpoints of ε are in disjoint maximal barriers.*

Proof. If the endpoints of ε were not in disjoint maximal barriers, then they are contained in the same maximal barrier. If an edge were added between these vertices, Proposition 3.4 states that this edge would be free. Since ε is an even subdivision of such an edge, the edges incident to the endpoints are not extendable, making $H+\varepsilon$ not 1-extendable. ∎

Lemma 3.6. *Let $H \subset H+\varepsilon_1+\varepsilon_2$ be a non-refinable two ear augmentation between 1-extendable graphs.*

1. *The endpoints of ε_1 are within a maximal barrier of H.*
2. *The endpoints of ε_2 are within a different maximal barrier of H.*

Proof. (1) If the endpoints a, b of ε_1 span two different maximal barriers, adding the edge ab would add an extendable edge by Proposition 3.4. The perfect matchings of $H+ab$ and $H+\varepsilon_1$ would be in bijection depending on if ab was used: if a perfect matching M in $H+ab$ does not contain ab, M extends to a perfect matching in $H+\varepsilon_1$ by taking alternating edges within ε_1, with the edges incident to a and b not used; if M used ab, the alternating edges along ε_1 would use the edges incident to a and b. Hence, $H+\varepsilon_1$ is 1-extendable and this is a refinable graded ear decomposition. This contradiction shows that ε_1 spans vertices within a single maximal barrier.

(2) The endpoints x, y of ε_2 must be within a single maximal barrier by the same proof as (2), since otherwise $H+\varepsilon_2$ would be 1-extendable and the augmentation is refinable. However, if both ε_1 and ε_2 span the same maximal barrier, $H+\varepsilon_1+\varepsilon_2$ is not 1-extendable. By Proposition 3.4, edges within a barrier are free. Hence, the perfect matchings of $H+\varepsilon_1+\varepsilon_2$ do not use the internal edges of ε_1 and ε_2 which are incident to their endpoints. This contradicts 1-extendability, so the endpoints of ε_2 are in a different maximal barrier than the endpoints of ε_1. ∎

4 Searching for p-extremal elementary graphs

Given p and c, we aim to generate all elementary graphs G with $\Phi(G) = p$ and $c(G) \geq c$. If $c \leq c_p$, Theorem 2.1 implies $n(G) \leq N_p \leq 3 + \sqrt{16p - 8c - 23}$. In order to discover these graphs, we use the isomorph-free generation algorithm of [9] to generate 1-extendable graphs with up to p perfect matchings and up to N_p vertices. In this section, we briefly discuss this technique and how it is applied to the current problem. This algorithm is based on McKay's canonical deletion technique [6] and generates graphs using ear augmentations while visiting each unlabeled graph only once. This technique will generate 1-extendable graphs and almost 1-extendable graphs. Let $\mathcal{M}^p$ be the set of 2-connected graphs G with $\Phi(G) \in \{2, \dots, p\}$ that are either 1-extendable or almost 1-extendable. $\mathcal{M}^p_{N_p}$ is the set of graphs in $\mathcal{M}^p$ with at most N_p vertices.

The following lemma is immediate from Corollary 3.3.

Lemma 4.1. *For each graph $H \in \mathcal{M}^p$, either H is an even cycle or there exists an ear ε so that $H - \varepsilon$ is in $\mathcal{M}^p$.*

With this property, all graphs in $\mathcal{M}^p_{N_p}$ can be generated by a recursive process: Begin at an even cycle $H^{(1)} = C_{2\ell}$. For each $H^{(i)}$, try adding each all ears ε of order r to all pairs of vertices in $H^{(i)}$ where $0 \leq r \leq N_p - n(H^{(i)})$ to form $H^{(i+1)} + \varepsilon$. If $H^{(i+1)}$ is 1-extendable or $H^{(i)}$ is 1-extendable and $H^{(i+1)}$ is almost 1-extendable, recurse on $H^{(i+1)}$ until $\Phi(H^{(i+1)}) > p$. While this technique will generate all graphs in $\mathcal{M}^p_{N_p}$, it will generate each *unlabeled* graph several times. In fact, the number of times an unlabeled $H \in \mathcal{M}^p_{N_p}$ appears is *at least* the number of ear decompositions $H^{(1)} \subset \cdots \subset H^{(k)} \subset H$ which match the conditions of Corollary 3.3.

We will remove these redundancies in two ways. First, we will augment using pair orbits of vertices in $H^{(i)}$. Second, we will *reject* some augmentations if they do not correspond with a "canonical" ear decomposition of the larger graph.

Let $\mathrm{del}(H)$ be a function which takes a graph $H \in \mathcal{M}^p$ and returns an ear ε in H so that $H - \varepsilon$ is in $\mathcal{M}^p$. This function $\mathrm{del}(H)$ is a *canonical deletion* if for any two $H_1, H_2 \in \mathcal{M}^p$ so that $H_1 \cong H_2$, there exists an isomorphism $\sigma : H_1 \to H_2$ that maps $\mathrm{del}(H_1)$ to $\mathrm{del}(H_2)$.

Given a canonical deletion $\mathrm{del}(H)$, the *canonical ear decomposition* at H is given by the following iterative construction: (i) Set $H^{(0)} = H$ and $i = 0$. (ii) While $H^{(i)}$ is not a cycle, define $H^{(i-1)} = H^{(i)} - \mathrm{del}(H^{(i)})$ and decrement i. When this process terminates, what results is an ear decomposition $H^{(-k)} \subset H^{(-(k-1))} \subset \cdots \subset H^{(-1)} \subset H^{(0)}$ where $H^{(-k)}$ is isomorphic to a cycle and $H^{(0)} = H$.

A simple consequence of this definition is that if $H^{(-1)} = H - \mathrm{del}(H)$, then the canonical ear decomposition of H begins with the canonical ear decomposition of $H^{(-1)}$ then proceeds with the augmentation $H^{(-1)} \subset H^{(-1)} + \mathrm{del}(H) = H$. Applying isomorph-free generation algorithm of [9] will generate all unlabeled graphs in $\mathcal{M}^p$ without duplication by generating ear decompositions using all possible ear augmentations and rejecting any augmentations which are not isomorphic to the canonical deletion.

In order to guarantee the canonical deletion $\mathrm{del}(H)$ satisfies the isomorphism requirement, the choice will depend on a canonical labeling. A function $\mathrm{lab}(H)$ which takes a labeled graph H and outputs a bijection $\sigma_H : V(H) \to \{1, \dots, n(H)\}$ is a *canonical labeling* if for all $H_1 \cong H_2$ the map $\pi : V(H_1) \to V(H_2)$ defined as $\pi(x) = \sigma^{-1}_{H_2}(\sigma_{H_1}(x))$ is an isomorphism. The canonical labeling $\sigma_H = \mathrm{lab}(H)$ on the vertex set induces a label γ_H on the ears of H. Given an ear ε of order r between endpoints x and y, let $\gamma_H(\varepsilon)$ be the triple $(r, \min\{\sigma_H(x), \sigma_H(y)\}, \max\{\sigma_H(x), \sigma_H(y)\})$.

These labels have a natural lexicographic ordering which minimizes the order of an ear and then minimizes the pair of canonical labels of the endpoints. In this work, the canonical labeling $\text{lab}(H)$ is computed using McKay's `nauty` library [7, 2]. We now describe the canonical deletion $\text{del}(H)$ which will generate a canonical ear decomposition matching Corollary 3.3 whenever given a graph $H \in \mathcal{M}^p$.

By the proof of Lemma 4.1, we need all almost 1-extendable graphs H to have $H - \varepsilon$ be 1-extendable, but 1-extendable graphs H may have $H - \varepsilon$ be 1-extendable or almost 1-extendable, depending on availability. Also, since we are only augmenting by ears of even order, we must select the deletion to have this parity.

The following sequence of choices describe the method for selecting a canonical ear to delete from a graph H in $\mathcal{M}^p_{N_p}$:

1. If H is almost 1-extendable, select an ear ε so that $H - \varepsilon$ is 1-extendable. By the definition of almost 1-extendable graphs, there is a unique such choice.

2. If H is 1-extendable and there exists an ear ε so that $H - \varepsilon$ is 1-extendable, then select such an ear with minimum value $\gamma_H(\varepsilon)$.

3. If H is 1-extendable and no single ear ε has the deletion $H - \varepsilon$ 1-extendable, then select an even-order ear ε so that there is a disjoint even-order ear ε' so that $H - \varepsilon$ is almost 1-extendable and $H - \varepsilon - \varepsilon'$ is 1-extendable. Out of these choices for ε, select ε with minimum value $\gamma_H(\varepsilon)$.

The full generation algorithm, including augmentations, checking canonical deletions, as well as some optimizations and pruning techniques, is described in Section 8. We now investigate how to find p-extremal elementary graphs using 1-extendable graphs in $\mathcal{M}^p$. In the following section, we discuss how to fill a 1-extendable graph H with free edges without increasing the number of perfect matchings.

5 Structure of Free Subgraphs

By Proposition 3.4, the free edges within an elementary graph have endpoints within a common barrier. This implies that the structure of the free edges is coupled with the structure of barriers in G. In this section, we demonstrate that the structure of the free subgraph of a p-extremal elementary graph depends entirely on the structure of the barriers in the extendable subgraph. This leads to a method to generate all maximal sets of free edges that can be added to a 1-extendable graph. Section 6 describes a method for quickly computing the list of barriers of a 1-extendable graph using an ear decomposition. In particular, this provides an on-line algorithm which is implemented along with the generation of canonical ear decompositions. Finally, Section 7 combines the results of these sections into a very strict condition which is used to prune the search tree.

Let G be an elementary graph. The *barrier set* $\mathcal{B}(G)$ is the set of all barriers in G. The *barrier partition* $\mathcal{P}(G)$ is the set of all maximal barriers in G. The following lemmas give some properties of $\mathcal{P}(G)$ and $\mathcal{B}(G)$ when G is elementary.

Lemma 5.1 (Lemma 5.2.1 [5])**.** *For an elementary graph G, $\mathcal{P}(G)$ is a partition of $V(G)$.*

Lemma 5.2 (Theorem 5.1.6 [5])**.** *For an elementary graph G and $B \in \mathcal{B}(G)$, $B \neq \emptyset$, all components of $G - B$ have odd order.*

Given an elementary graph H, let $\mathcal{E}(H)$ be the set of elementary supergraphs with the same extendable subgraph: $\mathcal{E}(H) = \{G \supseteq H : V(G) = V(H), \Phi(G) = \Phi(H)\}$. We will refer to maximal elements of $\mathcal{E}(H)$ using the subgraph relation $\subseteq$, giving a poset $(\mathcal{E}(H), \subseteq)$. Note that $(\mathcal{E}(H), \subseteq)$ has a unique minimal element, H.

Proposition 5.3. *Let H be a 1-extendable graph. If G is a maximal element in $\mathcal{E}(H)$, then every barrier in $\mathcal{P}(G)$ is a clique of free edges in G.*

Proof. If some maximal barrier X in $\mathcal{P}(G)$ is not a clique, then there is a missing edge e between vertices x, y of X. Since $|X| = \text{odd}(G - X)$, all perfect matchings of $G + e$ must match at least one vertex of each odd component to some vertex in X, saturating X. This means that e is not extendable in $G + e$, and $G + e \in \mathcal{E}(H)$. This contradicts that G was maximal in $\mathcal{E}(H)$.

By Proposition 3.4, the edges within the barriers are free. ∎

Lemma 5.4. *Let H be a 1-extendable graph and $G \in \mathcal{E}(H)$ be an elementary supergraph of H. Every barrier B of G is also a barrier of H.*

Proof. Each odd component of $G - B$ is a combination of components of $H - B$, an odd number of which are odd components, giving $\text{odd}(H - B) \geq \text{odd}(G - B)$. There are no new vertices in G, so the components of $G - B$ partition $V(H) - B$ so that the partition of components of $H - B$ is a refinement of $G - B$.

Since B is a barrier of G, $\text{odd}(G - B) = |B|$. Since H is matchable, Tutte's Theorem implies $\text{odd}(H - B) \leq |B|$. Thus $|B| = \text{odd}(G - B) \leq \text{odd}(H - B) \leq |B|$ and equality holds, making B a barrier of H. ∎

Given a 1-extendable graph H, barriers B_1 and B_2 *conflict* if (a) $B_1 \cap B_2 \neq \emptyset$, (b) B_1 spans multiple components of $H - B_2$, or (c) B_2 spans multiple components of $H - B_1$. A set $\mathcal{I}$ of barriers in $\mathcal{B}(H)$ is a *cover set* if each pair B_1, B_2 of barriers in $\mathcal{I}$ are non-conflicting and $\mathcal{I}$ is a partition of $V(H)$. Let $\mathcal{C}(H)$ be the family of cover sets in $\mathcal{B}(H)$. If $\mathcal{I}_1, \mathcal{I}_2 \in \mathcal{C}(H)$ are cover sets, let the relation $\mathcal{I}_1 \preceq \mathcal{I}_2$ hold if for each set $B_1 \in \mathcal{I}_1$ there exists a set $B_2 \in \mathcal{I}_2$ so that $B_1 \subseteq B_2$. This defines a partial order on $\mathcal{C}(H)$ and the poset $(\mathcal{C}(H), \preceq)$ has a unique minimal element given by the partition of $V(H)$ into singletons.

Theorem 5.5. *Let H be a 1-extendable graph. A graph $G \in \mathcal{E}(H)$ is maximal in $(\mathcal{E}(H), \subseteq)$ if and only if each $B \in \mathcal{P}(G)$ is a clique, $\mathcal{P}(G)$ is a cover set, and $\mathcal{P}(G)$ is maximal in $(\mathcal{C}(H), \preceq)$.*

Proof. We define a bijection between $\mathcal{C}(H)$ and a subset of elementary supergraphs in $\mathcal{E}(H)$, as given in the following claim.

Claim 5.6. *Cover sets $\mathcal{I} \in \mathcal{C}(H)$ are in bijective correspondence with elementary graphs $G \in \mathcal{E}(H)$ where the free subgraph of G is a disjoint union of cliques, each of which is a (not necessarily maximal) barrier of G.*

Let G be a graph in $\mathcal{E}(H)$ where the free subgraph of G is a disjoint union of cliques X_1, X_2, ..., X_k, where each X_i is a barrier of G. Then, let $\mathcal{I} = \{X_1, \dots, X_k\}$ be the set of barriers. Note that $\mathcal{I}$ is a partition of $V(H)$, each part of which is a barrier of G which is a barrier of H by Lemma 5.4. Consider two barriers $B_1, B_2 \in \mathcal{I}$. Since we selected $\mathcal{I}$ to be a partition, $B_1 \cap B_2 = \emptyset$. If B_2 spans multiple components of $H - B_1$, then the vertices from these components are a single component in $G - B_1$, where B_2 is a clique of edges. However, Lemma 5.2 gives that all components of $H - B_1$ and $G - B_1$ are odd, since B_1 is a barrier. This implies that $|B_1| = \text{odd}(H - B_1) > \text{odd}(G - B_1) = |B_1|$, a contradiction. Hence, B_2 is contained within a single component of $H - B_1$, so B_1 and B_2 do not conflict in H. This gives that $\mathcal{I}$ is a cover set in $\mathcal{C}(H)$.

This map from $G \in \mathcal{E}(H)$ to $\mathcal{I} \in \mathcal{C}(H)$ is invertible by taking a cover set $\mathcal{I} \in \mathcal{C}(H)$ and filling each barrier $B \in \mathcal{I}$ with edges, forming a graph $H_{\mathcal{I}}$. Since each pair of barriers B_1, B_2 in $\mathcal{I}$ are non-conflicting, the components of $H - B_1$ do not change by adding edges between vertices in B_2. Therefore, each set $B \in \mathcal{I}$ is also a barrier in $H_{\mathcal{I}}$. By Proposition 3.4, the edges within each barrier of $H_{\mathcal{I}}$ are free, so all extendable edges of $H_{\mathcal{I}}$ are exactly those in H. This gives that $\Phi(H_{\mathcal{I}}) = \Phi(H)$ and $H_{\mathcal{I}} \in \mathcal{E}(H)$. The map from $\mathcal{I}$ to $H_{\mathcal{I}}$ is the inverse of the earlier map from $G \in \mathcal{E}(H)$ with free edges forming disjoint cliques to $\mathcal{I} \in \mathcal{C}(H)$. Hence, this is a bijection, proving the claim.

An important point in the previous claim is that the free edges formed cliques which are barriers, but those cliques were not necessarily *maximal* barriers. We now show that the above bijection maps edge-maximal graphs in $\mathcal{E}(H)$ to maximal cover sets in $\mathcal{C}(H)$.

Claim 5.7. *Let $\mathcal{I}$ be a cover set in $\mathcal{C}(H)$. The following are equivalent:*

(i) $\mathcal{I}$ *is maximal in* $(\mathcal{C}(H), \preceq)$.

(ii) $H_{\mathcal{I}}$ *is maximal in* $(\mathcal{E}(H), \subseteq)$.

(iii) $\mathcal{P}(H_{\mathcal{I}}) = \mathcal{I}$.

(ii) $\Rightarrow$ (iii) This is immediate from Proposition 5.3.

(iii) $\Rightarrow$ (ii) Any edge $e \notin E(H_{\mathcal{I}})$ must span two maximal barriers in $\mathcal{I}$. By Proposition 3.4, e is allowable in $H_{\mathcal{I}} + e$, so $H_{\mathcal{I}}$ is maximal in $(\mathcal{E}(H), \subseteq)$.

(i) $\Rightarrow$ (ii) Let $\mathcal{I}$ be a maximal cover set of barriers in $\mathcal{B}(H)$ and $H_{\mathcal{I}}$ the corresponding elementary supergraph in $\mathcal{E}(H)$. Suppose there exists a supergraph $H' \supset H_{\mathcal{I}}$ in $\mathcal{E}(H)$. Then, there is an edge e in $E(H') \setminus E(H_{\mathcal{I}})$ so that e is free in $H_{\mathcal{I}} + e$. This implies that e spans vertices within the same barrier B of $H_{\mathcal{I}} + e$ (by Proposition 3.4), and B is also a barrier of $H_{\mathcal{I}}$. However, B is split into k barriers $B_1, \dots, B_k$ in $\mathcal{I}$, for some $k \geq 2$. Therefore, the set $\mathcal{I}' = (\mathcal{I} \setminus \{B_1, \dots, B_k\}) \cup \{B\}$ is a refinement of $\mathcal{I}$.

We now show that $\mathcal{I}'$ is a cover set in $\mathcal{C}(H)$. Note that any two barriers $X_1, X_2 \in \mathcal{I}'$ where neither is equal to B is still non-conflicting. For any barrier $X \neq B$ in $\mathcal{I}'$, notice that X does not span more than one component of $H - B$, since B is a barrier in $H_{\mathcal{I}}$ and $H_{\mathcal{I}'}$. Also, if B spanned multiple components of $H - X$, then those components would be combined in $H_{\mathcal{I}'} - X$, but since X is a barrier, $|X| = \text{odd}(H_{\mathcal{I}'} - X) \leq \text{odd}(H - X) = |X|$. Therefore, B does not conflict with any other barrier X in $\mathcal{I}'$ giving $\mathcal{I}'$ is a cover set and $\mathcal{I} \preceq \mathcal{I}'$. This contradicts maximality of $\mathcal{I}$, so $H_{\mathcal{I}}$ is maximal.

(ii) $\Rightarrow$ (i) By (iii), $\mathcal{I} = \mathcal{P}(H_{\mathcal{I}})$. Let $\mathcal{I}'$ be a cover set so that $\mathcal{I} \preceq \mathcal{I}'$. $\mathcal{I}'$ also partitions $V(H)$, so $\mathcal{P}(H_{\mathcal{I}})$ is a refinement of $\mathcal{I}'$. Then, the graph $H_{\mathcal{I}'}$ is a proper supergraph of G. By the maximality of G, $H_{\mathcal{I}'}$ must not be an elementary supergraph in $\mathcal{E}(H)$. By the bijection of Claim 5.6, $\mathcal{I}'$ must not be a cover set of H. Therefore, $\mathcal{I}$ is a maximal covering set in $\mathcal{C}(H)$.

This proves the claim and the theorem follows. ∎

The previous theorem provides a method to search for the maximum elements of $\mathcal{E}(H)$ by generating all cover sets $\{B_1, \ldots, B_k\}$ in $\mathcal{C}(H)$ and maximizing the sum $\sum_{i=1}^{k} \binom{|B_i|}{2}$.

The naïve independent set generation algorithm runs with an exponential blowup on the number of barriers. This can be remedied in two ways. First, we notice empirically that the number of barriers frequently drops as more edges and ears are added, especially for dense extendable graphs. Second, the number of barriers is largest when the graph is bipartite, as there are exactly two maximal barriers each containing half of the vertices, with many subsets which are possibly barriers. We directly adress the case when H is bipartite as there are exactly two maximum elements of $\mathcal{E}(H)$.

Lemma 5.8 (Corollary 5.2 [3])**.** *The maximum number of free edges in an elementary graph with n vertices is $\binom{n/2}{2}$.*

Not only is this a general bound, but it is attainable for bipartite graphs. In a bipartite graph H, there are exactly two graphs in $\mathcal{E}(H)$ which attain this number of free edges.

Lemma 5.9. *If H is a bipartite 1-extendable graph, then there are exactly two maximal barriers, X_1 and X_2. Also, there are exactly two maximum elements G_1, G_2 of $\mathcal{E}(H)$. Each graph G_i is given by adding all possible edges within X_i.*

Proof. Let X_1 and X_2 be the two sides of the bipartition of H. Since H is matchable, $|X_1| = |X_2|$ and $V(H - X_1) = X_2$ and $V(H - X_2) = X_1$. Thus X_1 and X_2 are both barriers which partition $V(H)$ and by Lemma 5.1 these must be the maximal barriers of H.

The sets $\mathcal{I}_1 = \{X_1\} \cup \{\{v\} : v \in X_2\}$ and $\mathcal{I}_2 = \{X_2\} \cup \{\{v\} : v \in X_1\}$ are maximal cover sets in $\mathcal{C}(H)$. Using the bijection of Theorem 5.5, $\mathcal{I}_1$ corresponds with the maximal elementary graph G_1 in $\mathcal{E}(H)$ where all possible edges are added to X_1. Similarly, $\mathcal{I}_2$ corresponds to adding all possible edges to X_2, producing G_2. Each of these graphs has $\binom{n(H)/2}{2}$ free edges, the maximum possible for graphs in $\mathcal{E}(H)$ by Lemma 5.8.

We must show that any other graph G in $\mathcal{E}(H)$ has fewer free edges. We again use the bijection of Theorem 5.5 in order to obtain a maximal cover set $\mathcal{I}$ in $\mathcal{B}(H)$ which are filled with free edges in G. Then, the number of free edges in G is given by $s(\mathcal{I}) = \sum_{B \in \mathcal{I}} \binom{|B|}{2}$.

Without loss of generality, the barrier A of largest size within $\mathcal{I}$ is a subset of X_1. For convenience, we use $m = n(H)/2$ to be the size of each part X_1, X_2 and $k = |A|$, with $1 \le k < m$. Note that in $H_{\mathcal{I}}$, no free edges have endpoints in both A and $X_1 \setminus A$, leaving at least $k(m-k) = mk - k^2$ fewer free edges within X_1 in G than in G_1. If $H_{\mathcal{I}}$ has $\binom{n(H)/2}{2}$ edges, then the barriers in X_2 add at least $mk - k^2$ free edges.

The problem of maximizing $s(\mathcal{I})$ over all maximal cover sets can be relaxed to a linear program with quadratic optimization function as follows: First, fix the barriers of $\mathcal{I}$ within X_1, including the largest barrier, A. Then, fix the number of barriers of $\mathcal{I}$ within X_2 to be some integer ℓ. Then, let $\{B_1, \dots, B_\ell\}$ be the list of barriers in X_2. Now, create variables $x_i = |B_i|$ for all $i \in \{1, \dots, \ell\}$. The barriers in X_1 are fixed, so to maximize $s(\mathcal{I})$, we must maximize $\sum_{i=1}^{\ell} \binom{x_i}{2}$.

We now set some constraints on the x_i. Since the barriers B_i are not empty, we require $x_i \ge 1$. Since B_i does not conflict with A, each B_i is within a single component of $H - A$. Since there are $|A|$ such components, there are at least $|A| - 1$ other vertices in X_2 that are not in B_i, giving $x_i \le m - k + 1$. Also, since A is the largest barrier, $x_i \le k$. Finally, the barriers B_i partition X_2, giving $\sum_{i=1}^{\ell} x_i = m$ and that there are is at least one barrier per component, giving $\ell \ge k$.

Since for $x < y$, $\binom{x-1}{2} + \binom{y+1}{2} > \binom{x}{2} + \binom{y}{2}$, optimal solutions to this linear program have maximum value when the maximum number of variables have maximum feasible value. Suppose $1 \le x_i \le t$ are the tightest bounds on the variables $x_1, \dots, x_\ell$. Then $\frac{m-\ell}{t-1}\binom{t}{2}$ is an upper bound on the value of the system.

Case 1: Suppose $k \ge m-k+1$. Now, the useful constraints are $\sum_{i=1}^{\ell} x_i = m, 1 \le x_i \le m-k+1$ and we are trying to maximize $\sum_{i=1}^{\ell}\binom{x_i}{2}$. The optimal value is bounded by $\frac{m-\ell}{m-k}\binom{m-k+1}{2}$. As a function of ℓ, this bound is maximized by the smallest feasible value of ℓ, being $\ell = k$. Hence, we have an optimum value at most $\frac{m-k}{m-k}\frac{(m-k+1)(m-k)}{2} = \frac{1}{2}m(m+1) - \left(m + \frac{1}{2}\right)k - \frac{1}{2}k^2$. Since $k \ge m - k + 1$, the inequality $k \ge \frac{1}{2}(m+1)$ holds, and (ii) $\Rightarrow$ (iii) This is immediate from Proposition 5.3.

the optimum value of this program is at most

$$\frac{1}{2}m\left(m + \frac{1}{2}\right) - \left(m + \frac{1}{2}\right)k - \frac{1}{2}k^2 \le \underbrace{mk}_{k \ge \frac{1}{2}(m+1)} - \underbrace{k^2}_{k \le m} - \frac{1}{2}k^2 < mk - k^2.$$

Therefore, $H_{\mathcal{I}}$ must not have $\binom{n(H)/2}{2}$ free edges.

Case 2: Suppose $k < m-k+1$. The constraints are now $\sum_{i=1}^{\ell} x_i = m, 1 \le x_i \le k$ while maximizing $\sum_{i=1}^{\ell}\binom{x_i}{2}$. This program has optimum value bounded above by $\frac{m-\ell}{k-1}\binom{k}{2}$, which is maximized by the smallest feasible value of ℓ. If $m/k > k$ and $\ell < m/k$, the program is not even feasible, as a sum of ℓ integers at most k could not sum to m. Hence, $\ell \ge \max\{k, m/k\}$.

Case 2.a: Suppose $k \ge m/k$. Setting $\ell = k$ gives a bound of $\frac{m-k}{k-1}\binom{k}{2} = \frac{1}{2}(mk - k^2)$. This is clearly below $mk - k^2$, so $H_{\mathcal{I}}$ does not have $\binom{n(H)/2}{2}$ free edges.

Case 2.b: Suppose $k < m/k$. Setting $\ell = \lceil m/k \rceil$ gives a bound of $\frac{m - \lceil m/k \rceil}{k-1}\binom{k}{2} = \frac{1}{2}(mk - m)$. Since $k < m/k$, $k^2 < m$ and $\frac{1}{2}(mk - m) \le mk - k^2$. Hence, $H_{\mathcal{I}}$ does not have $\binom{n(H)/2}{2}$ free edges. ∎

Experimentation over the graphs used during the generation algorithm for p-extremal graphs shows that a naïve generation of cover sets in $\mathcal{C}(H)$ is sufficiently fast to compute the maximum excess in $\mathcal{E}(H)$ when the list of barriers $\mathcal{B}(H)$ is known. The following section describes a method for computing $\mathcal{B}(H)$ very quickly using the canonical ear decomposition.

6 The Evolution of Barriers

In this section, we describe a method to efficiently compute the barrier list $\mathcal{B}(H)$ of a 1-extendable graph H utilizing a graded ear decomposition. Consider a non-refinable graded ear decomposition $H^{(1)} \subset H^{(2)} \subset \cdots \subset H^{(k)} = H$ of a 1-extendable graph H starting at a cycle $C_{2\ell} = H^{(1)}$. Not only are the maximal barriers of $C_{2\ell}$ easy to compute (the sets X, Y forming the bipartition) but also the barrier list (every non-empty subset of X and Y is a barrier).

Lemma 6.1. *Let $H^{(i)} \subset H^{(i+1)}$ be a non-refinable ear decomposition of a 1-extendable graph $H^{(i+1)}$ from a 1-extendable graph $H^{(i)}$ using one or two ears. If B' is a barrier in $H^{(i+1)}$, then $B = B' \cap V(H)$ is a barrier in $H^{(i)}$.*

Proof. There are $|B'|$ odd components in $H^{(i+1)} - B'$. There are at most $|B|$ odd components in $H^{(i)} - B$, which may combine when the ear(s) are added to make $H^{(i+1)}$.

Let $x_1, x_2, \ldots, x_r$ be the vertices in $B' \setminus B$. Each x_i is not in $V(H^{(i)})$ so it is an internal vertex of an augmented ear. Therefore, x_i has degree two in $H^{(i+1)}$, so removing x_i from $H^{(i+1)} - (B \cup \{x_1, \ldots, x_{i-1}\})$ increases the number of odd components by at most one. Hence, the number of odd components of $H^{(i+1)} - B'$ is at most the number of odd components of $H^{(i)} - B$ plus the number of vertices in $B' \setminus B$. These combine to form the inequalities

$$|B'| = \text{odd}(H^{(i+1)} - B') \leq \text{odd}(H^{(i+1)} - B) + |B' \setminus B| \leq \text{odd}(H^{(i)} - B) + |B' \setminus B| \leq |B| + |B' \setminus B| = |B'|.$$

Equality holds above, so B is a barrier in $H^{(i)}$. ∎

As one-ear augmentations and two-ear augmentations are applied to each $H^{(i)}$, we update the list $\mathcal{B}(H^{(i+1)})$ of barriers in $H^{(i+1)}$ using the list $\mathcal{B}(H^{(i)})$ of barriers in $H^{(i)}$.

Lemma 6.2. *Let B be a barrier of a 1-extendable graph $H^{(i)}$. Let $H^{(i)} \subset H^{(i+1)}$ be a 1-extendable ear augmentation of $H^{(i)}$ using one (ε_1) or two ($\varepsilon_1, \varepsilon_2$) ears.*

1. *If any augmenting ear connects vertices from different components of $H^{(i)} - B$, then B is not a barrier in $H^{(i+1)}$, and neither is any $B' \supset B$ where $B = B' \cap V(H^{(i)})$.*
2. *Otherwise, if B does not contain any endpoint of the augmented ear(s), then B is a barrier of $H^{(i+1)}$, but $B \cup S$ for any non-empty subset $S \subseteq V(H^{(i+1)}) \setminus V(H^{(i)})$ is not a barrier of $H^{(i+1)}$.*
3. *If B contains both endpoints of some ear ε_i, then B is not a barrier in $H^{(i+1)}$ and neither is any $B' \supset B$.*
4. *If B contains exactly one endpoint (x) of one of the augmented ears (ε_j), then*

(a) *B is a barrier of $H^{(i+1)}$.*

(b) *For $S \subseteq V(H^{(i+1)}) \setminus V(H^{(i)})$, $B \cup S$ is a barrier of $H^{(i+1)}$ if and only if S contains only internal vertices of ε_j of even distance from x along ε_j.*

5. *If $B = \emptyset$, then for any subset $S \subseteq V(H^{(i+1)}) \setminus V(H^{(i)})$ $B \cup S$ is a barrier of $H^{(i+1)}$ if and only if the vertices in S are on a single ear ε_j and the pairwise distances along ε_j are even.*

Proof. Let B' be a barrier in $H^{(i+1)}$. Lemma 6.1 gives $B = B' \cap V(H^{(i)})$ is a barrier of $H^{(i)}$, and $H^{(i)} - B$ has $|B|$ odd connected components. Thus, the barriers of $H^{(i+1)}$ are built from barriers B in $H^{(i)}$ and adding edges from the new ear(s).

Case 1: If an ear ε_j spans two components of $H^{(i)} - B$, then the number of components in $H^{(i+1)} - B$ is at most $|B| - 2$. Any vertices from ε_j added to B can only increase the number of odd components by at most one at a time, but also increases the size of B by one. Hence, vertices in $V(H^{(i+1)}) \setminus V(H^{(i)})$ can be added to B to form a barrier in $H^{(i+1)}$.

Case 2: If each ear ε_j spans points in the same components of $H^{(i)} - B$, then the number of odd connected components in $H^{(i+1)} - B$ is the same as in $H^{(i)} - B$, which is $|B|$. Hence, B is a barrier of $H^{(i+1)}$. However, adding a single vertex from any e_i does not separate any component of $H^{(i+1)} - B$, but adds a count of one to $|B|$. Adding any other vertices from ε_j to B can only increase the number of components by one but increases $|B|$ by one. Hence, no non-empty set of vertices from the augmented ears can be added to B to form a barrier of $H^{(i+1)}$.

Case 3: Suppose B contains both endpoints of an ear ε_j. If ε_j is a trivial ear, then it is an extendable edge. If $B' \supseteq B$ is a barrier in $H^{(i+1)}$, this violates Proposition 3.4 which states edges within barriers are free edges. If ε_j has internal vertices, they form an even component in $H^{(i+1)} - B$. By Lemma 5.2, this implies that B is not a barrier. Any addition of internal vertices from ε_j to form $B' \supset B$ will add at most one odd component each, but leave an even component in $H^{(i+1)} - B'$. It follows that no such B' is a barrier in $H^{(i+1)}$.

Case 4: Note that If an ear ε_j has an endpoint within B, then in $H^{(i+1)} - B$, the internal vertices of ε_j are attached to the odd component of $H^{(i+1)} - B$ containing the opposite endpoint. Since there are an even number of internal vertices on ε_j, then $H^{(i+1)} - B$ has the same number of odd connected components as $H^{(i)} - B$, which is $|B|$. Hence, B is a barrier in $H^{(i+1)}$.

Let the ear ε_j be given as a path of vertices $x_0 x_1 x_2 \dots x_k$, where $x_0 = x$ and x_k is the other endpoint of ε_j. Let S be a subset of $\{x_1, \dots, x_{k-1}\}$, the internal vertices of ε_j. The number of components given by removing S from the path $x_1 x_2 \cdots x_{k-1} x_k$ is equal to the number of *gaps* in S: the values a so that x_a is in S and x_{a+1} is not in S. These components are all odd if and only if for each x_a and $x_{a'}$ in S, $|a - a'|$ is even. Thus, $B \cup S$ is a barrier in $H^{(i+1)}$ if and only if S is a subset of the internal vertices which are an even distance from x_0. ∎

Lemma 6.2 describes all the ways a barrier $B \in \mathcal{B}(H)$ can extend to a barrier $B' \in \mathcal{B}(H + \varepsilon_1)$ or $B' \in \mathcal{B}(H + \varepsilon_1 + \varepsilon_2)$. Note that the barriers B' which use the internal vertices of ε_1 are independent of those which use the internal vertices of ε_2, unless one of the ears spans multiple components of $H + \varepsilon_1 + \varepsilon_2 - B'$. This allows us to define a *pseudo-barrier list* $\mathcal{B}(H + \varepsilon)$ for almost 1-extendable graphs $H + \varepsilon$, where H is 1-extendable. During the generation algorithm, we consider a single-ear augmentation $H^{(i)} \subset H^{(i)} + \varepsilon_i = H^{(i+1)}$. Regardless of if $H^{(i)}$ or $H^{(i+1)}$ is almost 1-extendable, we can update $\mathcal{B}(H^{(i+1)})$ by taking each $B \in \mathcal{B}(H^{(i)})$ and adding each $B \cup S$ that satisfies Lemma 6.2 to $\mathcal{B}(H^{(i+1)})$. This process generates all barriers $B' \in \mathcal{B}(H^{(i+1)})$ so that $B' \cap V(H^{(i)}) = B$, so each barrier is generated exactly once.

In addition to updating the barrier list in an ear augmentation $H^{(i)} \subset H^{(i+1)}$, we determine the conflicts between these barriers.

Lemma 6.3. *Let $H^{(i)} \subset H^{(i+1)}$ be a 1-extendable ear augmentation using one (ε_1) or two $(\varepsilon_1, \varepsilon_2)$ ears. Suppose B_1' and B_2' are barriers in $H^{(i+1)}$ with barriers $B_1 = V(H^{(i)}) \cap B_1'$ and $B_2 = V(H^{(i)}) \cap B_2'$ of $H^{(i)}$. The barriers B_1' and B_2' conflict in $H^{(i+1)}$ if and only if one of the following holds: (1) $B_1' \cap B_2' \neq \emptyset$, (2) B_1 and B_2 conflict in $H^{(i)}$, or (3) B_1' and B_2' share vertices in some ear (ε_j), with vertices $x_0x_1x_2\dots x_k$, and there exist indices $0 \leq a_1 < a_2 < a_3 < a_4 \leq k$ so that $x_{a_1}, x_{a_3} \in B_1'$ and $x_{a_2}, x_{a_4} \in B_2'$.*

Proof. Note that by definition, if $B_1' \cap B_2' \neq \emptyset$, then B_1' and B_2' conflict. We now assume that $B_1' \cap B_2' = \emptyset$.

If B_1 or B_2 conflict in $H^{(i)}$, then without loss of generality, B_2 has vertices in multiple components of $H^{(i)} - B_1$. Since B_1' is a barrier in $H^{(i+1)}$, Lemma 6.2 gives that no ear ε_j spans multiple components of $H^{(i)} - B_1$, and the components of $H^{(i)} - B_1$ correspond to components of $H^{(i+1)} - B_1$. Hence, B_2 also spans multiple components of $H^{(i+1)} - B_1$ and B_1' and B_2' conflict in $H^{(i+1)}$.

Now, consider the case that the disjoint barriers B_1 and B_2 did not conflict in $H^{(i)}$. Since B_1 and B_2 are barriers of $H^{(i)}$, then the vertices in $B_1' \setminus B_1$ are limited to one ear ε_{j_1} of the augmentation, and similarly the vertices of $B_2' \setminus B_2$ are within a single ear ε_{j_2}. Since B_1 and B_2 do not conflict, all of the vertices within B_2 lie in a single component of $H^{(i)} - B_1$: the component containing the ear ε_{j_1}. Similarly, the vertices of B_1 are contained in the component of $H^{(i)} - B_2$ that contains the endpoints of ε_{j_2}.

The components of $H^{(i+1)} - B_1$ are components in $H^{(i+1)} - B_1'$ except the component containing the ear ε_{j_1} is cut into smaller components for each vertex in ε_{j_1} and B_1'. In order to span these new components, B_2' must have a vertex within ε_{j_1}. Therefore, the ears ε_{j_1} and ε_{j_2} are the same ear, given by vertices $x_0, x_1, \dots, x_k$.

Suppose there exist indices $0 \leq a_1 < a_2 < a_3 < a_4 \leq k$ so that x_{a_1} and x_{a_3} are in B_1' and x_{a_2} and x_{a_4} are in B_2'. Then, the vertices x_{a_1} and x_{a_3} of B_1' are in different components of $H^{(i+1)} - B_2'$, since every path from x_{a_3} to x_{a_1} in $H^{(i+1)}$ passes through one of the vertices x_{a_2} or x_{a_4}. Hence, B_1' and B_2' conflict.

If B_1' and B_2' do not admit such indices $a_1, \dots, a_4$, then listing the vertices $x_0, x_1, x_2, \dots, x_k$ in order will visit those in B_1' and B_2' in two contiguous blocks. In $H^{(i+1)} - B_1'$, the block containing the vertices in B_2' remain connected to the endpoint closest to the block, and hence B_2' will not span more than one component of $H^{(i+1)} - B_1'$. Similarly, B_1' will not span more than one component of $H^{(i+1)} - B_2'$. B_1' and B_2' do not conflict in this case. ∎

The following corollary is crucial to the bound in Lemma 7.1.

Corollary 6.4. *Let $H^{(i)} \subset H^{(i+1)}$ be a 1-extendable ear augmentation using one (ε_1) or two ($\varepsilon_1, \varepsilon_2$) ears. Let $\mathcal{I}$ be a maximal cover set in $\mathcal{C}(H^{(i+1)})$ and S be the set of internal vertices x of an ear ε_j such that the barrier in $\mathcal{I}$ containing x has at least one vertex in $V(H^{(i)})$. Then, S contains at most half of the internal vertices of ε_j.*

Proof. Let $A' \subset \mathcal{I}$ be the set of barriers containing a vertex x in ε_j and a vertex y in $V(H^{(i)})$. For a barrier B to contain an internal vertex of ε_j and a vertex in $V(H^{(i)})$, Lemma 6.2 states that B must contain at least one of the endpoints of the ear ε_j. Since each barrier in A' contains and endpoint of ε_j and non-conflicting barriers are non-intersecting, there are at most two barriers in A'.

If there is exactly one barrier B in A', by Lemma 6.2 it must contain vertices an even distance away from the endpoint contained in B, and hence at most half of the internal vertices of ε_j are contained in B.

If there are two non-conflicting barriers B_1 and B_2 in A', then by Lemma 6.3 the vertices of B_1 and B_2 within ε_j come in two consecutive blocks along ε_j. Since each barrier includes only vertices of even distance apart, B_1 contains at most half of the vertices in one block and B_2 contains at most half of the vertices in the other block. Hence, there are at most half of the internal vertices of ε_j in S. ∎

7 Bounding the maximum reachable excess

In order to prune search nodes, we wish to detect when it is impossible to extend the current 1-extendable graph H with q perfect matchings to a 1-extendable graph H' with p perfect matchings so that H' has an elementary supergraph $G' \in \mathcal{E}(H')$ with excess $c(G') \geq c$. The following lemma gives a method for bounding $c(G')$ using the maximum excess $c(G)$ over all elementary supergraphs G in $\mathcal{E}(H)$.

Lemma 7.1. *Let H be a 1-extendable graph on n vertices with $\Phi(H) = q$. Let H' be a 1-extendable supergraph of H built from H by a graded ear decomposition. Let $\Phi(H') = p > q$ and $N = n(H')$. Choose $G \in \mathcal{E}(H)$ and $G' \in \mathcal{E}(H')$ with the maximum number of edges in each set. Then,*

$$c(G') \leq c(G) + 2(p - q) - \frac{1}{4}(N - n)(n - 2).$$

Proof. Let

$$H = H^{(0)} \subset H^{(1)} \subset \cdots \subset H^{(k-1)} \subset H^{(k)} = H'$$

be a non-refinable graded ear decomposition as in Theorem 3.2. For each $i \in \{0, 1, \ldots, k\}$, let $G^{(i)} \in \mathcal{E}(H^{(i)})$ be of maximum size. Without loss of generality, assume $G^{(0)} = G$ and $G^{(k)} = G'$. The following claims bound the excess $c(G^{(i)})$ in terms of $c(G^{(i-1)})$ using the ear augmentation $H^{(i-1)} \subset H^{(i)}$.

Claim 7.2. *If $H^{(i-1)} \subset H^{(i)}$ is a single ear augmentation $H^{(i)} = H^{(i-1)} + \varepsilon_1$ where ε_1 has order $\ell^{(i)}$, then*

$$c(G^{(i)}) \le c(G^{(i-1)}) + 1 + \frac{3}{4}\ell^{(i)} - \frac{1}{8}(\ell^{(i)})^2 - \frac{1}{4}\ell^{(i)} n(H^{(i-1)}).$$

By Lemma 3.5, ε_1 spans two maximal barriers $X, Y \in \mathcal{P}(H^{(i)})$. $H^{(i)}$ has $\ell^{(i)}+1$ more extendable edges than $H^{(i-1)}$.

We now bound the number of free edges $G^{(i)}$ has compared to the number of free edges in $G^{(i-1)}$. The elementary supergraph $G^{(i)}$ has a clique partition of free edges given by a maximal cover set $\mathcal{I}$ in $\mathcal{C}(H^{(i)})$. For each barrier $B \in \mathcal{I}$, the set $B \cap V(H^{(i-1)})$ is also a barrier of $H^{(i-1)}$, by Lemma 6.1. Through this transformation, the maximal cover set $\mathcal{I}$ admits an cover set $\mathcal{I}' = \{B \cap V(H^{(i-1)}) : B \in \mathcal{I}\}$ in $\mathcal{C}(H^{(i-1)})$. This cover set $\mathcal{I}'$ generates an elementary supergraph $G_*^{(i-1)} \in \mathcal{E}(H^{(i-1)})$ through the bijection in Claim 5.6. The free edges in $G^{(i)}$ which span endpoints within $V(H^{(i-1)})$ are exactly the free edges of $G_*^{(i-1)}$. By the selection of $G^{(i-1)}$, $e(G_*^{(i-1)}) \le e(G^{(i-1)})$.

When $\ell^{(i)} > 0$, the $\ell^{(i)}$ internal vertices of ε_1 may be incident to free edges whose other endpoints lie in the barriers X and Y. By Corollary 6.4, at most half of the vertices in ε_1 have free edges to vertices in X and Y. Since the barriers X and Y are in $H^{(i-1)}$, they have size at most $\frac{n(H^{(i-1)})}{2}$. So, there are at most $\frac{\ell^{(i)}}{2}\frac{n(H^{(i-1)})}{2}$ free edges between these internal vertices and the rest of the graph. Also, there are at most $\binom{\ell^{(i)}/2}{2} = \frac{1}{8}(\ell^{(i)})^2 - \frac{1}{4}\ell^{(i)}$ free edges between the internal vertices themselves. Combining these edge counts leads to the following inequalities:

$$\begin{aligned}
c(G^{(i)}) &= e(G^{(i)}) - \frac{(n(H^{(i-1)}) + \ell^{(i)})^2}{4} \\
&\le \left[e(G_*^{(i-1)}) + \left(1 + \ell^{(i)}\right) + \frac{n(H^{(i-1)})\ell^{(i)}}{2} + \frac{1}{8}(\ell^{(i)})^2 - \frac{1}{4}\ell^{(i)}\right] \\
&\qquad - \left[\frac{n(H^{(i-1)})^2}{4} + \frac{n(H^{(i-1)})\ell^{(i)}}{2} + \frac{(\ell^{(i)})^2}{4}\right] \\
&\le e(G^{(i-1)}) + 1 + \frac{3}{4}\ell^{(i)} - \frac{n(H^{(i-1)})^2}{4} - \frac{1}{8}(\ell^{(i)})^2 \\
&= c(G^{(i-1)}) + 1 + \frac{3}{4}\ell^{(i)} - \frac{1}{8}(\ell^{(i)})^2 - \frac{1}{4}\ell^{(i)} n_{i-1}.
\end{aligned}$$

This proves Claim 7.2. We now investigate a similar bound for two-ear autmentations.

Claim 7.3. *Let $H^{(i-1)} \subset H^{(i)}$ be a two-ear augmentation $H^{(i)} = H^{(i-1)} + \varepsilon_1 + \varepsilon_2$ where the ears ε_1 and ε_2 have $\ell_1^{(i)}$ and $\ell_2^{(i)}$ internal vertices, respectively. Set $\ell^{(i)} = \ell_1^{(i)} + \ell_2^{(i)}$. Then,*

$$c(G^{(i)}) \le c(G^{(i)}) + 2 + \frac{3}{4}\ell^{(i)} - \frac{1}{8}(\ell^{(i)})^2 - \frac{1}{4}\ell_1^{(i)}\ell_2^{(i)} - \frac{1}{4}\ell^{(i)} n(H^{(i-1)}.$$

By Lemma 3.6, the first ear spans endpoints x_1, x_2 in a maximal barrier $X \in \mathcal{P}(H^{(i)})$ and the second ear spans endpoints y_1, y_2 in a different maximal barrier $Y \in \mathcal{P}(H^{(i)})$. Note that after these augmentations, x_1 and x_2 are not in the same barrier, and neither are y_1 and y_2, by Lemma 6.2.

The graph $G^{(i)}$ is an elementary supergraph of $H^{(i)}$ given by adding cliques of free edges corresponding to a maximal cover set $\mathcal{I}$ in $\mathcal{C}(H^{(i)})$. By Lemma 6.1, each barrier $B \in \mathcal{I}$ generates the barrier $B \cap V(H^{(i-1)})$ in $V(H^{(i-1)})$. This induces a cover set $\mathcal{I}' = \{B \cap V(H^{(i-1)}) : B \in \mathcal{I}\}$ in $\mathcal{C}(H^{(i-1)})$ which in turn defines an elementary supergraph $G_*^{(i-1)}$ through the bijection in Claim 5.6. By the choice of $G^{(i-1)}$, $e(G_*^{(i-1)}) \leq e(G^{(i-1)})$.

Consider the number of free edges in $G^{(i)}$ compared to the free edges in $G_*^{(i-1)}$. First, the number of edges between the $\ell_1^{(i)} + \ell_2^{(i)}$ new vertices and the $n(H^{(i-1)})$ original vertices is at most $\left(\frac{\ell_1^{(i)}}{2} + \frac{\ell_2^{(i)}}{2}\right) \frac{n(H^{(i-1)})}{2}$, since the additions must occur within barriers, at most half of the internal vertices of each ear can be used (by Corollary 6.4), and barriers in $H^{(i-1)}$ have at most $\frac{n(H^{(i-1)})}{2}$ vertices. Second, consider the number of free edges within the $\ell_1^{(i)} + \ell_2^{(i)}$ vertices. Note that no free edges can be added between ε_1 and ε_2 since the internal vertices of ε_1 and ε_2 are in different maximal barriers of $H^{(i)}$. Thus, there are at most $\binom{\ell_1^{(i)}/2}{2} + \binom{\ell_2^{(i)}/2}{2}$ free edges between the internal vertices. Since $\binom{\ell_1^{(i)}/2}{2} + \binom{\ell_2^{(i)}/2}{2} = \frac{1}{8}(\ell_1^{(i)} + \ell_2^{(i)})^2 - \frac{1}{4}(\ell_1^{(i)} + \ell_2^{(i)} + \ell_1^{(i)}\ell_2^{(i)})$, we have

$$\begin{aligned}
c(G^{(i)}) &= e(G^{(i)}) - \frac{(n_{i-1}) + \ell_1^{(i)} + \ell_2^{(i)})^2}{4} \\
&\leq e(G_*^{(i-1)}) + \left(1 + \ell_1^{(i)} + 1 + \ell_2^{(i)}\right) + \frac{n(H^{(i-1)})(\ell_1^{(i)} + \ell_2^{(i)})}{4} \\
&\qquad + \frac{1}{8}\left(\ell_1^{(i)} + \ell_2^{(i)}\right)^2 - \frac{1}{4}\left(\ell_1^{(i)} + \ell_2^{(i)} + \ell_1^{(i)}\ell_2^{(i)}\right) \\
&\qquad - \left[\frac{n(H^{(i-1)})^2}{4} + \frac{n(H^{(i-1)})(\ell_1^{(i)} + \ell_2^{(i)})}{2} + \frac{(\ell_1^{(i)} + \ell_2^{(i)})^2}{4}\right] \\
&\leq e(G^{(i-1)}) - \frac{n(H^{(i-1)})^2}{4} + \left(2 + \ell_1^{(i)} + \ell_2^{(i)}\right) \\
&\qquad - \frac{1}{4}\left(\ell_1^{(i)} + \ell_2^{(i)}\right) - \frac{1}{8}\left(\ell_1^{(i)} + \ell_2^{(i)}\right)^2 - \frac{1}{4}\ell_1^{(i)}\ell_2^{(i)} - \frac{1}{4}n(H^{(i-1)})\ell^{(i)} \\
&= c(G^{(i-1)}) + 2 + \frac{3}{4}\left(\ell^{(i)}\right) - \frac{(\ell^{(i)})^2}{8} - \frac{1}{4}\ell_1^{(i)}\ell_2^{(i)} - \frac{1}{4}n(H^{(i-1)})\ell^{(i)}.
\end{aligned}$$

We have now proven Claim 7.3. We now combine a sequence of these bounds to show the global bound.

Since each ear augmentation forces $\Phi(H^{(i)}) > \Phi(H^{(i-1)})$, there are at most $p-q$ augmentations. Moreover, the increase in $c(G^{(i)})$ at each step is bounded by $1 + \frac{3}{4}\ell^{(i)} - \frac{1}{8}(\ell^{(i)})^2 - \frac{1}{4}\ell^{(i)}n(H^{(i-1)})$ in a single ear augmentation and $2 + \frac{3}{4}\ell^{(i)} - \frac{1}{8}(\ell^{(i)})^2 - \frac{1}{4}\ell_1^{(i)}\ell_2^{(i)} - \frac{1}{4}\ell^{(i)}n(H^{(i-1)})$ in a double ear augmentation. Independent of the number of ears,

$$c(G^{(i)}) - c(G^{(i-1)}) \leq 2 + \ell^{(i)} - \frac{1}{8}(\ell^{(i)})^2 - \frac{1}{4}\ell^{(i)}n(H^{(i-1)}).$$

Note also that if $\ell^{(i)}$ is positive, then it is at least two. Combining those inequalities gives

$$\begin{aligned}
c(G') &\leq c(G) + \sum_{i=1}^{k}\left(2 + \frac{3}{4}\ell^{(i)} - \frac{1}{8}(\ell^{(i)})^2 - \frac{1}{4}\ell^{(i)}n(H^{(i-1)})\right)\\
&\leq c(G) + \sum_{i=1}^{k} 2 + \frac{3}{4}\sum_{i=1}^{k}\ell^{(i)} - \frac{1}{8}\sum_{i=1}^{k}(\ell^{(i)})^2 - \frac{1}{4}\sum_{i=1}^{k}\ell^{(i)}n(H^{(i-1)})\\
&\leq c(G) + 2k + \frac{3}{4}(N-n) - \frac{1}{8}\sum_{i=1}^{k}2\ell^{(i)} - \frac{1}{4}\sum_{i=1}^{k}\ell^{(i)}n\\
&\leq c(G) + 2(p-q) - \frac{1}{4}(N-n)(n-2).
\end{aligned}$$

This proves the result. ∎

Corollary 7.4. *Let $p, c \geq 1$ be integers. If H is a 1-extendable graph with $q = \Phi(H)$, c' is the maximum excess $c(G)$ over all graphs $G \in \mathcal{E}(H)$, and $c' + 2(p-q) < c$, then there is no 1-extendable graph $H \subset H'$ reachable from H by a graded ear decomposition so that $\Phi(H') = p$ and there exits a graph $G' \in \mathcal{E}(H')$ with excess $c(G') \geq c$.*

Corollary 7.4 gives the condition to test if we can prune the current node, since there does not exist a sequence of ear augmentations that lead to a graph with excess at least our known lower bound on c_p. Moreover, Lemma 7.1 provides a dynamic bound on the maximum order r of ears that can be added to the current graph while maintaining the possibility of finding a graph with excess at least the known lower bound on c_p by selecting r to be maximum so that $c' + 2(p - \Phi(H)) - \frac{1}{4}r(n-2) \geq c$.

8 Full Algorithm, Results, and Data

The full algorithm to search for p-extremal elementary graphs combines three types of algorithms. First, the canonical deletion from Section 3 is used to enumerate the search space with no duplication of isomorphism classes. Second, the pruning procedure from Section 7 greatly reduces the number of generated graphs by backtracking when no dense graphs are reachable. Third, Section 5 provided a method for adding free edges to a 1-extendable graph with p perfect matchings to find maximal elementary supergraphs.

The recursive generation algorithm Search($H^{(i)}, N, p, c$) is given in Algorithm 1. Given a previously computed lower bound $c \leq c_p$, the full search Generate(p, c) (Algorithm 2) operates by running Search(C_{2k}, N_p, p, c) for each even cycle C_{2k} with $4 \leq 2k \leq N_p$. All elementary graphs G with $\Phi(G) = p$ and $c(G) \geq c$ are generated by this process.

Theorem 8.1. *Given p and $c \leq c_p$, Generate(p, c) (Algorithm 2) outputs all unlabeled elementary graphs with p perfect matchings and excess at least c.*

Algorithm 1 Search($H^{(i)}, N^{(i)}, p, c$)

```
Check all pairs of vertices, up to symmetries
for all vertex-pair orbits 𝒪 in H^{(i)} do
  {x, y} ← representative pair of 𝒪
  Augment by ears of all even orders
  for all orders r ∈ {0, 2, ..., N^{(i)} − n(H^{(i)})} do
    H^{(i+1)} ← H^{(i)} + Ear(x, y, r)
    if H^{(i)} is almost 1-extendable and H^{(i+1)} is not 1-extendable then
      Skip H^{(i+1)} (decomposition is not graded).
    else if Φ(H^{(i+1)}) > p then
      Skip H^{(i+1)}.
    else
      Check the canonical deletion
      (x', y', r') ← del(H^{(i+1)})
      if r = r' and {x', y'} in orbit with {x, y} in H^{(i+1)} then
        This augmentation matches the canonical deletion
        n^{(i+1)} ← n(H^{(i+1)}).
        p^{(i+1)} ← Φ(H^{(i+1)}).
        c^{(i+1)} ← max{c(H_𝓘^{(i+1)}) : 𝓘 ∈ 𝒞(H^{(i+1)})}.
        if p^{(i+1)} = p and c^{(i+1)} ≥ c then
          There are solutions within ℰ(H^{(i+1)}).
          for all cover sets 𝓘 ∈ 𝒞(H^{(i+1)}) do
            if c(H_𝓘^{(i+1)}) ≥ c then
              Output H_𝓘.
            end if
          end for
        else if p^{(i+1)} < p and c^{(i+1)} + 2(p − p^{(i+1)}) ≥ c then
          Use Lemma 7.1 to bound the number of vertices for future augmentations.
          N^{(i+1)} = max{N' : c^{(i+1)} + 2(p − p^{(i+1)}) − (1/4)(N' − n^{(i+1)}))(n^{(i+1)} − 2) ≥ c}.
          Search(H^{(i+1)}, N^{(i+1)}, p, c).
        end if
      end if
    end if
  end for
end for
return
```

Algorithm 2 Generate(p, c)

```
N ← max{2r : 2r ≤ 3 + √(16p − 8c − 23)}.
for r ∈ {1, ..., N/2} do
  Search(C_{2r}, N, p, c)
end for
return
```

p	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27
n_p	8	6	8	8	6	8	8	8	8	8	8	8	8	8	8	8	8
c_p	3	5	3	4	6	4	4	5	4	5	5	5	5	6	5	5	6
C_p	4	5	5	5	6	6	6	6	6	6	6	6	6	6	6	6	6

Table 2: New values of n_p and c_p. Conjecture 1.2 states that $c_p \leq C_p$.

Proof. Given an unlabeled graph G with $\Phi(G) = p$ and $c(G) \geq c$, note that Theorem 2.1 implies $n(G) \leq 3 + \sqrt{16p - 8c - 23}$. With respect to the canonical deletion $\text{del}(H)$, let $H^{(0)} \subset H^{(1)} \subset \cdots \subset H^{(k)}$ be the canonical ear decomposition of the extendable subgraph H in G. By the choice of canonical deletion, this decomposition takes the form of Corollary 3.3. Moreover, $H^{(0)}$ is an even cycle C_{2r} for some r. The Generate(p, c) method initializes Search(C_{2r}, N, p, c).

By the definition of canonical ear decomposition, the canonical ear $\varepsilon^{(i)} = \text{del}(H^{(i)})$ of $H^{(i)}$ is the ear used to augment from $H^{(i-1)}$ to $H^{(i)}$. Let $x^{(i)}, y^{(i)}$ be the endpoints of $\varepsilon^{(i)}$. When Search$(H^{(i)}, N^{(i)}, p, c)$ is called, the pair orbit $\mathcal{O}$ containing $\{x^{(i+1)}, y^{(i+1)}\}$ is visited and an ear ε of the same order as $\varepsilon^{(i+1)}$ is augmented to $H^{(i)}$ to form a graph $H_*^{(i+1)}$. Note that $H_*^{(i+1)} \cong H^{(i+1)}$ with an isomorphism mapping ε to $\varepsilon^{(i+1)}$. By the definition of the canonical deletion $\text{del}(H)$, the algorithm accepts this augmentation.

For each i, let $G^{(i)}$ be a maximum-size elementary supergraph in $\mathcal{E}(H^{(i)})$. By Theorem 5.5, there exists a maximal cover set $\mathcal{I} \in \mathcal{C}(H^{(i)})$ so that $G^{(i)} = H_{\mathcal{I}}^{(i)}$. Since $c(G^{(k)}) = c(G) \geq c$, Lemma 7.1 gives $c(G) \leq c(G^{(i+1)}) + 2(p - p^{(i+1)}) - \frac{1}{4}(n(G) - n(H^{(i+1)}))(n(H^{(i+1)}) - 2)$, so the algorithm recurses with $N^{(i+1)} \geq n(G)$.

When $H^{(k)}$ is reached, the algorithm notices that $\Phi(H^{(k)}) = p$ and enumerates all cover sets $\mathcal{I} \in \mathcal{C}(H^{(k)})$ which generates the elementary supergraphs $H_{\mathcal{I}}^{(k)} \in \mathcal{E}(H^{(k)})$ with excess at least c. Since $H^{(k)}$ is the extendable subgraph of G and $c(G) \geq c$, this procedure will output G. ∎

The framework for this search was implemented within the EarSearch library[4]. This implementation was executed on the Open Science Grid [8] using the University of Nebraska Campus Grid [12]. The nodes available on the University of Nebraska Campus Grid consist of Xeon and Opteron processors with a speed range of between 2.0 and 2.8 GHz.

A naïve search (using `geng`) on graphs with at most 10 vertices generated lower bounds on c_p for $p \in \{11, \ldots, 27\}$. A full enumeration of p-extremal graphs for this range of p was then completed using Algorithm 2 seeded with these lower bounds. The resulting values of c_p and n_p are given in Table 2. The computation time for these values ranged from less than a minute to more than 10 years. Table 3 gives the full list of computation times. The resulting p-extremal elementary graphs for $11 \leq p \leq 27$ are given in Figure 1.

To describe the complete structural characterization of p-extremal graphs on n vertices for all even $n \geq n_p$, we apply Theorem 2.2. An important step in applying Theorem 2.2 is to consider every factorization $p = \prod p_i$ and to check which spires are generated by the p_i-extremal elementary graphs.

[4]The EarSearch library is available at https://github.com/derrickstolee/EarSearch

p	N_p	c_p	CPU Time	p	N_p	c_p	CPU Time
5	8	2	0.02s	16	16	4	2.02h
6	10	3	0.04s	17	16	4	6.77h
7	10	3	0.18s	18	18	5	11.75h
8	12	3	0.72s	19	18	4	2.71d
9	12	4	1.46s	20	18	5	4.21d
10	12	4	5.95s	21	18	5	13.71d
11	14	3	43.29s	22	20	5	42.84d
12	14	5	44.01s	23	20	5	118.32d
13	14	3	6.66m	24	20	6	209.42d
14	16	4	12.17m	25	20	5	2.52y
15	16	6	12.71m	26	20	5	7.21y
			.	27	22	6	10.68y

Table 3: Time analysis of the search for varying p values.

We describe these structures based on the types of constructions given by these factorizations. It is necessary to consider the p-extremal elementary graphs for $1 \leq p \leq 10$, in Figure 2.

For $p \in \{11, 13, 17, 19, 23\}$, p is prime, and there is no non-trivial factorization of p. Hence, a p-extremal graph is a spire using exactly one p-extremal elementary graph with all other vertices within chambers isomorphic to K_2. In most cases, the p-extremal elementary graph must appear at the top of the spire. Only when $p = 11$ and the 11-extremal elementary graph chosen is the one with a barrier of size 4 can this chamber be positioned anywhere in the spire.

For each $p \in \{15, 22, 25, 26\}$, p has at least one non-trivial factorization $p = \prod p_i$, but the sum of c_{p_i} over the factors is strictly below c_p. Hence, no p-extremal spire could contain more than one non-trivial chamber. Also, all p-extremal elementary graphs have a barrier with relative size strictly below $\frac{1}{2}$, so the non-trivial chamber must appear at the top of the spire.

For each $p \in \{21, 27\}$, there exists at least one factorization $p = \prod p_i$, all with $\sum c_{p_i} \leq c_p$, and at least one factorization which reaches c_p with equality. For example, $21 = 3 \cdot 7$, and $c_3 + c_7 = 2 + 3 = 5 = c_{21}$. However, in these cases of equality, p_i-extremal elementary graphs with large barriers do not exist and it is impossible to achieve an excess of c_p over the entire spire using multiple non-trivial chambers. Hence, the p-extremal graphs for these values of p have exactly one non-trivial chamber with p perfect matchings and these chambers have small barriers, so they must appear at the top of the spire.

For each $p \in \{14, 18, 20, 24\}$, there is at least one factorization $p = \prod p_i$ so that $\sum c_{p_i} = c_p$ and there are p_i-extremal graphs with large enough barriers to admit a spire with excess c_p. These factorizations are $14 = 2 \cdot 7$, $18 = 3 \cdot 6 = 2 \cdot 9$, $20 = 2 \cdot 10$, and $24 = 2 \cdot 12$. There are also the p-extremal spires with exactly one non-trivial chamber, most of which must appear at the top of the spire. For $p \in \{14, 24\}$, there exists one p-extremal elementary graph with a large barrier that can appear anywhere in a p-extremal spire.

The case $p = 16$ is special: every factorization admits at least one configuration for a 16-extremal spire. The q-extremal elementary graphs for $q \in \{1, 2, 4, 8\}$ as found by Hartke, Stolee, West, and

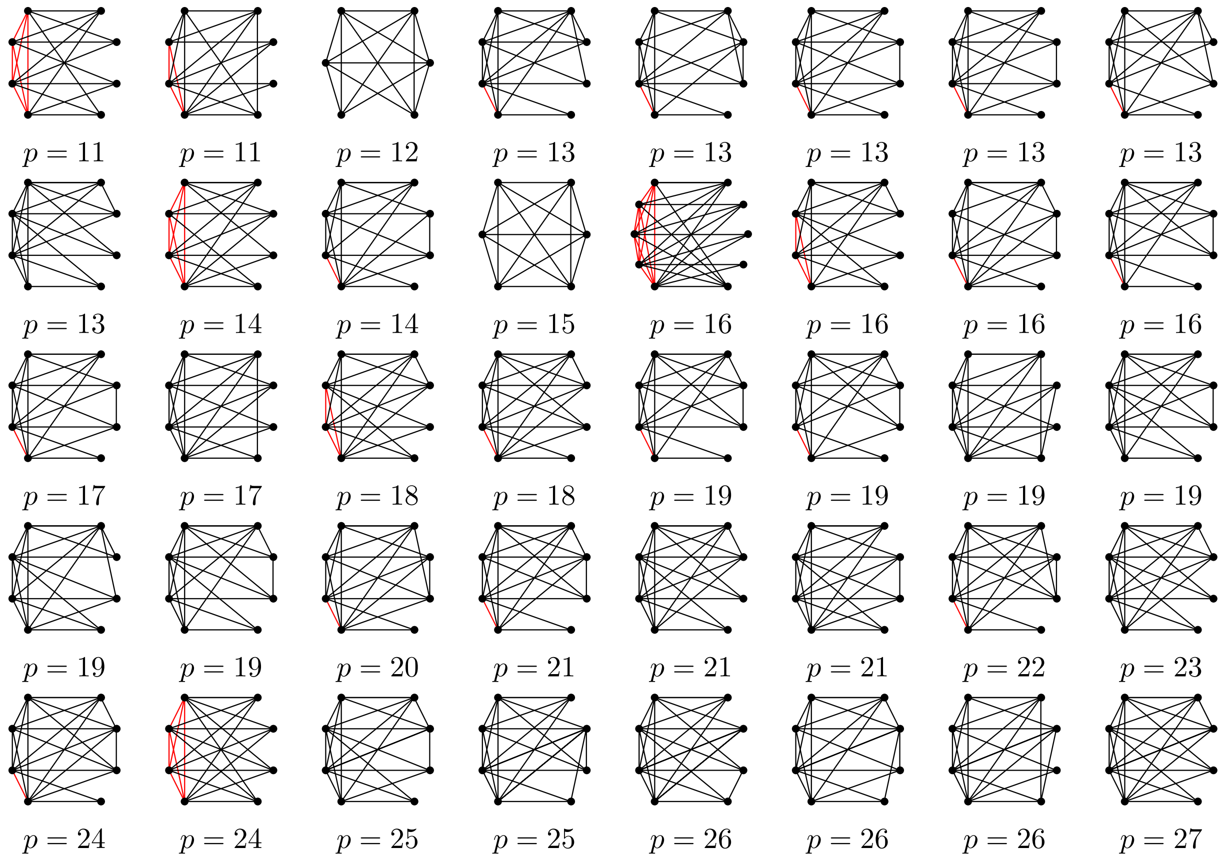

Figure 1: The p-extremal elementary graphs where $11 \leq p \leq 27$.

Yancey [3] are given in Figure 2. Note that for each such q, there exists at least one q-extremal graph with a barrier with relative size $\frac{1}{2}$. This allows any combination of values of q that have product 16 give a spire with 16 perfect matchings and excess equal to the sum of the excesses of the chambers, which always adds to $c_{16} = 4$. There are two 8-extremal elementary graphs and three 16-extremal elementary graphs which have small barriers and must appear at the top of a 16-extremal spire. All other chambers of a 16-extremal spire can take any order.

9 Future work

The $O(\sqrt{p})$ bound N_p on the number of vertices in a p-extremal elementary graph was sufficient for the computational technique described in this work to significantly extend the known values of c_p. However, all of the elementary graphs we discovered to be p-extremal for $p \leq 27$ have at most 10 vertices. If a smaller bound on n_p could be proven, these p-extremal graphs could be generated using existing software, such as McKay's `geng` program [7].

A smaller N_p bound would also improve the distributed search developed in this work. Computation time would still be exponential in p because the depth of the search is a function of p, but the branching factor at each level would be reduced. This delays the exponential behavior and

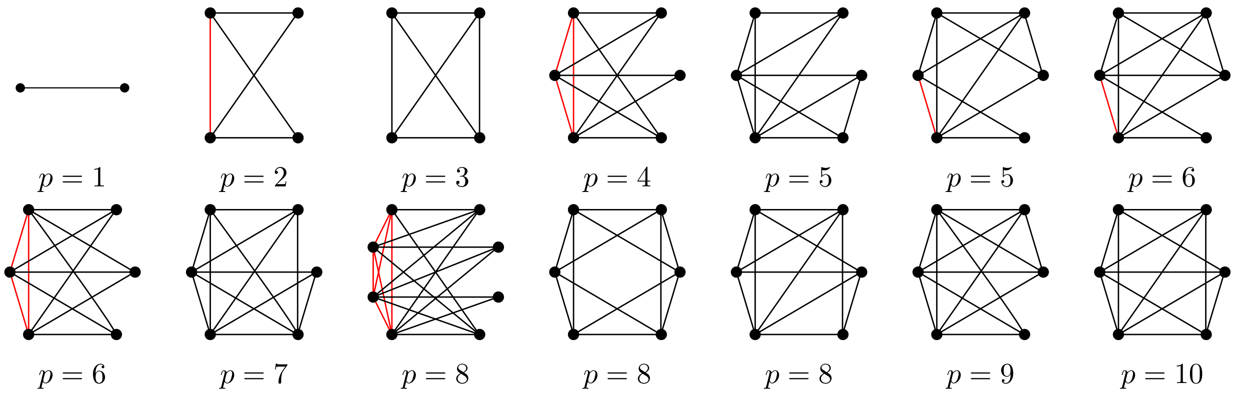

Figure 2: The p-extremal elementary graphs with $1 \leq p \leq 10$ [1, 3].

potentially makes searches over larger values of p become tractable.

The following conjecture is motivated by the orders of the known p-extremal elementary graphs as well as the potential algorithmic implications.

Conjecture 9.1. *Every p-extremal elementary graph has at most $2(\log_2 p + 1)$ vertices.*

This conjecture is tight for $p = 2^k$, with $k \in \{1, 2, 3, 4\}$ and holds for all $p \leq 27$. Note that $n_8 = 6$, but there is an 8-extremal elementary graph with eight vertices. Similarly, $n_{16} = 8$, but there is a 16-extremal elementary graph with ten vertices.

The structure theorem requires searching over all factorizations of p in order to determine which factorizations yield a spire with the largest excess. However, all known values of p admit p-extremal elementary graphs. Moreover, all composite values $p = p_1 p_2$ admit $c_p \geq c_{p_1} + c_{p_2}$. Does this always hold?

Conjecture 9.2. *For all $p \geq 1$, there exists a p-extremal elementary graph.*

Conjecture 9.3. *For all products $p = \prod_{i=1}^{k} p_i$ with $p \geq 1$, $c_p \geq \sum_{i=1}^{k} c_{p_i}$.*

The closest known bound to Conjecture 9.3 is $c_p \geq c_{p_1} + \sum_{i=2}^{k} w(p_i)$, where $w(n)$ is the number of 1's in the binary representation of n [3, Proposition 7.1].

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References

[1] A. Dudek and J. Schmitt. On the size and structure of graphs with a constant number of 1-factors, 2010. preprint.

[2] S. G. Hartke and A. Radcliffe. Mckay's canonical graph labeling algorithm. In *Communicating Mathematics*, volume 479 of *Contemporary Mathematics*, pages 99–111. American Mathematical Society, 2009.

[3] S. G. Hartke, D. Stolee, D. B. West, and M. Yancey. On extremal graphs with a given number of perfect matchings, 2011. preprint.

[4] L. Lovasz. Ear-decompositions of matching-covered graphs. *Combinatorica*, 3(1):105–117, 1983.

[5] L. Lovász and M. Plummer. *Matching theory.* Elsevier Science Ltd, 1986.

[6] B. D. McKay. Isomorph-free exhaustive generation. *J. Algorithms*, 26(2):306–324, 1998.

[7] B. D. McKay. nauty user's guide (version 2.4). *Dept. Computer Science, Austral. Nat. Univ.*, 2006.

[8] R. Pordes, D. Petravick, B. Kramer, D. Olson, M. Livny, A. Roy, P. Avery, K. Blackburn, T. Wenaus, et al. The Open Science Grid. In *Journal of Physics: Conference Series*, volume 78, pages 12–57. IOP Publishing, 2007.

[9] D. Stolee. Isomorph-free generation of 2-connected graphs with applications. Technical Report 120, University of Nebraska–Lincoln Computer Science and Engineering Department, 2011.

[10] Z. Szigeti. The two ear theorem on matching-covered graphs. *J. Combin. Theory Ser. B*, 74(1):104–109, 1998.

[11] W. T. Tutte. The factorization of linear graphs. *J. London Math. Soc.*, 22:107–111, 1947.

[12] D. J. Weitzel. *Campus Grids: A framework to facilitate resource sharing.* Masters thesis, University of Nebraska - Lincoln, 2011.

[13] H. Whitney. Congruent Graphs and the Connectivity of Graphs. *Amer. J. Math.*, 54(1):150–168, 1932.