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Cograph editing: Merging modules is equivalent to editing P_4s*

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Abstract

The modular decomposition of a graph $G = (V, E)$ does not contain prime modules if and only if G is a cograph, that is, if no quadruple of vertices induces a simple connected path P_4. The cograph editing problem consists in inserting into and deleting from G a set F of edges so that $H = (V, E \triangle F)$ is a cograph and $|F|$ is minimum. This NP-hard combinatorial optimization problem has recently found applications, e.g., in the context of phylogenetics. Efficient heuristics are hence of practical importance. The simple characterization of cographs in terms of their modular decomposition suggests that instead of editing G one could operate directly on the modular decomposition. We show here that editing the

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induced P_4s is equivalent to resolving prime modules by means of a suitable defined merge operation on the submodules. Moreover, we characterize so-called module-preserving edit sets and demonstrate that optimal pairwise sequences of module-preserving edit sets exist for every non-cograph. This eventually leads to an exact algorithm for the cograph editing problem as well as fixed-parameter tractable (FPT) results when cograph editing is parameterized by the so-called modular-width. In addition, we provide two heuristics with time complexity $O(|V|^3)$, resp., $O(|V|^2)$.

Keywords: Cograph editing, modular decomposition, module merge, prime modules, P_4.

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1 Introduction

Cographs are of particular interest in computer science because many combinatorial optimization problems that are NP-complete for arbitrary graphs become polynomial-time solvable on cographs [4, 8, 20]. This makes them an attractive starting point for constructing heuristics that are exact on cographs and yield approximate solutions on other graphs. In this context it is of considerable practical interest to determine "how close" an input graph is to a cograph.

An independent motivation recently arose in biology, more precisely in molecular phylogenetics [14, 21, 35, 36, 37, 47]. In particular, *orthology*, a key concept in evolutionary biology in phylogenetics, is intimately tied to cographs [35]. Two genes in a pair of related species are said to be orthologous if their last common ancestor was a speciation event. The orthology relation on a set of genes forms a cograph [30], see [33] for a detailed discussion and [21, 22, 23, 31, 47] for generalizations of these concepts. This relation can be estimated directly from biological sequence data, albeit in a necessarily noisy form. Correcting such an initial estimate to the nearest cograph thus has recently become a computational problem of considerable practical interest in computational biology [35]. However, the (decision version of the) problem to edit a given graph with a minimum number of edits into a cograph is NP-complete [32, 34, 38, 39].

As noted already in [7], the input for several combinatorial optimization problems, such as exam scheduling or several variants of clustering problems, is naturally expected to have few induced paths on four vertices (P_4s). Since graphs without an induced P_4 are exactly the cographs, available cograph editing algorithms focus on efficiently removing P_4s, see e.g. [16, 24, 25, 38, 39, 53]. The FPT-algorithm introduced in [38, 39] takes as input a graph that is first edited to a so-called P_4-sparse graph and then to a cograph. The basic strategy is to destroy the P_4s in the subgraphs by branching into six cases that eventually leads to an $O(4.612^k|V|^{9/2})$-time algorithm, where k is the number of required edits. Algorithms that compute the kernel of the (parameterized) cograph editing problem [24, 25] as well as the exact $O(3^{|V|}|V|)$-time algorithm [53] use the modular-decomposition tree as a guide to locate the forbidden P_4s using the fact that these are associated with prime modules. Nevertheless, the basic operation in all of these algorithms is still the direct destruction of the P_4s.

Cographs are recursively defined as follows: K_1 is a cograph, the disjoint union of

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cographs is a cograph, and the join of cographs is a cograph. This recursive definition associates a vertex labeled tree, the cotree, with each cograph, where a vertex label "0" denotes a disjoint union, while "1" indicates the join of the children is formed. It has been shown in [7] that each cograph has a unique cotree and conversely, every tree whose interior vertices are labeled alternatingly defined a unique cograph. A simple recognition algorithm starts with an input graph G. If G is connected, then a node labeled "1" is inserted into the tree, the complement graph $\overline{G}$ is formed and the algorithm proceeds recursively on the connected components of $\overline{G}$. If G is not connected, the tree-node is labeled "0", and the algorithm recurses on the components of G. If both G and $\overline{G}$ are connected, then G is not a cograph, and the algorithm terminates with a negative answer. A natural heuristic for cograph editing proceeds by finding a minimal cut in G or $\overline{G}$, removes the cut-edges and proceeds with the modified graph. This idea is pursued in [14, 15].

A very different heuristic for cograph modification was recently proposed by Crespelle [11]. It corrects the neighborhood of each vertex separately. More precisely, an inclusion-minimal cograph editing H_k of the induced subgraph $G_k := G[\{x_1, \dots x_k\}]$ is computed from the correction H_{i-1} of G_{i-1} in such a way that only edges involving x_i are inserted or deleted. It has the useful property that in each step the number of inserted or deleted edges is minimum, and it inserts or deletes no more than $|E(G)|$ edges in total. It is based on a general property of single-vertex augmentations in hereditary graph classes that are stable under the addition of universal vertices and isolated vertices, see e.g. [48]. A key advantage is that it has linear time complexity, i.e., $O(|V| + |E|)$.

Cotrees are a special case of the much more general modular decomposition tree, which is well-defined for every graph and conveys detailed information about its structure in a hierarchical manner [19]. A subset $M \subseteq V$ is called a module of a graph $G = (V, E)$, if all members of M share the same neighbors in $V \setminus M$. A prime module is a module that is characterized by the property that both, the induced subgraph $G[M]$ and its complement $\overline{G[M]}$, are connected subgraphs of G. Cographs play a particular role in this context as their modular decompositions are of a special form: they are characterized by the absence of prime modules. In particular, the cotree of a cograph coincides with its modular decomposition tree [19]. It is natural to ask, therefore, whether the modular decomposition tree can be manipulated in a such a way that all prime modules of a given graph are converted into "series" or "parallel" modules for which either $G[M]$ and or $\overline{G[M]}$ is disconnected. This is equivalent to converting G into a cograph G^*. Every minimum edit set clearly is inclusion-minimal. However, not every minimum edit set – and in particular not every inclusion-minimal edit set – respects the module structure of G. Figure 1 below shows a pertinent example. In contrast to the editing approach of [11], we pursue an approach that is modul-preserving in the sense that each module of G is also a module of the edited graph G^*. We argue that this property is desirable in the context of orthology detection, because the corrected modular decomposition tree, i.e., the cotree of G^* has a direct interpretation as event-labeled gene tree [30, 35].

An alternative way of looking at the connection between cographs and their modular decomposition trees is to interpret the destruction of all P_4s in a cograph editing algorithm as the resolution of all prime modules in the edited graph G^*. This simple observation suggests to edit the modules of G. The min-cut approach of [14] is one possibility to achieve this. Here, we consider the merging of modules instead. Every union $\bigcup_{i \in I} M_i$ of the connected components $M_1, \dots, M_k$ of the edited graph $G^*[M]$ or $\overline{G^*[M]}$ forms a module G^*, while $\bigcup_{i \in I} M_i$ was not a module in the graph G before editing. In this situation, we say that "*the modules* M_i, $i \in I$ *of* G *are merged w.r.t.* G^*". Vertices within a module $\bigcup_{i\in I} M_i$ share the same neighbors in $V \setminus (\bigcup_{i\in I} M_i)$. It is sufficient therefore to adjust the neighbors of certain submodules M_i of M to merge the M_i in a way that resolves the prime module M to obtain G^*. In this setting, it seems natural to edit the modular decomposition tree of a graph directly with the aim of converting it step-by-step into the closest modular decomposition tree of a cograph. To this end, one would like to break up individual prime modules by means of the module merge operation.

The key results of this contribution are that (1) every prime node M can be resolved by a sequence of *pairwise* merges of modules that are children of M in the modular decomposition tree, and (2) optimal cograph editing can be expressed as optimal *pairwise* module merging. To prove these statements, we start with an overview of important properties on cographs and the modular decomposition (Section 2 and 3). In Section 4, we then show that so-called module-preserving edit sets are characterized by resolving any prime node by module-merges. In particular, we show that any graph has an optimal edit set that can be entirely expressed by merging modules that are children of prime modules in the modular decomposition tree. Finally in Section 5, we summarize the results and show how they can be used for establishing efficient heuristics for the cograph editing problem. We provide an exact algorithm that allows to optimally edit a cograph via pairwise module-merges. As by-product, we obtain an FPT algorithm for the case that cograph editing is parameterized by the so-called modular-width [1, 18]. We finish this paper with a short discussion on how the latter method can be used to obtain a simple $O(|V|^2)$-time heuristic.

2 Basic definitions

We consider simple finite undirected graphs $G = (V, E)$ without loops. The complement $\overline{G}$ of a graph $G = (V, E)$ has vertex set V and edge set $E(\overline{G}) = \{xy \mid x, y \in V, x \neq y, xy \notin E\}$. The notation $G \triangle F$ is used to denote the graph $(V, E \triangle F)$, where $\triangle$ denotes the symmetric difference. The disjoint union $G \cupdot H$ of two distinct graphs $G = (V, E)$ and $H = (W, F)$ is simply the graph $(V \cupdot W, E \cupdot F)$. The join $G \oplus H$ of G and H is defined as the graph $(V \cupdot W, E \cupdot F \cupdot \{xy \mid x \in V, y \in W\})$. A graph $H = (W, F)$ is a *subgraph* of a graph $G = (V, E)$, in symbols $H \subseteq G$, if $W \subseteq V$ and $F \subseteq E$. If $H \subseteq G$ and $xy \in F$ if and only if $xy \in E$ for all $x, y \in W$, then H is called an *induced* subgraph. We will often denote an induced subgraph $H = (W, F)$ by $G[W]$. A *connected component* of G is a connected induced subgraph that is maximal w.r.t. inclusion. We write $G \simeq H$ for two isomorphic graphs G and H.

Let $G = (V, E)$ be a graph. The *neighborhood* $N(v)$ of $v \in V$ is defined as $N(v) = \{x \mid vx \in E\}$. If there is a risk of confusion we will write $N_G(v)$ to indicate that the respective neighborhood is taken w.r.t. G. The *degree* $\deg(v)$ of a vertex is defined as $\deg(v) = |N(v)|$.

A *tree* is a connected graph that does not contain cycles. A *path* is a tree where every vertex has degree 1 or 2. A *rooted* tree $T = (V, E)$ is a tree with one distinguished vertex $\rho \in V$. We distinguish two further types of vertices in a tree: the *leaves* which are distinct from the root and are contained in only one edge and the *inner* vertices which are contained in at least two edges. The first inner vertex $\operatorname{lca}(x, y)$ that lies on both unique paths from two vertices x, resp., y to the root, is called *lowest common ancestor* of x and y. We say that a rooted tree T *displays* the *triple* $\mathrm{xy|z}$ if x, y, and z are leaves of T and the path from x to y does not intersect the path from z to the root of T.

It is well-known that there is a one-to-one correspondence between (isomorphism classes of) rooted trees on V and so-called hierarchies on V. For a finite set V, a *hierarchy on* V is a subset $\mathcal{C}$ of the power set $\mathcal{P}(V)$ such that (i) $V \in \mathcal{C}$, (ii) $\{x\} \in \mathcal{C}$ for all $x \in V$ and (iii) $p \cap q \in \{p, q, \emptyset\}$ for all $p, q \in \mathcal{C}$.

Theorem 2.1 ([51]). *Let $\mathcal{C}$ be a collection of non-empty subsets of V. Then, there is a rooted tree $T = (W, E)$ on V with $\mathcal{C} = \{L(v) \mid v \in W\}$ if and only if $\mathcal{C}$ is a hierarchy on V.*

3 Cographs and the modular decomposition

3.1 Introduction to cographs

Cographs are defined as the class of graphs formed from a single vertex under the closure of the operations of union and complementation, namely: (i) a single-vertex graph K_1 is a cograph; (ii) the disjoint union $G = (V_1 \cupdot V_2, E_1 \cupdot E_2)$ of cographs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ is a cograph; (iii) the complement $\overline{G}$ of a cograph G is a cograph. Condition (ii) can be replaced by the equivalent condition that the join $G_1 \oplus G_2$ is a cograph, since $G_1 \oplus G_2$ is the complement of $\overline{G}_1 \cupdot \overline{G}_2$.

The name cograph originates from *complement reducible graphs*, as by definition, cographs can be "reduced" by stepwise complementation of connected components to totally disconnected graphs [50].

It is well-known that for each induced subgraph H of a cograph G either H is disconnected or its complement $\overline{H}$ is disconnected [4]. This, in particular, allows representing the structure of a cograph $G = (V, E)$ in an unambiguous way as a rooted tree $T = (W, F)$, called *cotree*: If the considered cograph is the single vertex graph K_1, then output the tree $(\{u\}, \emptyset)$. Else if the given cograph G is connected, create an inner vertex u in the cotree with label "series", build the complement $\overline{G}$ and add the connected components of $\overline{G}$ as children of u. If G is not connected, then create an inner vertex u in the cotree with label "parallel" and add the connected components of G as children of u. Proceed recursively on the respective connected components that consists of more than one vertex. Eventually, this cotree will have leaf-set $V \subseteq W$ and the inner vertices $u \in W \setminus V$ are labeled with either "parallel" or "series" such that $xy \in E$ if and only if $u = \mathrm{lca}_T(x, y)$ is labeled "series".

The complement of a path on four vertices P_4 is again a P_4 and hence, such graphs are not cographs. Intriguingly, cographs have indeed a quite simple characterization as P_4*-free* graphs, that is, no four vertices induce a P_4. A number of further equivalent characterizations are given in [4] and Theorem 3.2. Determining whether a graph is a cograph can be done in linear time [5, 8].

3.2 Modules and the modular decomposition

The concept of *modular decompositions (MD)* is defined for arbitrary graphs G and allows us to present the structure of G in the form of a tree that generalizes the idea of cotrees. However, in general much more information needs to be stored at the inner vertices of this tree if the original graph has to be recovered.

The MD is based on the notion of modules. These are also known as autonomous sets [43, 44], closed sets [19], clans [17], stable sets, clumps [2] or externally related sets [27]. A *module* of a given graph $G = (V, E)$ is a subset $M \subseteq V$ with the property that for all vertices in $x, y \in M$ it holds that $N(y) \setminus M = N(x) \setminus M$. Therefore, the vertices within a given module M are not distinguishable by the part of their neighborhoods that lie "outside" M. We denote with $\mathrm{MD}(G)$ the set of all modules of $G = (V, E)$. Clearly, the vertex set V and the singletons $\{v\}$, $v \in V$ are modules, called *trivial* modules. A graph G is called *prime* if it only contains trivial modules. For a module M of G and a vertex $v \in M$, we define the out_M-neighborhood of v as $N(v) \setminus M$. Since for any two vertices contained in M the out_M-neighborhoods are identical, we can equivalently define $N(v) \setminus M$ as the out_M-neighborhood of the module M, where $v \in M$.

We say that a module M of G is *parallel*, resp., *series* if the induced subgraph $G[M]$, resp., the complement $\overline{G[M]}$ is disconnected. If both $G[M]$ and $\overline{G[M]}$ are connected, then M is called *prime*.

For a graph $G = (V, E)$ let M and M' be disjoint subsets of V. We say that M and M' are adjacent (in G) if each vertex of M is adjacent to all vertices of M'; the sets are non-adjacent if none of the vertices of M is adjacent to a vertex of M'. Two disjoint modules are either adjacent or non-adjacent [43]. One can therefore define the *quotient graph* G/P for an arbitrary subset $P \subseteq \mathrm{MD}(G)$ of pairwise disjoint modules: G/P has P as its vertex set and $M_iM_j \in E(G/P)$ if and only if M_i and M_j are adjacent in G.

A module M is called *strong* if for any module $M' \neq M$ either $M \cap M' = \emptyset$, or $M \subseteq M'$, or $M' \subseteq M$, i.e., a strong module does not *overlap* any other module. The set of all strong modules $\mathrm{MDs}(G) \subseteq \mathrm{MD}(G)$ thus forms a hierarchy, the so-called *modular decomposition* of G. While arbitrary modules of a graph form a potentially exponential-sized family, the sub-family of strong modules has size $O(|V(G)|)$ [26].

Let $\mathbb{P} = \{M_1, \dots, M_k\}$ be a partition of the vertex set of a graph $G = (V, E)$. If every $M_i \in \mathbb{P}$ is a module of G, then $\mathbb{P}$ is a *modular partition* of G. A non-trivial modular partition $\mathbb{P} = \{M_1, \dots, M_k\}$ that contains only maximal (w.r.t. inclusion) strong modules is a *maximal modular partition*. We denote the (unique) maximal modular partition of G by $\mathbb{P}_{\max}(G)$. We will refer to the elements of $\mathbb{P}_{\max}(G[M])$ as the *the children of* M. This terminology is motivated by the following considerations:

The hierarchical structure of $\mathrm{MDs}(G)$ gives rise to a canonical tree representation of G, which is usually called the *modular decomposition tree* $T_{\mathrm{MDs}}(G)$ [28, 44]. The root of this tree is the trivial module V and its $|V|$ leaves are the trivial modules $\{v\}$, $v \in V$. The set of leaves L_v associated with the subtree rooted at an inner vertex v induces a strong module of G. In other words, each inner vertex v of $T_{\mathrm{MDs}}(G)$ *represents* the strong module L_v. An inner vertex v is then labeled "parallel", "series", resp., "prime" if L_v is a parallel, series, resp., prime module. The strong module L_v of the induced subgraph $G[L_v]$ associated to a vertex v labeled "prime" is called prime module. Note, the latter does not imply that the graph $G[L_v]$ is prime, however, in all cases the quotient graph $G[L_v]/\,\mathbb{P}_{\max}(G[L_v])$ is prime [28]. Similar to cotrees it holds that $xy \in E$ if $u = \mathrm{lca}_{T_{\mathrm{MDs}}(G)}(xy)$ is labeled "series", and $xy \notin E$ if $u = \mathrm{lca}_{T_{\mathrm{MDs}}(G)}(xy)$ is labeled "parallel". However, to trace back the full structure of a given graph G from $T_{\mathrm{MDs}}(G)$ one has to store additionally the information of the subgraph $G[L_v]/\,\mathbb{P}_{\max}(G[L_v])$ in the vertices v labeled "prime". Although, $\mathrm{MDs}(G) \subseteq \mathrm{MD}(G)$ does not represent all modules, we state the following remarkable fact [12, 43]: Any subset $M \subseteq V$ is a module if and only if $M \in \mathrm{MDs}(G)$ or M is the union of children of non-prime modules. Thus, $T_{\mathrm{MDs}}(G)$ represents at least implicitly all modules of G.

A simple polynomial time recursive algorithm to compute $T_{\mathrm{MDs}}(G)$ is as follows [28]: (1) compute the maximal modular partition $\mathbb{P}_{\max}(G)$; (2) label the root node according to the parallel, series or prime type of G; (3) for each strong module M of $\mathbb{P}_{\max}(G)$, compute $T_{\mathrm{MDs}}(G[M])$ and attach it to the root node and proceed with $\mathbb{P}_{\max}(G[M])$. The first polynomial time algorithm to compute the modular decomposition is due to Cowan *et al.* [10], and it runs in $O(|V|^4)$. Improvements are due to Habib and Maurer [27], who proposed a cubic time algorithm, and to Müller and Spinrad [45], who designed a quadratic time algorithm. The first two linear time algorithms appeared independently in 1994 [9, 40]. Since then a series of simplified algorithms has been published, some running in linear time [13, 41, 52], and others in almost linear time [13, 26, 29, 42].

For later reference we give the following lemma.

Lemma 3.1. *Let M be a module of a graph $G = (V, E)$ and $M' \subseteq M$. Then, M' is a module of $G[M]$ if and only if M' is a module of G. If M is a strong module of G, then M' is a strong module of $G[M]$ if and only if M' is a strong module of G. Moreover, if M_1 and M_2 are overlapping modules in G, then $M_1 \setminus M_2$, $M_1 \cap M_2$ and $M_1 \cup M_2$ are also modules in G.*

Proof. The first and the last statement were shown in [43]. We prove the second statement.

Let $M \in \mathrm{MDs}(G)$. Assume that $M' \subseteq M$ is a strong module of $G[M]$. Assume for contradiction that M' is not a strong module of G. Hence M' must overlap some module M'' in G. This module M'' cannot be entirely contained in M as otherwise, M'' and M' overlap in $G[M]$ implying that M' is not a strong module of $G[M]$, a contradiction. But then M and M'' must overlap, contradicting that M is strong in G.

If $M' \subseteq M$ is a strong module of G then it does not overlap *any* module of G. Since every module of $G[M]$ is also a module of G, there cannot be a module of $G[M]$ that overlaps M' and thus, M' is a strong module of $G[M]$. $\square$

3.3 Useful properties of modular partitions

First, we briefly summarize the relationship between cographs G and the modular decomposition $\mathrm{MDs}(G)$. While the first three items are from [4, 7], the proof of the fourth item can be found in [3, 30].

Theorem 3.2 ([4, 7, 30])**.** *Let $G = (V, E)$ be an arbitrary graph. Then the following statements are equivalent.*

1. *G is a cograph.*
2. *G does not contain induced paths on four vertices.*
3. *$T_{MDs}(G)$ is the cotree of G and hence, has no inner vertices labeled with "prime".*
4. *Define a set $\mathcal{R}(G)$ of triples as follows: For any three vertices $x, y, z \in V$ we add the triple $\mathrm{xy|z}$ to $\mathcal{R}(G)$ if either $xz, yz \in E$ and $xy \notin E$ or $xz, yz \notin E$ and $xy \in E$. There is a tree T that displays all triples in $\mathcal{R}(G)$.*

For later explicit reference, we summarize in the next theorem several results that we already implicitly referred to in the discussion above.

Theorem 3.3 ([25, 28, 43])**.** *The following statements are true for an arbitrary graph $G = (V, E)$:*

(T1) The maximal modular partition $\mathbb{P}_{\max}(G)$ and the modular decomposition $\mathrm{MDs}(G)$ of G are unique.

(T2) *Let* $\mathbb{P}_{\max}(G[M])$ *be the maximal modular partition of* $G[M]$*, where* M *denotes a prime module of* G *and* $\mathbb{P}' \subsetneq \mathbb{P}_{\max}(G[M])$ *be a proper subset of* $\mathbb{P}_{\max}(G[M])$ *with* $|\,\mathbb{P}'\,| > 1$*. Then,* $\bigcup_{M' \in \mathbb{P}'} M' \notin \mathrm{MD}(G)$*.*

(T3) *Any subset* $M \subseteq V$ *is a module of* G *if and only if* M *is either a strong module of* G *or* M *is the union of children of a non-prime module of* G*.*

Statements (T1) and (T3) are clear. Statement (T2) explains that none of the unions of elements of a maximal modular partition of $G[M]$ are modules of G, whenever M is a prime module of G. Moreover, Statement (T3) can be used to show that all prime modules are strong.

Lemma 3.4. *Let* $G = (V, E)$ *be an arbitrary graph. Then, every prime module* M *of* G *is strong.*

Proof. Let M be a prime module of G. Assume for contradiction that M is not strong in G. Theorem 3.3(T3) implies that M is the union of children of some non-prime module M'. Hence, there is a subset $\mathcal{M} \subsetneq \mathbb{P}_{\max}(G[M'])$ such that $M = \bigcup_{M'_i \in \mathcal{M}} M'_i$. Note that $1 < |\mathcal{M}| < |\,\mathbb{P}_{\max}(G[M'])|$, since all $M'_i \in \mathbb{P}_{\max}(G[M'])$ are strong and $\bigcup_{M'_i \in \mathbb{P}_{\max}(G[M'])} M'_i = M'$ is non-prime. As M' is non-prime, it is either parallel or series. Since M is a non-trivial union of elements in $\mathbb{P}_{\max}(G[M'])$, $G[M]$ is either disconnected (if M' is parallel) or its complement $\overline{G[M]}$ is disconnected (if M' is series). But then M is non-prime; a contradiction. Thus, M is a strong module of G. □

In what follows, whenever the term “prime module” is used it refers therefore always to a strong module.

3.4 Cograph editing

Given an arbitrary graph we are interested in understanding how the graph can be edited into a cograph. A well-studied problem is the following optimization problem.

Problem 3.5 (Optimal Cograph Editing)**.** Given a graph $G = (V, E)$. Find a set $F \subseteq \binom{V}{2}$ of minimum cardinality such that $H = (V, E \triangle F)$ is a cograph.

We will simply call an edit set of minimum cardinality an *optimal (cograph) edit set*. For later reference we recall Lemma 9 of [35]. It shows that it suffices to solve the cograph editing problem separately for each connected component of G.

Lemma 3.6 ([35])**.** *Let* $G = (V, E)$ *be a graph with optimal edit set* F*. Then* $\{x, y\} \in F \setminus E$ *implies that* x *and* y *are located in the same connected component of* G*.*

Let $G = (V, E)$ be a graph and F be an arbitrary edit set that transforms G to the cograph $H = (V, E \triangle F)$. If any module of G is a module of H, then F is called *module-preserving*.

Proposition 3.7 ([25])**.** *Every graph has an optimal module-preserving cograph edit set.*

The importance of module-preserving edit sets lies in the fact that they update either all or none of the edges between any two disjoint modules. It is worth noting that module preserving edit sets do not necessarily preserve the property of modules being strong, i.e., although M might be a strong module in G it needs not to be strong in H.

Definition 3.8. Let $G = (V, E)$ be a graph, F a cograph edit set for G and M be a non-trivial module of G. The induced edit set in $G[M]$ is

$$F[M] \coloneqq \{\{x, y\} \in F \mid x, y \in M\}.$$

The next result shows that any optimal edit set F can entirely expressed by the union of edits within prime modules and that $F[M]$ is an optimal edit set of $G[M]$ for any module M of G. Hence, if $F[M]$ is not optimal for some module M of G, then F cannot be an optimal edit set for G.

Lemma 3.9 ([25]). *Let $G = (V, E)$ be an arbitrary graph and let M be a non-trivial module of G. If F' is an optimal edit set of the induced subgraph $G[M]$ and F is an optimal edit set of G, then $(F \setminus F[M]) \cup F'$ is an optimal edit set of G. Thus, $|F[M]| = |F'|$.*

Moreover, the optimal cograph editing problem can be solved independently on the prime modules of G.

4 Module merge is the key to cograph editing

Since cographs are characterized by the absence of induced P_4s, we can interpret every optimal cograph-editing method as the removal of all P_4s in the input graph with a minimum number of edits. A natural strategy is therefore to detect P_4s and then to decide which edges must be edited. Optimal edit sets are not necessarily unique, see Figure 1. The computational difficulty arises from the fact that editing an edge of a P_4 can produce new P_4s in the updated graph. Hence, we cannot expect *a priori* that local properties of G alone will allow us to identify optimal edits.

By Lemma 3.9, on the other hand, it is sufficient to edit within the prime modules. Moreover, as shown in Figure 1, there are strong modules $M^\star$ in an optimal edited cograph H that are not modules in G. Hence, instead of editing P_4s in G, it might suffice to edit the out_{M_i}-neighborhoods for some $M_i \in \mathbb{P}_{\max}(G[M])$ in such a way that they result in the new module $M^\star$ in H. The following definitions are important for the concepts of the "module merge process" that we will extensively use in our approach.

Definition 4.1 (Module Merge). Let G and H be arbitrary graphs with $V(H) \subseteq V(G)$ and let $\text{MD}(G)$ and $\text{MD}(H)$ denote their corresponding sets of all modules. Consider a set $\mathcal{M} \coloneqq \{M_1, M_2, \dots, M_k\} \subseteq \text{MD}(G)$. We say that the modules in $\mathcal{M}$ are *merged (w.r.t. H)* if

(i) $M_1, \dots, M_k \in \text{MD}(H)$,

(ii) $M \coloneqq \bigcup_{i=1}^k M_i \in \text{MD}(H)$, and

(iii) $M \notin \text{MD}(G)$.

We use the symbols $\uplus$ and $\rightarrow$ as operations that allows us to illustrate the merge process, that is, we write $M_1 \uplus \dots \uplus M_k = \uplus_{i=1}^k M_i \rightarrow M$, whenever the modules $M_1, M_2, \dots, M_k$ are merged w.r.t. H resulting in the module $M = \bigcup_{i=1}^k M_i$ of H.

The intuition is that the modules M_1 through M_k of G are merged into a single new module M, their union, that is present in H but not in G. This, in particular, already defines all required edits to adjust the neighbors of the vertices in $\bigcup_{i=1}^k M_i$ in G resulting in the module $M = \bigcup_{i=1}^k M_i$ of H. It is easy to verify that $\uplus$ is commutative in the sense that

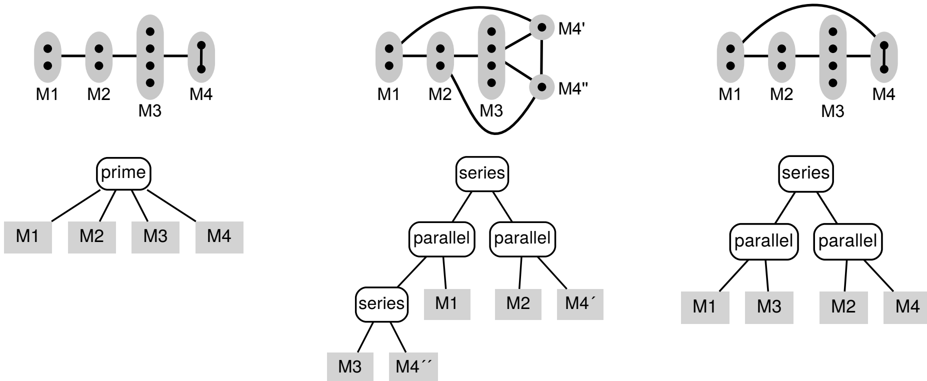

Figure 1: Shown are three graphs G, H_1, H_2 (from left to right). Maximal non-trivial strong modules are indicated by gray ovals in each graph and edges are used to show whether two modules are adjacent or not. The dots/lines within the modules are used to depict the vertices/edges within the modules. The modular decomposition trees up to a certain level are depicted below the respective graphs. This tree differs from the modular decomposition tree of the original graph G, H_1, and H_2, respectively, only from the unresolved leaf-nodes (gray boxes).
Left: A non-cograph G is shown. The optimal edit set F has cardinality 4. *Center:* An optimal edited cograph $H_1 = G \triangle F$ is shown, where F is not module-preserving. None of the new strong modules of H_1 that are not modules of G can be expressed as the union of the sets $M_1, \dots, M_4$. Hence, none of these modules are the result of a module merge process.
Right: An optimal edited cograph $H_2 = G \triangle F$ is shown, where F is module-preserving. The new strong modules $M_1^\star, M_2^\star$ of H_2 that are not modules of G are two parallel modules. They can be written as $M_1^\star = M_1 \cup M_3$ and $M_2^\star = M_2 \cup M_4$. Hence, they are obtained by merging modules of G, in symbols: $M_1 \uplus M_3 \to M_1^\star$ and $M_2 \uplus M_4 \to M_2^\star$. Here we have $F_{H_2}(M_1 \uplus M_3 \to M_1^\star) = F_{H_2}(M_2 \uplus M_4 \to M_2^\star) = F = \{\{x, y\} \mid x \in M_1, y \in M_4\}$.

if $M_1 \uplus M_2 \to M$, then $M_2 \uplus M_1 \to M$. However, $\uplus$ is not necessarily associative. To see this, consider the example in Figure 2. Although the module $M_3^\star$ in H is obtained by merging the modules $\{3\}$, $\{4\}$ and $\{5\}$, the set $\{3\} \cup \{4\}$ does not form a module in H. Hence, although $\{3\} \uplus \{4\} \uplus \{5\} \to M_3^\star$, it does not hold that $\{3\} \uplus \{4\} \to M^\star$ for any module $M^\star$ in H. Thus, we cannot write $(\{3\} \uplus \{4\}) \uplus \{5\} \to M_3^\star$.

It follows directly from Definition 4.1 that every new module M of H that is not a module of G can be obtained by merging trivial modules: simply set $M = \bigcup_{x \in M}\{x\}$ and $\biguplus_{x \in M}\{x\} \to M$ follows immediately. In what follows we will show, however, that each strong module of H that is not a module of G can be obtained by merging the modules that are contained in $\mathbb{P}_{\max}(G[M])$ of some prime module M of G.

When modules $M_1, \dots, M_k$ of G are merged w.r.t. H then all vertices in $M = \bigcup_{h=1}^{k} M_h$ must have the same out$_M$-neighbors in H, while at least two vertices $x \in M_i$, $y \in M_j$, $1 \leq i \neq j \leq k$ must have different out$_M$-neighbors in G. Hence, in order to merge these modules it is necessary to change the out$_M$-neighbors in G. However, edit operations between vertices *within* M are dispensable for obtaining the module M.

Definition 4.2 (Module Merge Edit)**.** Let $G = (V, E)$ be an arbitrary graph and F be an arbitrary edit set resulting in the graph $H = (V, E \triangle F)$. Let $H' \subseteq H$ be an induced subgraph of H and suppose $M_1, \ldots, M_k \in \mathrm{MD}(G)$ are modules that have been merged w.r.t. H' resulting in the module $M = \bigcup_{i=1}^{k} M_i \in \mathrm{MD}(H')$. We then call

$$F_{H'}(\uplus_{i=1}^{k} M_i \to M) := \{\{x, v\} \in F \mid x \in M, v \in V(H') \setminus M\} \tag{4.1}$$

the *module merge edits* associated with $\uplus_{i=1}^{k} M_i \to M$ w.r.t. H'.

By construction, the edit set $F_{H'}(\uplus_{i=1}^{k} M_i \to M)$ comprises exactly those (non)edges of F that have been edited so that all vertices in M have the same out_M-neighborhood in $H' = (V', E')$. In particular, it contains only (non)edges of F that are not entirely contained in $G[M]$, but entirely contained in H'. Moreover, (non)edges of F that contain a vertex in $V(H')$ and a vertex in $V \setminus V(H')$ are not considered as well.

Let G be an arbitrary graph and F be an optimal edit set that applied to G results in the cograph H. We will show that every optimal module-preserving edit set F can be expressed completely by means of module merge edits. To this end, we will consider the prime modules M of the given graph G (in particular certain children of M that do not share the same out-neighborhood) and adjust their out-neighbors to obtain new modules. Illustrative examples are given in Figure 1 and 2.

We are now in the position to derive the main results, Theorems 4.3 – 4.7. We begin with showing that each strong module of H that is not a module of G can be obtained by merging some children of a particular chosen prime module of G. Moreover, we prove that any strong module of H that is a module of G must also be strong in G.

Theorem 4.3. *Let $G = (V, E)$ be an arbitrary graph, F an optimal module-preserving cograph edit set, and $H = (V, E \triangle F)$ the resulting cograph. Then, each strong module $M^\star$ of H is either a module in G or there exists a prime module $P_{M^\star}$ of G that contains $M^\star$ and is minimal w.r.t. inclusion, i.e., there is no prime module $P'_{M^\star}$ of G with $M^\star \subseteq P'_{M^\star} \subsetneq P_{M^\star}$. In the latter case $M^\star$ is obtained by merging some modules in $\mathbb{P}_{\max}(G[P_{M^\star}])$.*

Furthermore, if a strong module $M^\star$ of H is a module in G, then $M^\star$ is a strong module of G.

Proof. Let $M^\star$ be an arbitrary strong module of H that is not a module of G. We show first that for the module $M^\star$ there is a prime module $P_{M^\star}$ of G with $M^\star \subseteq P_{M^\star}$ such that there is no other prime module $P'_{M^\star}$ of G with $M^\star \subseteq P'_{M^\star} \subsetneq P_{M^\star}$.

Since $M^\star$ is a module of H but not of G there are vertices $x \in M^\star$ and $y \in V \setminus M^\star$ with $\{x, y\} \in F$. Now, let $P_{M^\star}$ be the strong module of G containing x and y that is minimal w.r.t. inclusion, that is, there is no other strong module of G that is properly contained in $P_{M^\star}$ and that contains x and y. Thus $\{x, y\} \in F[P_{M^\star}]$. Lemma 3.9 implies that $F[P_{M^\star}]$ is an optimal edit set of $G[P_{M^\star}]$. Since $P_{M^\star}$ is minimal w.r.t. inclusion it holds that x and y are from distinct children $M_x, M_y \in \mathbb{P}_{\max}(G[P_{M^\star}])$. We continue to show that this strong module $P_{M^\star}$ is indeed prime. Assume for contradiction, that $P_{M^\star}$ is a non-prime module of G. If $P_{M^\star}$ is parallel, then editing $\{x, y\}$ would connect the two connected components M_x, M_y of $G[P_{M^\star}]$. Then, it follows by Lemma 3.6 that $F[P_{M^\star}]$ is not optimal; a contradiction. By similar arguments for the complement $\overline{G[P_{M^\star}]}$ it can be shown that $P_{M^\star}$ cannot be a series module. Thus $P_{M^\star}$ must be prime. Since F is module-preserving, $P_{M^\star}$ is module in H. Hence, $P_{M^\star}$ and $M^\star$ cannot overlap, since $M^\star$ is strong in H. However, since $x \in P_{M^\star} \cap M^\star$ and $y \in P_{M^\star}$ but $y \notin M^\star$ we have $M^\star \subseteq P_{M^\star}$.

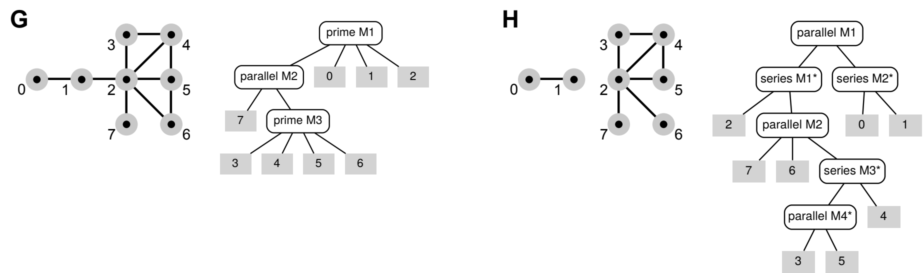

Figure 2: Illustration of the main results. Consider the non-cograph G, the cograph $H = G \triangle F$ and the module-preserving edit set $F = \{\{1,2\},\{5,6\}\}$. The modular decomposition trees are depicted right to the respective graphs.
According to Theorem 4.3, both strong modules M_1 and M_2 of H that are modules of G are also strong modules of G and correspond to the prime module M_1 and the parallel module M_2 in G, respectively. Moreover, each of the new strong modules $M_1^\star, \dots, M_4^\star$ of H are obtained by merging children of a prime module of G. To be more precise, $M_1^\star$ and $M_2^\star$ are obtained by merging children of the prime module M_1 of G: $M_2 \uplus \{2\} \to M_1^\star$ and $\{0\} \uplus \{1\} \to M_2^\star$ with $F_{H[M_1]}(M_2 \uplus \{2\} \to M_1^\star) = F_{H[M_1]}(\{0\} \uplus \{1\} \to M_2^\star) = \{\{1,2\}\}$. The new strong modules $M_3^\star$ and $M_4^\star$ are obtained by merging children of the prime module M_3 of G: $\{3\} \uplus \{5\} \to M_4^\star$ and $\{3\} \uplus \{4\} \uplus \{5\} \to M_3^\star$ with $F_{H[M_3]}(\{3\} \uplus \{5\} \to M_4^\star) = F_{H[M_3]}(\{3\} \uplus \{4\} \uplus \{5\} \to M_3^\star) = \{\{5,6\}\}$. According to Corollary 4.7, the set F can be written as the union of the edit sets used to obtain the new merged modules of H.
It is worth noting that not all strong modules of G remain strong in H (e.g. the prime module M_3) and that there are (non-strong) modules in H (e.g. the module $\{6,7\}$) that are not obtained by merging children of prime modules of G.

Finally, since $P_{M^\star}$ is chosen to be minimal w.r.t. inclusion, there exists in particular no prime module $P'_{M^\star}$ of G with $M^\star \subseteq P'_{M^\star} \subsetneq P_{M^\star}$.

We continue to show that $M^\star$ is obtained by merging some child modules of $P_{M^\star}$ in G, say $M_1, \dots, M_k \in \mathbb{P}_{\max}(G[P_{M^\star}])$. Note that we just formally prove the existence of such a subset $\{M_1, \dots, M_k\} \subset \mathbb{P}_{\max}(G[P_{M^\star}])$ without explicitly constructing it. To this end, we need to verify the three conditions of Definition 4.1, i.e., (i) $M_1, \dots, M_k \in \mathrm{MD}(H)$, (ii) $M^\star := \bigcup_{i=1}^k M_i \in \mathrm{MD}(H)$, and (iii) $M^\star \notin \mathrm{MD}(G)$. Since each $M_i \in \mathbb{P}_{\max}(G[P_{M^\star}])$ is module of G and F is module-preserving, Condition (i) is always satisfied. Moreover, by assumption $M^\star \notin \mathrm{MD}(G)$ and thus Condition (iii) is satisfied.

It remains to show that Condition (ii) is satisfied. To this end, we show that there are modules $M_1, \dots, M_k$ of G (without explicitly constructing them) such that $M^\star = \bigcup_{i=1}^k M_i$. We prove this by showing that each module from $P_{M^\star}$ is either completely contained in, or disjoint from $M^\star$. First, note that $M^\star \neq P_{M^\star}$, since $M^\star$ is not a module of G. Second, $M^\star$ cannot overlap any $M_i \in \mathbb{P}_{\max}(G[P_{M^\star}])$, since M_i is a module of H and $M^\star$ is strong in H. We continue to show that there is no $M_i \in \mathbb{P}_{\max}(G[P_{M^\star}])$ such that $M^\star \subsetneq M_i$. Assume for contradiction that there is a module $M_i \in \mathbb{P}_{\max}(G[P_{M^\star}])$ with $M^\star \subsetneq M_i$. Note that M_i cannot be prime in G, as otherwise $M^\star \subseteq M_i = P'_{M^\star} \subsetneq P_{M^\star}$, contradicting the minimality of $P_{M^\star}$. Moreover, $M^\star$ cannot overlap any $M_j^i \in \mathbb{P}_{\max}(G[M_i])$, since $M^\star$ is strong in H and any M_j^i is a module of H, since F is module-preserving. Furthermore, since M_i is non-prime in G for any subset $\{M^i_1, \dots, M^i_l\} \subsetneq \mathbb{P}_{\max}(G[M_i])$ it holds that the set $M' = \bigcup_{j=1}^{l} M^i_j$ is a module of G (cf. Theorem 3.3(T3)). Since $M^\star$ is no module of G it cannot be a union of elements in $\mathbb{P}_{\max}(G[M_i])$. Note that this especially implies that $M^\star \neq M_i$ and $M^\star \neq M^i_j$ for all $M^i_j \in \mathbb{P}_{\max}(G[M_i])$. Now it follows, that $M^\star \subset M^i_j$ for some $M^i_j \in \mathbb{P}_{\max}(G[M_i])$. Repeating the latter arguments and since G is finite, there must be a minimal set M^a_b with $M^\star \subset M^a_b \subset \dots \subset M^i_j \subset M_i$. Now we apply the latter arguments again and obtain that $M^\star \subset M' \in \mathbb{P}_{\max}(G[M^a_b])$ which is not possible, since M^a_b is chosen to be the minimal module that contains $M^\star$. Thus, there is no $M_i \in \mathbb{P}_{\max}(G[P_{M^\star}])$ such that $M^\star \subseteq M_i$.

Now, since $M^\star \neq P_{M^\star}$, and $M^\star$ does not overlap any $M_i \in \mathbb{P}_{\max}(G[P_{M^\star}])$, and there is no $M_i \in \mathbb{P}_{\max}(G[P_{M^\star}])$ such that $M^\star \subseteq M_i$, there must be a set $\{M_1, \dots, M_k\} \subsetneq \mathbb{P}_{\max}(G[P_{M^\star}])$ such that $M^\star = \bigcup_{i=1}^{k} M_i$. Thus, Condition (ii) is satisfied and therefore $M^\star$ is obtained by merging modules in $\mathbb{P}_{\max}(G[P_{M^\star}])$.

Hence, any strong module of H is either a module of G or obtained by merging the children of a prime module of G.

Finally, assume that there is a strong module $M^\star$ in H that is a module of G. Assume that $M^\star$ is not strong in G. Then there is a module M in G that overlaps $M^\star$. Since F is module-preserving, M is a module in H and thus, M overlaps $M^\star$ in H; a contradiction. Thus, any strong module $M^\star$ of H that is also a module of G must be strong in G. □

Theorem 4.3 allows us to give the following definitions that we will use in the subsequent part.

Definition 4.4. Let $G = (V, E)$ be an arbitrary graph, F an optimal module-preserving cograph edit set, and $H = (V, E \triangle F)$ the resulting cograph. Let $M^\star$ be a strong module of H but no module of G.

We denote by $P_{M^\star}$ the prime module of G that contains $M^\star$ and is minimal w.r.t. inclusion, i.e., there is no prime module $P'_{M^\star}$ of G with $M^\star \subseteq P'_{M^\star} \subsetneq P_{M^\star}$. Furthermore, we denote by $\mathcal{C}(M^\star) \subset \mathbb{P}_{\max}(G[P_{M^\star}])$ the set of children of $P_{M^\star}$ that satisfies $\bigcup_{M_i \in \mathcal{C}(M^\star)} M_i = M^\star$.

The next result provides a characterization of module-preserving edit sets by means of module merge of the children of prime modules.

Theorem 4.5. *Let $G = (V, E)$ be an arbitrary graph, F an optimal cograph edit set, and $H = (V, E \triangle F)$ the resulting cograph. Then F is module-preserving for G if and only if each new strong module $M^\star$ of H that is not a module of G is obtained by merging the modules in $\mathcal{C}(M^\star) \subset \mathbb{P}_{\max}(G[P_{M^\star}])$, in symbols $\uplus_{M_i \in \mathcal{C}(M^\star)} M_i \to M^\star$.*

Proof. If F is an optimal and module-preserving edit-set for G, we can apply Theorem 4.3.

For the converse, assume for contraposition that F is not module-preserving. Then, there is a module M_i in G that is not a module in H. Hence, there is a vertex $z \in V \setminus M_i$ and two vertices $x, y \in M_i$ such that $xz \in E(H)$ and $yz \notin E(H)$ and thus, either $\{x, z\} \in F$ or $\{y, z\} \in F$. There are two cases, either $xy \in E(H)$ or $xy \notin E(H)$. Since H is a cograph we can apply Theorem 3.2 and conclude that either $\mathrm{yz|x} \in \mathcal{R}(H)$ or $\mathrm{xz|y} \in \mathcal{R}(H)$. Assume that $\mathrm{xz|y} \in \mathcal{R}(H)$ and let T be the cotree of H. Since T displays $\mathrm{xz|y}$, the strong module $M^\star$ of H located at the $\mathrm{lca}_T(x, z)$ contains the vertices x and z but not y. Moreover, since there is an edit $\{x, z\}$ or $\{y, z\}$ in F there is a strong prime module $P_{M^\star}$ in G that contains x, y, z and is minimal w.r.t. inclusion. Note, $M_i \neq P_{M^\star}$ since

$x, y \in M_i$ and $z \notin M_i$. Moreover, since M_i is a module in G, but none of the unions of the children of $P_{M^\star}$ is a module of G (cf. Theorem 3.3(T3)), we can conclude that $M_i \subseteq M'$, where M' is a child of $P_{M^\star}$ in G. Since $P_{M^\star}$ is the minimal prime module that contains x, y, z and there is an edit $\{x, z\}$ or $\{y, z\}$ in F, the vertex z must be located in a module different from the module M' that contains both x and y. Thus, $z \notin M'$. Therefore, there is no module in G that contains x and z but not y. Thus, $M^\star$ is no module of G. Since there is no module in G that contains x and z but not y, the set $M^\star$ cannot be written as the union of children of any strong prime module $P_{M^\star}$ and thus, $M^\star$ is not obtained by merging modules of $\mathbb{P}_{\max}(G[P_{M^\star}])$. The case yz|x $\in \mathcal{R}(H)$ is shown analogously. □

Combining the latter results, it can be shown that for every graph G there is always an optimal edit set such that the resulting cograph H contains all modules of G and any newly created strong module $M^\star$ of H is obtained by merging the respective modules in $\mathcal{C}(M^\star)$.

Theorem 4.6. *Any graph $G = (V, E)$ has an optimal edit-set F such that each strong module $M^\star$ in $H = (V, E \triangle F)$ that is not a module of G is obtained by merging modules in $\mathbb{P}_{\max}(G[P_{M^\star}])$, where $P_{M^\star}$ is a prime module of G.*

Proof. Proposition 3.7 implies that any graph has a module-preserving optimal edit set. Hence, we can apply Theorem 4.5 to derive the statement. □

Finally, the following result shows that each module-preserving edit set can indeed be derived by considering the module merge edits only.

Theorem 4.7. *Let $G = (V, E)$ be an arbitrary graph, F an optimal module-preserving cograph edit set, $H = (V, E \triangle F)$ the resulting cograph, and $\mathcal{M}$ the set of all strong modules of H that are no modules of G. Then,*

$$F = \bigcup_{M^\star \in \mathcal{M}} \left(F_{H[P_{M^\star}]}(\uplus_{M_i \in \mathcal{C}(M^\star)} M_i \to M^\star) \right).$$

Proof. We set $F^\star = \bigcup_{M^\star \in \mathcal{M}} \left(F_{H[P_{M^\star}]}(\uplus_{M_i \in \mathcal{C}(M^\star)} M_i \to M^\star) \right)$. Clearly, it holds that $F^\star \subseteq F$. It remains to show that, $F \subseteq F^\star$. First, observe, that every edit $\{x, y\} \in F$ is between distinct children $M_x, M_y \in \mathbb{P}_{\max}(G[P_{M^\star}])$ of a prime module $P_{M^\star}$ of G. To see this, let $P_{M^\star}$ be a strong module of G such that x and y are in distinct children $M_x, M_y \in \mathbb{P}_{\max}(G[P_{M^\star}])$ and assume for contradiction that $P_{M^\star}$ is non-prime in G. Let $F' := \bigcup_{M_i \in \mathbb{P}_{\max}(G[P_{M^\star}])} F[M_i]$. Since $P_{M^\star}$ is non-prime in G it follows that F' is an edit set for $G[P_{M^\star}]$, that is, $G[P_{M^\star}]\Delta F'$ is a cograph. But $|F'| < |F[P_{M^\star}]|$; contradicting Lemma 3.9. Thus, every edit $\{x, y\} \in F$ is between distinct children $M_x, M_y \in \mathbb{P}_{\max}(G[P_{M^\star}])$ of a prime module $P_{M^\star}$ of G.

Assume that $\{x, y\} \in F$, but $\{x, y\} \notin F^\star$. By the latter arguments, there is a prime module $P_{M^\star}$ of G with $x \in M_x$ and $y \in M_y$ and $M_x, M_y \in \mathbb{P}_{\max}(G[P_{M^\star}])$. Now let M'_x be the strong module of H that contains x but not y and that is maximal w.r.t. inclusion. Since F is module-preserving, M_x is a module in H. Moreover, since M'_x is a strong module of H, the modules M'_x and M_x do not overlap in H. Therefore, either $M_x \subsetneq M'_x$ or $M'_x \subseteq M_x$. We show first that the case $M_x \subsetneq M'_x$ is not possible. Assume for contradiction, that $M_x \subsetneq M'_x$. Thus, there is a vertex $z \in M'_x \setminus M_x$. Since $P_{M^\star}$ is prime in G and $M_x \in \mathbb{P}_{\max}(G[P_{M^\star}])$, we can apply Theorem 3.3(T2) and conclude that there is no other module than M_x in G that entirely contains M_x but not y. Since

$M_x \subsetneq M'_x \subsetneq P_{M^\star}$ it follows that M'_x is a new strong module of H and therefore, by Theorem 4.3, obtained by merging modules $M_1, \dots, M_k \in \mathcal{C}(M'_x) \subsetneq \mathbb{P}_{\max}(G[P_{M^\star}])$. But then $\{x, y\} \in F_{H[P_{M^\star}]}(\uplus_{M_i \in \mathcal{C}(M'_x)} M_i \to M'_x) \subseteq F^\star$; contradicting that $\{x, y\} \notin F^\star$. Hence, $M'_x \subseteq M_x$. Similarly, $M'_y \subseteq M_y$ for the strong module M'_y of H that contains y but not x and that is maximal w.r.t. inclusion.

Consider now the strong module $M^\star$ of H that is identified with the lowest common ancestor of the modules $\{x\}$ and $\{y\}$ within the cotree of H. Then, there are distinct children in $\mathbb{P}_{\max}(H[M^\star])$, containing x and y, respectively. Since M'_x is the strong module of H that contains x but not y and that is maximal w.r.t. inclusion, we have $M'_x \in \mathbb{P}_{\max}(H[M^\star])$. Analogously, $M'_y \in \mathbb{P}_{\max}(H[M^\star])$.

Both, M_x as well as M_y are modules in H and G. Since F is module-preserving, either all or none of the edges between M_x and M_y are edited. Since $\{x, y\} \in F$ we have, therefore, $\{x', y'\} \in F$ for all $x' \in M'_x \subseteq M_x$ and $y' \in M'_y \subseteq M_y$. Let $F' := \{\{x', y'\} \mid x' \in M'_x, y' \in M'_y\}$. By the latter argument $F' \neq \emptyset$ and $F' \subseteq F$.

Note, the subgraphs $H[M'_x]$ and $H[M'_y]$ are cographs. Since $M^\star$ is either a parallel or a series module in H, we have either (i) $H[M'_x \cup M'_y] = H[M'_x] \,\dot\cup\, H[M'_y]$ or (ii) $H[M'_x \cup M'_y] = H[M'_x] \oplus H[M'_y]$, respectively. Since F' comprises the edits $\{x', y'\}$ between *all* vertices $x' \in M'_x$ and $y' \in M'_y$, the graph $H[M'_x \cup M'_y] \triangle F'$ is in case (i) the graph $H[M'_x] \oplus H[M'_y]$ and in case (ii) $H[M'_x] \,\dot\cup\, H[M'_y]$. By definition, in both cases $H[M'_x \cup M'_y] \triangle F'$ is a cograph. Note that F' did not change the out$_{M'_x \cup M'_y}$-neighborhood and thus, the graph $H[M^\star] \triangle F' = G[M^\star] \triangle (F[M^\star] \setminus F')$ is a cograph as well. Since $\{x, y\} \in F' \cap F[M^\star]$ it holds that $|F[M^\star] \setminus F'| < |F[M^\star]|$. But then, $F[M^\star]$ is not optimal, and therefore, by Lemma 3.9 the set F is not optimal; a contradiction.

In summary, there exists no edit $\{x, y\} \in F$ with $\{x, y\} \notin F^\star$. Hence, $F \subseteq F^\star$ and the statement follows. □

From an algorithmic perspective, Theorem 4.7 implies that it is sufficient to correctly determine the set of strong modules of a resulting cograph H that are no modules of the given graph G. Afterwards, the module-preserving edit set F is obtained by taking all the edits needed for the corresponding module merge operations. On the other hand, by Theorem 4.6 it is ensured that such a closest cograph H that contains all modules of G always exists.

5 Pairwise module merge and algorithmic issues

So far, we have shown that for an arbitrary graph $G = (V, E)$ there is an optimal module-preserving edit set F that transforms G into the cograph $H = (V, E \triangle F)$ (cf. Theorem 4.6). Moreover, this edit set F can be expressed in terms of edits derived by module merge operations on the strong modules of H that are no modules of G (cf. Theorem 4.7). In what follows, we show that there is an explicit order in which these individual merge operations can be consecutively applied to G such that all intermediate edit-steps result in graphs that contain all modules of G, and, moreover, all new strong modules produced in this edit-step are preserved in any further step. In Section 5.1, we show that an optimal edit set can always be obtained by a series of "ordered" pairwise merge operations. In Section 5.2, we show that the latter "order"-condition can even be relaxed and that particular modules can be pairwisely merged in an arbitrary order to obtain an optimal edited graph.

The next Lemma shows that the number of edits in an optimal edit set F can be expressed as the sum of individual edits based on the $\uplus$-operator to obtain the strong modules in a cograph $H = G \triangle F$ that are no modules in G.

Lemma 5.1. *Let $G = (V, E)$ be a graph, F an optimal module-preserving cograph edit-set, and $H = (V, E \triangle F)$ the resulting cograph. Let $\mathcal{M} = \{M_1^\star, \dots, M_n^\star\}$ be the set of all strong modules of H that are no modules of G and assume that the elements in $\mathcal{M}$ are partially ordered w.r.t. inclusion, i.e., $M_i^\star \subseteq M_j^\star$ implies $i \leq j$.*

Let $M^\star \in \mathcal{M}$. We set $F_{M^\star} := \{\{x, v\} \in F \mid x \in M^\star, v \in P_{M^\star} \setminus M^\star\}$, that is, the set $F_{M^\star} \subseteq F$ comprises all edits in F that are used to obtain the module $M^\star$ within $G[P_{M^\star}]$.

Furthermore, we set $\sigma_{M_1^\star} = F_{M_1^\star}$ and $\sigma_{M_i^\star} = F_{M_i^\star} \setminus (\bigcup_{j=1}^{i-1} F_{M_j^\star})$, $2 \leq i \leq n$. Then

$$F = \dot{\bigcup_{i=1}^{n}} \sigma_{M_i^\star} \text{ and, thus, } |F| = \sum_{i=1}^{n} |\sigma_{M_i^\star}| .$$

Moreover, for each intermediate graph $G_j = G \triangle \left(\bigcup_{i=1}^{j} \sigma_{M_i^\star}\right)$ and any $M_i^\star \in \mathcal{M}$ with $i - 1 \leq j$ we have

$$G_j[M_i^\star] = H[M_i^\star] .$$

In each step j the induced subgraphs $G_j[M_i^\star]$ are already cographs for all sets $M_i^\star$ with $i - 1 \leq j$ and hence $F[M_i^\star] \setminus \bigcup_{k=1}^{j} \sigma_{M_k^\star} = \emptyset$, for all $i - 1 \leq j$.

Proof. By Theorem 4.3, for each $M^\star \in \mathcal{M}$ there is an inclusion-minimal prime module $P_{M^\star}$ in G and a set of children $\mathcal{C}(M^\star) \subseteq \mathbb{P}_{\max}(G[P_{M^\star}])$ such that $\uplus_{M_i \in \mathcal{C}(M^\star)} M_i \to M^\star$. Thus, $P_{M^\star}$ and $\mathcal{C}(M^\star)$ exists and $\mathcal{C}(M^\star)$ is not empty.

Now, we show that $|F|$ can be expressed by the sum of the size of the edits in $\sigma_{M_i^\star}$ To this end, observe that by Theorem 4.7, $F = \bigcup_{M^\star \in \mathcal{M}} \left(F_{H[P_{M^\star}]}(\uplus_{M_i \in \mathcal{C}(M^\star)} M_i \to M^\star)\right)$. Thus, $F = \bigcup_{M^\star \in \mathcal{M}} F_{M^\star}$. By construction of $\sigma_{M_i^\star}$ it holds first that $\bigcup_{i=1}^{n} \sigma_{M_i^\star} = \bigcup_{i=1}^{n} F_{M_i^\star}$ and second that $\sigma_{M_i^\star} \cap \sigma_{M_j^\star} = \emptyset$ for all $i \neq j$. Hence, $F = \dot{\bigcup}_{i=1}^{n} \sigma_{M_i^\star}$ and thus, $|F| = \sum_{i=1}^{n} |\sigma_{M_i^\star}|$.

By construction, $\mathcal{M}$ is partially ordered w.r.t. inclusion. We want to show that $G_j[M_i^\star] = H[M_i^\star]$ for all $i - 1 \leq j$. To this end, we show that $F[M_i^\star] \setminus \bigcup_{k=1}^{j} \sigma_{M_k^\star} = \emptyset$, in which case after each step j there are no more edits left to modify an edge between vertices within $M_i^\star$. We show first that the latter is satisfied for all $1 \leq i \leq n$ and a fixed $j = i - 1$. Assume for contradiction that $\{x, y\} \in F[M_i^\star] \setminus \bigcup_{k=1}^{i-1} \sigma_{M_k^\star}$ and thus, $x, y \in M_i^\star$. Since $\{x, y\} \in F = \bigcup_{k=1}^{n} F_{M_k^\star}$, there must be a module $M_\ell^\star \in \mathcal{M}$ such that $\{x, y\} \in F_{M_\ell^\star}$. By construction, $F_{M_\ell^\star}$ contains only the edits that affect the out$_{M_\ell^\star}$-neighborhood. Thus, w.l.o.g. we can assume that $x \in M_\ell^\star$ and $y \notin M_\ell^\star$. Since $M_\ell^\star$ and $M_i^\star$ are strong modules, they do not overlap, and therefore, $M_\ell^\star \subsetneq M_i^\star$. However, since $\mathcal{M}$ is partially ordered, we can conclude that $\ell < i$ and therefore, $\{x, y\} \in \bigcup_{k=1}^{i-1} \sigma_{M_k^\star}$. Hence, $\{x, y\} \notin F[M_i^\star] \setminus \bigcup_{k=1}^{i-1} \sigma_{M_k^\star}$; a contradiction. Thus, $F[M_i^\star] \setminus \bigcup_{k=1}^{i-1} \sigma_{M_k^\star} = \emptyset$ for all $1 \leq i \leq n$. But then, clearly $F[M_i^\star] \setminus \bigcup_{k=1}^{j} \sigma_{M_k^\star} = \emptyset$ holds for any $j \geq i - 1$. Thus, $G_j[M_i^\star] = H[M_i^\star]$ for all $i - 1 \leq j$. □

The following Lemma shows that, given the explicit order $\mathcal{M} = \{M_1^\star, \dots, M_n^\star\}$ from Lemma 5.1, in which the edits are applied to the graph G, the intermediate graphs G_i retain all modules of G and also all new modules $M_j^\star$, $j \leq i$.

Lemma 5.2. *Let $G = (V, E)$ be an arbitrary graph, F an optimal module-preserving cograph edit set, and $H = (V, E \triangle F)$ the resulting cograph. Moreover, let $\mathcal{M} = \{M_1^\star, \dots, M_n^\star\}$ be the partially ordered (w.r.t. inclusion) set of all strong modules of H that are no modules of $G_0 := G$, and choose $\sigma_{M_i^\star}$, $F_{M_i^\star}$ and the intermediate graphs G_i, $1 \leq i \leq n$ as in Lemma 5.1.*

Then, any module M' of G is a module of G_i and the set $M_j^\star$ is a module of G_i for $1 \leq i \leq n$ and any $j \leq i$.

Proof. First note that $\sigma_{M_i^\star}$ affects only modules that are entirely contained in $P_{M_i^\star}$ and only their out-neighbors within $P_{M_i^\star}$. Moreover $M_j^\star \subseteq M_i^\star$ implies that $P_{M_j^\star} \subseteq P_{M_i^\star}$. The partial ordering of the elements in $\mathcal{M}$ implies that $P_{M_i^\star}$ remains a module in G_i.

Before we prove the main statement, we show first that the following statement is satisfied:

Claim 1. *For every M' with $M_i^\star \subsetneq M' \subsetneq P_{M_i^\star}$ we have $M' \neq M_j^\star \in \mathcal{M}$, $j \leq i$ and M' cannot be a module of G.*

Proof of Claim 1. Let M' be an arbitrary set with $M_i^\star \subsetneq M' \subsetneq P_{M_i^\star}$. By the partial order of the elements in $\mathcal{M}$ we immediately observe that $M' \neq M_j^\star \in \mathcal{M}$ for any $j \leq i$. Now assume for contradiction that M' is a module of G. Note, all elements in $\mathbb{P}_{\max}(G[P_{M_i^\star}])$ are strong modules of G, and thus, do not overlap the module M'. Moreover, since $P_{M_i^\star}$ is prime in G, we can apply Theorem 3.3(T2) and conclude that the union of elements of any proper subset $\mathbb{P}' \subsetneq \mathbb{P}_{\max}(G[P_{M_i^\star}])$ with $|\,\mathbb{P}'\,| > 1$ is not a module of G. Taken the latter arguments together and because $M' \subsetneq P_{M_i^\star}$, we have $M' \subseteq M_\ell \in \mathbb{P}_{\max}(G[P_{M_i^\star}])$ for some ℓ. Hence, $M_i^\star \subsetneq M' \subseteq M_\ell$. However, since $M_i^\star$ is the union of some children $\mathbb{P}' \subseteq \mathbb{P}_{\max}(G[P_{M_i^\star}])$ of $P_{M_i^\star}$ it follows that $M_\ell \subseteq M_i^\star$; a contradiction. This proves Claim 1. $\triangleleft$

We continue with proving the main statement by induction over i. Since $G_0 = G$, the statement is satisfied for G_0. We continue to show that the statement is satisfied for G_{i+1} under the assumption that it is satisfied for G_i.

For further reference, we note that $P_{M_{i+1}^\star}$ is a module of G_i, since $P_{M_{i+1}^\star}$ is a module of G and by induction assumption. Moreover, $P_{M_{i+1}^\star}$ remains a module of G_{i+1}, since $G_{i+1} = G_i \triangle \sigma_{M_{i+1}^\star}$ and $\sigma_{M_{i+1}^\star}$ does not affect the $\text{out}_{P_{M_{i+1}^\star}}$-neighborhood. Furthermore, $M_{i+1}^\star$ is a module of H and thus, of $H[P_{M_{i+1}^\star}]$. Since $\sigma_{M_{i+1}^\star}$ contains all such edits to adjust $M_{i+1}^\star$ to a module in $H[P_{M_{i+1}^\star}]$, we can conclude that $M_{i+1}^\star$ is a module in $G_{i+1}[P_{M_{i+1}^\star}]$. Therefore, Lemma 3.1 implies that $M_{i+1}^\star$ is a module of G_{i+1}.

Now, let M' be an arbitrary module of G. We proceed to show that M' is a module of G_{i+1}. By induction assumption, each module M' of G is a module of G_i. Since F is module-preserving, M' is also a module of H. Hence, $M' \in \text{MD}(G) \cap \text{MD}(G_i) \cap \text{MD}(H)$. Moreover, by Claim 1 the case $M_{i+1}^\star \subsetneq M' \subsetneq P_{M_{i+1}^\star}$ cannot occur for any module M' of G.

Note, the module M' cannot overlap $P_{M_{i+1}^\star}$, since $P_{M_{i+1}^\star}$ is strong in G. Hence, for M' one of the following three cases can occur: either $P_{M_{i+1}^\star} \subseteq M'$, $P_{M_{i+1}^\star} \cap M' = \emptyset$, or $M' \subsetneq P_{M_{i+1}^\star}$. In the first two cases, M' remains a module of G_{i+1}, since $\sigma_{M_{i+1}^\star}$ contains only edits between vertices within $P_{M_{i+1}^\star}$, and thus, the $\text{out}_{M'}$-neighborhood is not affected. Therefore, assume that $M' \subsetneq P_{M_{i+1}^\star}$. The module M' cannot overlap $M_{i+1}^\star$, since $M^\star_{i+1}$ is strong in H. As shown above, the case $M^\star_{i+1} \subsetneq M' \subsetneq P_{M^\star_{i+1}}$ cannot occur, and thus we have either (1) $M' \subseteq M^\star_{i+1}$, or (2) $M^\star_{i+1} \cap M' = \emptyset$.

Case (1): Since $\sigma_{M^\star_{i+1}}$ affects only the $\text{out}_{M^\star_{i+1}}$-neighborhood, there is no edit between vertices in M' and $M^\star_{i+1} \setminus M'$ and, moreover, $G_{i+1}[M^\star_{i+1}] = G_i[M^\star_{i+1}]$. By assumption, M' is a module of G_i. Thus, M' is a module in any induced subgraph of G_i that contains M' and hence, in particular in $G_i[M^\star_{i+1}]$. Hence, M' is a module of $G_{i+1}[M^\star_{i+1}]$. Now, we can apply Lemma 3.1 and conclude that M' is also a module of G_{i+1}.

Case (2): Assume for contradiction that M' is no module of G_{i+1}. Thus, there must be an edge $xy \in E(G_{i+1})$, $x \in M', y \in V \setminus M'$ such that for some other vertex $x' \in M'$ we have $x'y \notin E(G_{i+1})$. Since M' is a module of G_i it must hold that $\{x, y\} \in \sigma_{M^\star_{i+1}}$ or $\{x', y\} \in \sigma_{M^\star_{i+1}}$. Since $x, x' \notin M^\star_{i+1}$ and each edit in $\sigma_{M^\star_{i+1}}$ affects a vertex within $M^\star_{i+1}$, we can conclude that $y \in M^\star_{i+1}$. Now, by construction of $F_{M^\star_{i+1}}$ and since $M' \subsetneq P_{M^\star_{i+1}}$, all edits between vertices of $M^\star_{i+1}$ and M' are entirely contained in $F_{M^\star_{i+1}}$. But this implies that none of the sets $\sigma_{M^\star_\ell}$ with $\ell > i+1$ contains $\{x, y\}$ or $\{x', y\}$. Hence, it holds that $xy \in E(H)$ and $x'y \notin E(H)$, which implies that M' is no module of H; a contradiction.

Therefore, each module M' of G is a module of G_{i+1}.

We proceed to show that $M^\star_j \in \mathcal{M}$ is a module of G_{i+1} for all $j \leq i+1$. As we have already shown this for $j = i+1$, we proceed with $j < i+1$. By induction assumption, each module $M^\star_j$ is a module of G_i for all $j < i+1$. Note, the module $M^\star_j$ cannot overlap $P_{M^\star_{i+1}}$, since $M^\star_j$ is strong in H and $P_{M^\star_{i+1}}$ is a module of H, because F is module-preserving. Hence, for $M^\star_j$ one of the following three cases can occur: either $P_{M^\star_{i+1}} \subseteq M^\star_j$, $P_{M^\star_{i+1}} \cap M^\star_j = \emptyset$, or $M^\star_j \subsetneq P_{M^\star_{i+1}}$. In the first two cases, $M^\star_j$ remains a module of G_{i+1}, since $\sigma_{M^\star_{i+1}}$ contains only edits between vertices within $P_{M^\star_{i+1}}$, and thus, the $\text{out}_{M^\star_j}$-neighborhood is not affected. Therefore, assume that $M^\star_j \subsetneq P_{M^\star_{i+1}}$. The module $M^\star_j$ cannot overlap $M^\star_{i+1}$, since both are strong in H. Due to the partial ordering of the elements in $\mathcal{M}$, the case $M^\star_{i+1} \subsetneq M^\star_j$ cannot occur. Hence there are two cases, either (A) $M^\star_j \subseteq M^\star_{i+1}$, or (B) $M^\star_{i+1} \cap M^\star_j = \emptyset$.

Case (A): Since $\sigma_{M^\star_{i+1}}$ affects only the $\text{out}_{M^\star_{i+1}}$-neighborhood, there is no edit between vertices in $M^\star_j$ and $M^\star_{i+1} \setminus M^\star_j$. By analogous arguments as in Case (1), we can conclude that $M^\star_j$ remains a module of $G_{i+1}[M^\star_{i+1}]$. Lemma 3.1 implies that $M^\star_j$ is also a module of G_{i+1}.

Case (B): Assume for contradiction that $M^\star_j$ is no module of G_{i+1}. Thus, there must be an edge $xy \in E(G_{i+1})$, $x \in M^\star_j, y \in V \setminus M^\star_j$ such that for some other vertex $x' \in M^\star_j$ we have $x'y \notin E(G_{i+1})$. Since $M^\star_j$ is a module of G_i it must hold that $\{x, y\} \in \sigma_{M^\star_{i+1}}$ or $\{x', y\} \in \sigma_{M^\star_{i+1}}$. Now, we can argue analogously as in Case (2) and conclude that $xy \in E(H)$ and $x'y \notin E(H)$, which implies that $M^\star_j$ is no module of H; a contradiction.

Therefore, each module $M^\star_j$, $j \leq i+1$ is a module of G_{i+1}. □

The latter two Lemmata show that there exists an explicit order, in which all new modules $M^\star_i$ of H can be constructed such that whenever a module $M^\star_i$ is produced step i the induced subgraph $G_{i-1}[M^\star_i]$ is already a cograph and, moreover, is not edited any further in subsequent steps.

5.1 Pairwise module-merge

Regarding Lemma 5.1, each module $M_i^\star$ is created by applying the remaining edits $\sigma_{M_i^\star} \subseteq F_{M_i^\star}$ of the module merge $\uplus_{M' \in \mathcal{C}(M_i^\star)} M' \to M_i^\star$ to the previous intermediate graph G_{i-1}. Now, there might be linear many modules in $\mathcal{C}(M_i^\star)$ which have to be merged at once to create $M_i^\star$. However, from an algorithmic point of view the module $M_i^\star$ is not known in advance. Hence, in each step, for a given prime module M of G an editing algorithm has to choose one of the exponentially many sets from the power set $\mathcal{P}(\mathbb{P}_{\max} G[M])$ to determine which new module $M_i^\star$ have to be created. For an algorithmic approach, however, it would be more convenient to only merge modules in a pairwise manner, since then only quadratic many combinations of choosing two elements of $\mathbb{P}_{\max} G[M]$ have to be considered in each step.

The aim of this section is to show that for each of the n steps of creating one of the new strong modules $\mathcal{M} = \{M_1^\star, \dots, M_n^\star\}$ of H it is possible to replace the merge operation $\uplus_{M' \in \mathcal{C}(M_i^\star)} M' \to M_i^\star$ with a series of pairwise merge operations.

Before we can state this result we have to define the following partition of strong modules of a resulting cograph H that are no modules of a given graph G.

Definition 5.3. Let $G = (V, E)$ be an arbitrary graph, F a module-preserving cograph edit set, and $H = (V, E \triangle F)$ the resulting cograph. Moreover, let $M^\star \in \mathcal{M}$ be a strong module of H that is no module of G and consider the partitions $\mathbb{P}_{\max}(H[M^\star]) = \{\widetilde{M}_1, \dots, \widetilde{M}_k\}$ and $\mathcal{C}(M^\star) = \{\widehat{M}_1, \dots, \widehat{M}_l\}$. We define with $\mathcal{X}(M^\star) = \{M_0, \dots, M_n\}$ the set of modules that contains the maximal (w.r.t. inclusion) modules of $\mathbb{P}_{\max}(H[M_i^\star]) \cup \mathcal{C}(M_i^\star)$ as follows

$$\mathcal{X}(M^\star) := \{\widetilde{M}_i \in \mathbb{P}_{\max}(H[M^\star]) \mid \exists \widehat{M}_j \in \mathcal{C}(M^\star) \text{ s.t. } \widehat{M}_j \subseteq \widetilde{M}_i\} \cup \{\widehat{M}_j \in \mathcal{C}(M^\star) \mid \exists \widetilde{M}_i \in \mathbb{P}_{\max}(H[M^\star]) \text{ s.t. } \widetilde{M}_i \subseteq \widehat{M}_j\}.$$

Note that for technical reasons the index of the elements in $\mathcal{X}$ starts with 0.

Furthermore, assume that $\mathcal{M} = \{M_1^\star, \dots, M_n^\star\}$ is a partially ordered (w.r.t. inclusion) set of all strong modules of H that are no modules of G. For each $M_i^\star \in \mathcal{M}$ let $\mathcal{X}(M_i^\star) = \{M_{i,0}, \dots, M_{i,l_i}\}$ and set $M_i^\star(j) = \bigcup_{k=0}^{j} M_{i,k}$ for all $1 \leq i \leq n$ and $1 \leq j \leq l_i$. Then, we denote with

$$\mathcal{N}(\mathcal{M}) = \{N_1^\star = M_1^\star(1), \dots, N_m^\star = M_n^\star(l_n)\}$$

the set of all such $M_i^\star(j)$. In particular, we assume that $\mathcal{N}(\mathcal{M})$ is ordered as follows: if $N_k^\star = M_i^\star(j)$ and $N_l^\star = M_{i'}^\star(j')$, then $k < l$ if and only if either $i < i'$, or $i = i'$ and $j < j'$, i.e., within $\mathcal{N}(\mathcal{M})$ the elements $M_i^\star(j)$ are ordered first w.r.t. i, and second w.r.t. j.

Although, we have already shown by Theorem 4.5 that any new strong module $M^\star \in \mathcal{M}$ of H can be obtained by merging the modules from $\mathcal{C}(M^\star)$, we will see in the following that $M^\star$ can also be obtained by merging the modules form $\mathcal{X}(M^\star)$. In particular, we will see that if all elements in $\mathcal{X}(M^\star)$ are already modules of the intermediate graph $G^\star$, then we can use any order of the elements within $\mathcal{X}(M^\star)$ and successively merge them in a pairwise manner to construct $M^\star$. As a consequence of doing pairwise module merges we obtain in each step an intermediate module $N^\star \in \mathcal{N}(\mathcal{M})$.

To see the intention to use the partition $\mathcal{X}(M^\star)$ instead of $\mathcal{C}(M^\star)$ observe the following. Due to the order of the elements in $\mathcal{M}$, the modules $M_1^\star, \dots, M_n^\star$ are constructed from bottom to top, i.e., when module $M^\star$ is processed then all child modules from $\mathbb{P}_{\max}(H[M^\star])$ are already constructed. So, instead of obtaining $M^\star$ by merging $\mathcal{C}(M^\star)$ we can indeed obtain $M^\star$ also by merging $\mathbb{P}_{\max}(H[M^\star])$. However, it might be the case that a non-trivial subset $\bigcup_{i\in I}\widetilde{M}_i = \widehat{M}_j$ for some j, e.g., if $\widehat{M}_j$ is a (strong) prime module of G but not a strong module of H. But also in this case, we have to assure that $\widehat{M}_j$ remains a module of H. In particular, we do not want to destroy $\widehat{M}_j$ by merging the elements from $\mathbb{P}_{\max}(H[M^\star])$ in the incorrect order. Thus, we choose $\widehat{M}_j \in \mathcal{X}(M^\star)$ and do not include the individual $\widetilde{M}_i, i \in I$ into $\mathcal{X}(M^\star)$.

Before we can continue, we have to show that $\mathcal{X}(M^\star)$ as given in Definition 5.3 is indeed a partition of $M^\star$.

Proposition 5.4. *Let $G = (V, E)$ be an arbitrary graph, F a module-preserving cograph edit set, and $H = (V, E \triangle F)$ the resulting cograph. Moreover, let $M^\star$ be a strong module of H that is no module of G and consider the partitions $\mathbb{P}_{\max}(H[M^\star]) = \{\widetilde{M}_1, \ldots, \widetilde{M}_k\}$ and $\mathcal{C}(M^\star) = \{\widehat{M}_1, \ldots, \widehat{M}_l\}$. Then $\mathcal{X}(M^\star)$ is a partition of $M^\star$. As a consequence, for each $M \in \mathcal{X}(M^\star)$ there are index sets $I \subseteq \{1, \ldots, k\}$ and $J \subseteq \{1, \ldots, l\}$ such that $M = \bigcup_{i\in I}\widetilde{M}_i$ and $M = \bigcup_{j\in J}\widehat{M}_j$.*

Proof. First note that all $\widetilde{M}_i \in \mathbb{P}_{\max}(H[M^\star])$ are strong modules of H. Moreover, all $\widehat{M}_j \in \mathcal{C}(M^\star)$ are strong modules of G. Since F is module-preserving it follows that none of the elements $\widetilde{M}_i \in \mathbb{P}_{\max}(H[M^\star])$ overlap any $\widehat{M}_j \in \mathcal{C}(M^\star)$, and vice versa. Hence, for each $\widetilde{M}_i \in \mathbb{P}_{\max}(H[M^\star])$ there are three distinct cases: Either $\widetilde{M}_i \subseteq \widehat{M}_j$, or $\widehat{M}_j \subsetneq \widetilde{M}_i$, or $\widetilde{M}_i \cap \widehat{M}_j = \emptyset$ for all $\widehat{M}_j \in \mathcal{C}(M^\star)$. Now, since $\mathbb{P}_{\max}(H[M^\star])$ and $\mathcal{C}(M^\star)$ are partitions of $M^\star$ it follows for each $x \in M^\star$ that x is contained in exactly one $\widetilde{M}_i \in \mathbb{P}_{\max}(H[M^\star])$ and exactly one $\widehat{M}_j \in \mathcal{C}(M^\star)$ and either $\widetilde{M}_i \subseteq \widehat{M}_j$ or $\widehat{M}_j \subsetneq \widetilde{M}_i$. By construction of $\mathcal{X}(M^\star)$ then either $\widetilde{M}_i = \widehat{M}_j \in \mathcal{X}(M^\star)$; or $\widetilde{M}_i \in \mathcal{X}(M^\star)$ and $\widehat{M}_j \notin \mathcal{X}(M^\star)$; or $\widetilde{M}_i \notin \mathcal{X}(M^\star)$ and $\widehat{M}_j \in \mathcal{X}(M^\star)$. Thus, $\mathcal{X}(M^\star)$ is a partition of $M^\star$. □

Using the partitions $\mathcal{X}(M^\star), M^\star \in \mathcal{M}$ we now show that there is a sequence of pairwise module merge operations that construct the intermediate modules $N_j^\star \in \mathcal{N}(\mathcal{M})$ while keeping all modules from G as well as all previous modules $N_i^\star, i < j$.

Lemma 5.5. *Let $G = (V, E)$ be an arbitrary graph, F an optimal module-preserving cograph edit set, $H = (V, E \triangle F)$ the resulting cograph and $\mathcal{M} = \{M_1^\star, \ldots, M_n^\star\}$ be the partially ordered (w.r.t. inclusion) set of all strong modules of H that are no modules of G.*

For each $M_i^\star \in \mathcal{M}$ let $\mathcal{X}(M_i^\star) = \{M_{i,0}, \ldots, M_{i,l_i}\}$ and assume that $\mathcal{N} := \mathcal{N}(\mathcal{M}) = \{N_1^\star, \ldots, N_m^\star\}$. Note, each $N_l^\star$ coincides with some $M_i^\star(j) = \bigcup_{k=0}^{j} M_{i,k}$. We define $F_{M_i^\star(j)} \subseteq F$ as the set

$$F_{M_i^\star(j)} := \{\{x, v\} \in F \mid x \in M_i^\star(j), v \in P_{M_i^\star} \setminus M_i^\star(j)\}.$$

Furthermore, set $G'_0 = G$ and for each $1 \leq l \leq m$ define $G'_l = G'_{l-1} \triangle \theta_l$ with

$$\theta_l = \begin{cases} \emptyset, & \text{if } N_l^\star \text{ is a module of } G'_{l-1} \\ F_{N_l^\star} \setminus \bigcup_{k=1}^{l-1} \theta_k, & \text{otherwise.} \end{cases}$$

If $N^\star_l$ is no module of G'_{l-1}, then θ_l contains exactly those edits that affect the out-neighborhood of $N^\star_l = M^\star_i(j)$ within $G[P_{M^\star_i}]$ that have not been used so far.

The following statements are true for the intermediate graphs G'_l, $1 \leq l \leq m$:

1. *Any set $N^\star_k$ is a module of G'_l for all $k \leq l$.*
2. *Any module M' of G is a module of G'_l, i.e., $\bigcup_{k=1}^{l} \theta_k$ is module-preserving.*
3. *Either $G'_{l-1} \simeq G'_l$, or there are two modules $M_1, M_2 \in G'_{l-1}$ such that $M_1 \uplus M_2 \to N^\star_l$ is a pairwise module merge w.r.t. G'_l.*

Proof. Before we start to prove the statements, we will first show

Claim 1. *For each $1 \leq l \leq m$ it holds that $N^\star_l$ is a module of H.*

Proof of Claim 1. By construction $N^\star_l = M^\star_i(j) = \bigcup_{k=0}^{j} M_{i,k}$ for some $1 \leq i \leq n$ and $1 \leq j \leq l_i$ with $M_{i,k} \in \mathcal{X}(M^\star_i)$. Moreover, for each $M_{i,k}$ it holds either that $M_{i,k} \in \mathbb{P}_{\max} H[M^\star_i]$ or $M_{i,k}$ is a union of elements in $\mathbb{P}_{\max} H[M^\star_i]$. Therefore, $N^\star_l$ is a union of elements in $\mathbb{P}_{\max} H[M^\star_i]$. Since $M^\star_i$ is a strong non-prime module of H, Theorem 3.3(T3) implies that each union of elements in $\mathbb{P}_{\max} H[M^\star_i]$ is a module of H and therefore, $N^\star_l$ is a module of H, which proves Claim 1. ◁

We proceed to prove Statements 1 and 2 for each intermediate graph G'_l by induction over l. Since $G'_0 = G$, the Statements 1 and 2 are satisfied for G'_0. We continue to show that Statements 1 and 2 are satisfied for G'_{l+1} under the assumption that they are satisfied for G_l.

We start to prove Statement 1. First assume that $N^\star_{l+1}$ is already a module of G'_l. Then, by construction it holds that $\theta_{l+1} = \emptyset$ and therefore, $G'_l = G'_{l+1}$. Now, by induction assumption, it holds that all modules of G and all modules $N^\star_k \in \mathcal{N}$, $k \leq l$ are modules of $G'_l = G'_{l+1}$. Hence, all modules $N^\star_k \in \mathcal{N}$, $k \leq l+1$ are modules of G'_{l+1}. Hence, if $N^\star_{l+1}$ is already a module of G'_l, then Statement 1 is satisfied for G'_{l+1}.

Now assume that $N^\star_{l+1}$ is not a module of G'_l. For the proof of Statement 1, we show first

Claim 2. *$N^\star_{l+1}$ is a module of G'_{l+1}.*

Proof of Claim 2. By construction it holds that $N^\star_{l+1} = M^\star_i(j)$ for some $1 \leq i \leq n$ and $1 \leq j \leq l_i$. Note that $P_{M^\star_i}$ is a module of G and therefore, by induction assumption it is a module of G'_l. Since $\theta_{l+1} \subseteq F_{M^\star_i(j)}$ did only affect the out$_{M^\star_i(j)}$-neighborhood within the prime module $P_{M^\star_i}$ of G it follows that $P_{M^\star_i}$ is a module of G'_{l+1}. Moreover, it holds that $F_{M^\star_i(j)} \subseteq \bigcup_{k=1}^{l+1} \theta_k$. Note that $F_{M^\star_i(j)}$ contains all those edits that affect the out$_{M^\star_i(j)}$-neighborhood within the prime module $P_{M^\star_i}$ of G. Hence, for all $x \in M^\star_i(j)$ and all $y \in P_{M^\star_i} \setminus M^\star_i(j)$ it holds that $xy \in E(H)$ if and only if $xy \in E(G'_{l+1})$. The latter arguments then imply that $M^\star_i(j)$ is a module of G'_{l+1} and therefore, $N^\star_{l+1}$ is a module of G'_{l+1}. This proves Claim 2. ◁

Now, we proceed with showing

Claim 3. *$N^\star_k$, $k \leq l$ is a module of G'_{l+1}.*

Proof of Claim 3. Let $N_k^\star = M_{i'}^\star(j')$ and $N_{l+1}^\star = M_i^\star(j)$. By induction assumption it holds that $N_k^\star$ is a module of G'_l. By the ordering of elements in $\mathcal{N}$ it holds that $i' \leq i$ and by the ordering of elements in $\mathcal{M}$ it then follows that $P_{M_{i'}^\star} \subseteq P_{M_i^\star}$ or $P_{M_{i'}^\star} \cap P_{M_i^\star} = \emptyset$.

If $P_{M_{i'}^\star} \cap P_{M_i^\star} = \emptyset$ then $N_k^\star$ is not affected by the edits in θ_{l+1} since they are all within $P_{M_i^\star}$ and thus, $N_k^\star$ remains a module of G'_{l+1}.

Now consider the case $P_{M_{i'}^\star} \subseteq P_{M_i^\star}$. For later reference, we show

Claim 3'. *$N_k^\star \subseteq N_{l+1}^\star$ or $N_k^\star \cap N_{l+1}^\star = \emptyset$.*

Proof of Claim 3'. If $i' = i$, then $j' < j$ and by construction, $M_{i'}^\star(j') \subsetneq M_i^\star(j)$ which implies that $N_k^\star \subseteq N_{l+1}^\star$. Assume now that $i' < i$ and thus, $N_k^\star = M_{i'}^\star(j') \subseteq M_{i'}^\star$. Since $M_i^\star$ and $M_{i'}^\star$ are strong modules of H they cannot overlap. Therefore, and due to the ordering of the elements in $\mathcal{M}$ it follows that either $M_{i'}^\star \subset M_i^\star$ or $M_{i'}^\star \cap M_i^\star = \emptyset$. If $M_{i'}^\star \cap M_i^\star = \emptyset$, then $N_k^\star \cap N_{l+1}^\star = \emptyset$. If $M_{i'}^\star \subset M_i^\star$, then there is a module $M' \in \mathbb{P}_{\max}(H[M_i^\star])$ such that $M_{i'}^\star \in M'$, since $M_i^\star$ and $M_{i'}^\star$ are strong modules of H. Furthermore, the set $M_i^\star(j)$ is a union of elements in $\mathcal{X}(M_i^\star)$ and for each $M_{i,h} \in \mathcal{X}(M_i^\star)$ it holds that either $M_{i,h} \in \mathbb{P}_{\max}(H[M_i^\star])$ or $M_{i,h}$ is the union of elements in $\mathbb{P}_{\max}(H[M_i^\star])$. Hence, it follows that either $M' \subseteq M_i^\star(j)$ or $M' \cap M_i^\star(j) = \emptyset$. If $M' \cap M_i^\star(j) = \emptyset$, then $M_{i'}^\star(j') \cap M_i^\star(j) = \emptyset$ and hence, $N_k^\star \cap N_{l+1}^\star = \emptyset$. If, on the other hand, $M' \subseteq M_i^\star(j)$, then $M_{i'}^\star(j') \subseteq M_i^\star(j)$ and thus, $N_k^\star \subseteq N_{l+1}^\star$. Therefore, in all cases we have either $N_k^\star \subseteq N_{l+1}^\star$ or $N_k^\star \cap N_{l+1}^\star = \emptyset$, which proves Claim 3'. ◇

By Claim 3', we are left with the following two cases.

Case $N_k^\star \subseteq N_{l+1}^\star$. Since θ_{l+1} did not effect edges within $N_{l+1}^\star$ it holds that $G'_l[N_{l+1}^\star] \simeq G'_{l+1}[N_{l+1}^\star]$. By induction assumption, $N_k^\star$ is a module of G'_l and hence, of $G'_l[N_{l+1}^\star] = G'_l[M_i^\star(j)]$. Thus, $N_k^\star$ is a module of $G'_{l+1}[M_i^\star(j)]$. Now, since $N_{l+1}^\star$ is a module of G'_{l+1} and by Lemma 3.1 it follows that $N_k^\star$ is a module of G'_{l+1}.

Case $N_k^\star \cap N_{l+1}^\star = \emptyset$. Recall that $N_k^\star = M_{i'}^\star(j')$ and $N_{l+1}^\star = M_i^\star(j)$ by the fact that $i' \leq i$. Moreover, as shown in the proof of Claim 2, we have $F_{M_i^\star(j)} \subseteq \bigcup_{k=1}^{l+1} \theta_k$. Therefore, for all $x \in M_i^\star(j)$ and all $y \in M_{i'}^\star(j')$ it holds that $xy \in E(H)$ if and only if $xy \in E(G'_{l+1})$. Now let $y, y' \in M_{i'}^\star(j')$ and $x \notin \setminus M_{i'}^\star(j')$. Since $M_{i'}^\star(j')$ is a module of H, xy as well as xy' are either both edges H or both are non-edges in H.

If $x \in M_i^\star(j)$, then there are no further edits $F \setminus F_{M_i^\star(j)}$ that may affect any of these edges, since $F_{M_i^\star(j)} \subseteq \bigcup_{k=1}^{l+1} \theta_k$. Thus, $xy \in E(G'_{l+1})$ if and only if $xy' \in E(G'_{l+1})$.

If $x \notin M_i^\star(j)$, then xy as well as xy' are not affected by θ_{l+1}. Hence, $xy' \in E(G'_{l+1})$ if and only if $xy' \in E(G'_l)$. By induction assumption, $M_{i'}^\star(j')$ is a module of G'_l and hence, $xy \in E(G'_l)$ if and only if $xy' \in E(G'_l)$ and therefore, $xy \in E(G'_{l+1})$ if and only if $xy' \in E(G'_{l+1})$. Hence, $N_k^\star = M_{i'}^\star(j')$ is a module of G'_{l+1}, which proves Claim 3. ◁

By Claim 1, 2 and 3, Statement 1 is satisfied for G'_{l+1}. We continue to prove Statement 2 and assume that M' is a module of G and by induction assumption M' is a module of G'_l.

Again, let $N_{l+1}^\star = M_i^\star(j)$ and consider the module $P_{M_i^\star}$ of G. Since $P_{M_i^\star}$ is strong in G, it cannot overlap M'. Thus, either $M' \cap P_{M_i^\star} = \emptyset$, or $P_{M_i^\star} \subseteq M'$, or $M' \subset P_{M_i^\star}$.

If $M' \cap P_{M_i^\star} = \emptyset$ or $P_{M_i^\star} \subseteq M'$ then M' is not affected by the edits in θ_{l+1} since they are all within $P_{M_i^\star}$ and thus, M' remains a module of G'_{l+1}.

Hence, we only have to consider the case $M' \subset P_{M_i^\star}$. We show

Claim 4. *Either $M' \subseteq N^\star_{l+1}$ or $M' \cap N^\star_{l+1} = \emptyset$.*

Proof of Claim 4. Note again, that the set $M_i^\star(j)$ is a union of elements in $\mathcal{X}(M_i^\star)$ and for each $M_{i,h} \in \mathcal{X}(M_i^\star)$ it holds that either $M_{i,h} \in \mathbb{P}_{\max}(G[P_{M_i^\star}])$ or $M_{i,h}$ is the union of elements in $\mathbb{P}_{\max}(G[P_{M_i^\star}])$. Hence, $M_i^\star(j)$ is a union of elements in $\mathbb{P}_{\max}(G[P_{M_i^\star}])$. Theorem 3.3(T2) implies that no union of elements in $\mathbb{P}_{\max}(G[P_{M_i^\star}])$ of the prime module $P_{M_i^\star}$ is a module of G and thus, $M_i^\star(j)$ cannot be a proper subset of M'. Therefore, either $M' \subseteq M_i^\star(j)$ or $M' \cap M_i^\star(j) = \emptyset$ or M' and $M_i^\star(j)$ overlap. However, the latter case cannot occur, since then M' would either overlap one of the strong modules in $\mathbb{P}_{\max}(G[P_{M_i^\star}])$ or be a union of elements in $\mathbb{P}_{\max}(G[P_{M_i^\star}])$. Thus, in all cases either $M' \subseteq N^\star_{l+1}$ or $M' \cap N^\star_{l+1} = \emptyset$, which proves Claim 4. ◁

Now the same argumentation that was used to show Statement 1 can be used to show Statement 2. Thus, Statement 2 is satisfied for G'_{l+1}.

Finally, we prove Statement 3. To this end, assume that $G'_l \not\simeq G'_{l+1}$ and that $N^\star_{l+1}$ is no module of G'_l. We show that there are modules $M_1, M_2 \in G'_l$ with $M_1 \uplus M_2 \to N^\star_{l+1}$ being a pairwise module merge w.r.t. G'_{l+1}. Clearly, Items (ii) and (iii) of Definition 4.1 are satisfied, since $N^\star_{l+1}$ is a module of G'_{l+1} but no module of G'_l. It remains to show that there are two modules $M_1, M_2 \in G'_l$ with $M_1 \cup M_2 = N^\star_{l+1}$ and $M_1, M_2 \in G'_{l+1}$, i.e., Item (i) of Definition 4.1 is satisfied. Note, $N^\star_{l+1} = M_i^\star(j)$ for some i and $j \geq 1$. Assume first that $j = 1$. Then, $M_i^\star(1) = M_{i,0} \cup M_{i,1}$ with $M_{i,0}, M_{i,1} \in \mathcal{X}(M_i^\star)$. For each $M_{i,h}$ it holds that $M_{i,h} \in \mathbb{P}_{\max}(H[P_{M_i^\star}])$ or $M_{i,h} \in \mathbb{P}_{\max}(G[P_{M_i^\star}])$. If $M_{i,h} \in \mathbb{P}_{\max}(G[P_{M_i^\star}])$ then $M_{i,h}$ is a module of G and by Statement 2, a module of G'_l and G'_{l+1}. If $M_{i,h}$ is no module of G, then $M_{i,h} \in \mathbb{P}_{\max}(H[P_{M_i^\star}])$ is a new strong module of H. Therefore, there exists a $k < i$ such that $M_{i,h} = M_k^\star$. Since $M_k^\star = M_k^\star(l_k)$ and by the ordering of elements in $\mathcal{N}$ it holds that $M_k^\star(l_k) = N^\star_{k'}$ for some $k' \leq l$. Thus, by Statement 1, all $M_{i,h}$ and therefore, $M_{i,0}$ and $M_{i,1}$ are modules of G'_l and G'_{l+1}.

Now, assume that $N^\star_{l+1} = M_i^\star(j)$ with $j > 1$. Then, $M_i^\star(j) = M_i^\star(j-1) \cup M_{i,j}$. By the same argumentation as before, it holds that $M_{i,j}$ is a module of G'_l and G'_{l+1}. Moreover, by Statement 1, $M_i^\star(j-1) = N_l^\star$ is a module of G'_l and G'_{l+1}.

Thus, there are modules M_1, M_2 of G'_l and G'_{l+1} with $M_1 \cup M_2 = N^\star_{l+1}$. Moreover, since for all $\{x, y\} \in \theta_{l+1}$ it holds that either $x \in N^\star_{l+1}$ and $y \in P_{M_i^\star} \setminus N^\star_{l+1}$, or vice versa, it follows that there are no additional edits contained in θ_{l+1} besides the edits of the module merge $M_1 \uplus M_2 \to N^\star_{l+1}$ that transforms G'_l into G'_{l+1}. □

We are now in the position to derive the main result of this section that shows that optimal pairwise module-merge is always possible.

Theorem 5.6 (Pairwise Module-Merge)**.** *For an arbitrary graph $G = (V, E)$ and an optimal module-preserving cograph edit set F with $H = (V, E \triangle F)$ being the resulting cograph there exists a sequence of pairwise module merge operations that transforms G into H.*

Proof. Set $\mathcal{M} = \{M_1^\star, \dots, M_n^\star\}$, $\mathcal{N} = \{N_1^\star, \dots, N_m^\star\}$, $\mathcal{X}(M_i^\star) = \{M_{i,0}, \dots, M_{i,l_i}\}$, as well as θ_k and G'_k for all $1 \leq k \leq m$ as in Lemma 5.5. Again, we set $G_0 := G$

and $H' := G_m$. By Lemma 5.5 for each $1 \leq k \leq m$ there is a pairwise module merge $M_1 \uplus M_2 \to N_k^\star$ that transforms G_{k-1} to G_k. Thus, there exists a sequence of module merge operations that transforms G to some graph H'.

In what follows, we will show that $\dot\bigcup_{k=1}^m \theta_k = F$ and therefore $H' \simeq H$, from which we can conclude the statement. For simplicity, we put $F' := \bigcup_{k=1}^m \theta_k$.

We start with showing

Claim 1. $F' \subseteq F$.

Proof of Claim 1. Note first that by construction it holds that $\theta_k \cap \theta_l = \emptyset$ for all $k \neq l$ and therefore, $F' = \bigcup_{k=1}^m \theta_k = \dot\bigcup_{k=1}^m \theta_k$. By construction of θ it holds that $\theta_k \subseteq F$ for all $1 \leq k \leq m$. Hence, $F' \subseteq F$. $\triangleleft$

Before we show that $F = F'$, we will prove

Claim 2. *All strong modules of H are modules of H'.*

Proof of Claim 2. Lemma 5.5(1) implies that all modules M' of G are modules of H'. Moreover, Lemma 5.5(2) implies that all $N_k^\star \in \mathcal{N}$ are modules of H'. Since for all $M_i^\star \in \mathcal{M}$ it holds that $M_i^\star = M_i^\star(l_i) = N_k^\star$ for some $1 \leq k \leq m$, the set $M_i^\star$ is a module of H'. Since each strong module of H is either a module of G or a new module $M_i^\star \in \mathcal{M}$, all strong modules of H are modules of H'. $\triangleleft$

We continue to show

Claim 3. *$F' \subsetneq F$ is not possible.*

Proof of Claim 3. By Claim 1, $F' \subseteq F$. Thus assume for contradiction that $F' \neq F$. Since F is an optimal edit set and $F' \subsetneq F$ it follows that H' is not a cograph. Thus, there exist a prime module M in H' that contains no other prime module.

We will now show that M is a module of H and that all $M_i \in \mathbb{P}_{\max}(H[M])$ are modules of H'. Therefore, consider the strong module P_M of H that entirely contains M and that is minimal w.r.t. inclusion. Since P_M is strong in H it is, by Claim 2, also a module of H'. Moreover, each module $M_i \in \mathbb{P}_{\max}(H[P_M])$ is strong in H and, again by Claim 2, a module of H' as well. If $P_M = M$, then M is a module of H and we are done. Assume now that $M \subsetneq P_M$. Note that since M and all $M_i \in \mathbb{P}_{\max}(H[P_M])$ are modules of H' and M is strong in H' it holds that M does not overlap any $M_i \in \mathbb{P}_{\max}(H[P_M])$. Moreover, $M \not\subseteq M_i$ since otherwise M_i would have been chosen instead of P_M. Thus, $M = \bigcup_{i \in I} M_i$ is the union of some elements M_i in $\mathbb{P}_{\max}(H[P_M])$. Since P_M is a non-prime module of H it follows by Theorem 3.3(T3) that M is a module of H. Since H is a cograph, the children $M_i \in \mathbb{P}_{\max}(H[P_M])$ of the non-prime module P_M are the connected components of either $H[P_M]$ (if P_M is parallel) or its complement $\overline{H[P_M]}$ (if P_M is series). Since $M = \bigcup_{i \in I} M_i$ is the union of some elements in $\mathbb{P}_{\max}(H[P_M])$ and $H[M] \subseteq H[P_M]$, we can conclude that $H[M]$, resp., its complement $\overline{H[M]}$, has as its connected components M_i, $i \in I$. Thus, $\mathbb{P}_{\max}(H[M]) \subset \mathbb{P}_{\max}(H[P_M])$. Hence, all M_i, $i \in I$ are strong modules in H and, by the discussion above, all M_i are modules of H'.

Since all $M_i \in \mathbb{P}_{\max}(H[M])$ are modules of H' and all $M'_j \in \mathbb{P}_{\max}(H'[M])$ are strong in H', it holds that no $M_i \in \mathbb{P}_{\max}(H[M])$ can overlap any $M'_j \in \mathbb{P}_{\max}(H'[M])$. Therefore, if $M_i \cap M'_j \neq \emptyset$ then either $M'_j \subsetneq M_i$ or $M_i \subseteq M'_j$ for any i and j. If $M'_j \subsetneq M_i$ then M_i must be the union of some elements in $\mathbb{P}_{\max}(H'[M])$. However, since

M is prime in H' no union of elements in $\mathbb{P}_{\max}(H'[M])$, besides M itself, is a module of H' (cf. Theorem 3.3(T2)). Thus, M_i cannot be a module of H'; a contradiction. Hence, $M_i \subseteq M'_j$ and therefore, each M'_j is the union of some elements in $\mathbb{P}_{\max}(H[M])$. Note that this holds for any $M'_j \in \mathbb{P}_{\max}(H'[M])$, i.e., there are distinct sets $I_1, \ldots, I_{|\mathbb{P}_{\max}(H'[M])|}$ with $I_j \subsetneq \{1, \ldots, |\mathbb{P}_{\max}(H[M])|\}$ such that $M'_j = \bigcup_{i \in I_j} M_i$. Hence, all M'_j are modules of H.

Since, M is prime in H' and M did not contain any other prime module, it holds that all $H'[M'_j]$ are cographs. Moreover, since all M'_j are modules in H and M is prime in H' it holds that there are at least two distinct $M'_k, M'_l \in \mathbb{P}_{\max}(H'[M])$ with $xy \in E(H')$ if and only if $xy \notin E(H)$. Thus, $F'' = \{\{x, y\} \mid x \in M'_k, y \in M'_l\} \subseteq F$. Now, since all $H'[M'_j]$ are cographs it holds that $H'[M'_k \cup M'_l]$ is a cograph.

Now, consider the graph $H'' = G \triangle F \setminus F''$, and in particular the subgraph $H''[M] = G[M] \triangle F[M] \setminus F''$. Again, since all $H'[M'_j]$ with $M'_j \in \mathbb{P}_{\max}(H'[M])$ are cographs it holds that $H[M'_j] \simeq H'[M'_j] \simeq H''[M'_j]$. By construction of F'' for the previously chosen M'_k and M'_l it holds that $H'[M'_k \cup M'_l] \simeq H''[M'_k \cup M'_l]$ as well as $H[M \setminus (M'_k \cup M'_l)] \simeq H''[M \setminus (M'_k \cup M'_l)]$ is a cograph. Moreover, since for all $x \in M'_k \cup M'_l$ and all $y \in M \setminus (M'_k \cup M'_l)$ we have $xy \in E(H)$ if and only if $xy \in E(H'')$ it holds that $H''[M]$ is a cograph as well. Note that $F'' \subseteq F[M]$ and $F'' \neq \emptyset$ and therefore, $|F[M] \setminus F''| < |F[M]|$. But then, since $F[M] \setminus F''$ is an edit set for $G[M]$ and by Lemma 3.9 the set F is not optimal; a contradiction. Thus, F' cannot be a proper subset of F, which proves Claim 3. ◁

Claim 1 and 3 immediately imply that $F = F'$. In particular, we have

$$F' = \dot{\bigcup_{i=1}^{n}} \dot{\bigcup_{j=1}^{l_i}} \theta'_{M_i^\star(j)} = \dot{\bigcup_{i=1}^{n}} \dot{\bigcup_{j=1}^{l_i}} \theta_{M_i^\star(j)} = F. \qquad \Box$$

It can easily be seen by the latter results that each of the modules in $\mathcal{N}(\mathcal{M}) = \{N_1^\star, \ldots, N_m^\star\}$ that is created by a pairwise module merge is either already a module of G, or a union of elements from $\mathbb{P}_{\max}(G[M])$ of some prime module M of G.

5.2 A modular-decomposition-based heuristic for cograph editing

Although the (decision version of the) optimal cograph-editing problem is NP-complete [38, 39], it is fixed-parameter tractable (FPT) [6, 39, 49]. However, the best-known run-time for an FPT-algorithm is $\mathcal{O}(4.612^k + |V|^{4.5})$, where the parameter k denotes the number of edits. These results are of little use for practical applications, because the parameter k can become quite large. An exact algorithm that runs in $O(3^{|V|}|V|)$-time is introduced in [53]. Moreover, approximation algorithms are described in [16, 46]. In the following we provide an alternative exact algorithm for the cograph-editing problem based on pairwise module-merge. The virtue of this algorithm is that it can be adopted very easily to design a cograph-editing heuristic.

Algorithm 1 contains two points at which the choice of a particular module or a particular pair of modules affects performance and efficiency. First, the function `get-module-pair()` returns two modules of $\mathcal{P}$ in the correct order of the sequence of pairwise module merge operations that transforms G into H (cf. Theorem 5.6). Second, subroutine `get-module-pair-edit()` is used to compute the edits needed to merge

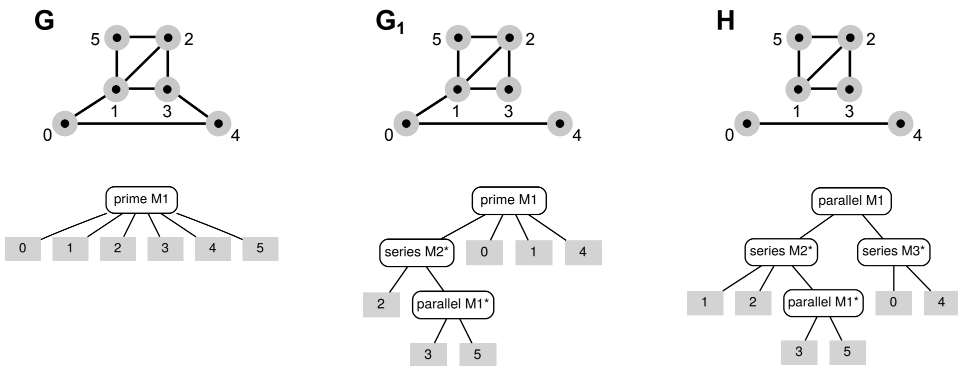

Figure 3: Illustration of Lemma 5.1 – 5.5, Theorem 5.6 and the exact algorithm. Consider the non-cograph G, the cograph $H = G \triangle F$ and the optimal module-preserving edit set $F = \{\{0,1\},\{3,4\}\}$. The modular decomposition trees are depicted below the respective graphs.
Let $\mathcal{M} = \{M_1^\star, M_2^\star, M_3^\star\}$ be the inclusion-ordered set of strong modules of H that are no modules of G. For all modules $M_i^\star \in \mathcal{M}$ the inclusion-minimal module $P_{M_i^\star}$ is the prime module M_1 in G.
In compliance with Lemma 5.2 we start with constructing the module $M_1^\star$. By definition $F_{M_1^\star} = \{\{3,4\}\} = \sigma_{M_1^\star}$. and we obtain $G_1 = G \triangle \sigma_{M_1^\star}$. Thus, $\{3\} \uplus \{5\} \to M_1^\star$ w.r.t. G_1. Next, we continue with $M_2^\star$. By construction, $F_{M_2^\star} = \{\{0,1\},\{3,4\}\}$ and $\sigma_{M_2^\star} = F_{M_2^\star} \setminus F_{M_1^\star} = \{\{0,1\}\}$. We then obtain $G_2 = G_1 \triangle \sigma_{M_2^\star} = H$. Thus, $\uplus_{M_i \in \mathcal{C}(M_2^\star)} M_i \to M_2^\star$ w.r.t. $G_2 = H$. The module $M_3^\star$ is now obtained for free, since $F_{M_3^\star} = \{\{0,1\},\{3,4\}\}$ and $\sigma_{M_3^\star} = F_{M_3^\star} \setminus (F_{M_1^\star} \cup F_{M_2^\star}) = \emptyset$.
In compliance with Lemma 5.5, i.e., when considering pairwise module merge only, we start with constructing the module $M_1^\star(1)$. Here, $\mathcal{X}(M_1^\star) = \{M_0 = \{3\}, M_1 = \{5\}\}$ and $M_1^\star(1) = \{3,5\} = M_1^\star$. By definition, $F_{M_1^\star(1)} = \{\{3,4\}\} = \theta_{M_1^\star(1)}$ and we obtain $G_{1,1} = G_1 = G \triangle \theta_{M_1^\star(1)}$. Thus, $\{3\} \uplus \{5\} \to M_1^\star$ w.r.t. $G_{1,1} = G_1$. Next, we continue with $M_2^\star(1)$ and $M_2^\star(2)$. Here, $\mathcal{X}(M_2^\star) = \{M_0 = \{1\}, M_1 = \{2\}, M_2 = M_1^\star\}$ and $M_2^\star(1) = \{1\} \cup \{2\}$ and $M_2^\star(2) = \{1,2,3,5\} = M_2^\star$. By definition $\theta_{M_2^\star(1)} = F_{M_2^\star(1)} \setminus F_{M_1^\star(1)} = \{\{0,1\}\}$ comprises the edits to obtain the new module $\{1,2\}$. Thus, $\{1\} \uplus \{2\} \to M_2^\star(1)$ w.r.t. $G_{2,1}$. Then, since $F_{M_2^\star(2)} = F_{M_2^\star} = \{\{0,1\},\{3,4\}\}$, we obtain $\theta_{M_2^\star(2)} = F_{M_2^\star(2)} \setminus (F_{M_1^\star} \cup \theta_{M_2^\star(1)} = \emptyset$. Thus, there are no edits left to apply in order to derive at H, since $G_{2,1} = G_{2,2} = G_2 = H$. Again, the module $M_3^\star$ is now obtained for free. In all steps, we obtained the new modules by merging pairs of existing modules.

Algorithm 1 Pairwise Module Merge

1: **INPUT:** A graph $G = (V, E)$.
2: $G^\star \leftarrow G$;
3: $F^\star \leftarrow \emptyset$;
4: MDs$(G) \leftarrow$ `compute-modular-decomposition(`G`)`.
5: $P_1, \dots, P_m$ be the prime modules of G that are partially ordered w.r.t. inclusion, i.e., $P_i \subseteq P_j$ implies $i \leq j$.
6: **for** $p = 1, \dots, m$ **do**
7: $\quad \mathcal{P}_p \leftarrow \mathbb{P}_{\max}(G[P_p])$
8: $\quad$ **while** $G^\star[P_p]$ is not a cograph **do**
9: $\quad\quad M_i, M_j \leftarrow$`get-module-pair(`$\mathcal{P}_p$`)`. {according to Theorem 5.6}
10: $\quad\quad$ **if** $M_i \cup M_j$ is no module of $G^\star$ **then**
11: $\quad\quad\quad \theta \leftarrow$ `get-module-pair-edit(`$M_i \uplus M_j \rightarrow N$ w.r.t. $G[P_p]$`)` {according to θ_l in Lemma 5.5}
12: $\quad\quad\quad G^\star \leftarrow G^\star \Delta\, \theta$
13: $\quad\quad$ **end if**
14: $\quad\quad \mathcal{P}_p \leftarrow \mathcal{P}_p \setminus \{M_i, M_j\} \cup \{N\}$
15: $\quad$ **end while**
16: **end for**
17: **OUTPUT:** $H = G^\star$;

the modules M_i and M_j to a new module such that these edits affect only the vertices within P_p (cf. Lemma 5.5).

Lemma 5.7. *Let $\mathcal{P}(G)$ be the set of all strong prime modules of G and suppose that Algorithm 1 is applied on the graph G with $n = |V(G)|$. If* `get-module-pair()` *is an "oracle" that always returns the correct pair M_i and M_j and* `get-module-pair-edit()` *returns the correct edit set θ, then Algorithm 1 computes an optimally edited cograph H in $O(m\Lambda h(G)) \leq O(n^2 h(G))$ time, where m denotes the number of strong prime modules in G and $\Lambda = \max_{P \in \mathcal{P}(G)} |\mathbb{P}_{\max}(G[P])|$ is the size of the largest maximal strong partition among all prime modules $P \in \mathcal{P}(G)$, and $h(G)$ is the maximal cost for evaluating* `get-module-pair()` *and* `get-module-pair-edit()`.

Proof. The correctness of Algorithm 1 follows directly from Lemma 5.5 and Theorem 5.6.

The modular decomposition tree of a graph $G = (V, E)$ can be computed in linear-time, i.e., $O(|V| + |E|) \leq O(n^2)$ with $n = |V(G)|$, see [9, 13, 40, 41, 52]. It yields the partial order $P_1, \dots, P_m$ of the prime modules of G (line 5) in time $O(n)$ by depth first search. Then, we have to resolve each of the m prime modules and in each step in the worst case all modules have to be merged stepwisely, resulting in an effort of $O(|\mathbb{P}_{\max}(G[P_p])|)$ merging steps in each iteration. Since $m \leq n$ and $\Lambda \leq n$ we obtain $O(n^2 h(G))$ as an upper bound. □

In practice, the exact computation of the optimal editing requires exponential effort. To be more precise, we show now the complexity $h(G)$ as in Lemma 5.7 using a naive brute-force method. Given a prime module P with $\lambda = |\mathbb{P}_{\max}(G[P])|$ child modules there are $\binom{\lambda}{2}$ possibilities for selecting the first module pair that has to be merged. After merging those two modules there are at most $\lambda - 1$ modules left from which possibly two more have to be merged. In general in the i-th merging step there are at most $\binom{\lambda - i}{2}$ possible merge pairs left. This process have to repeat at most $(\lambda - 4)$ times, since any module with less than four child modules cannot be prime. In the worst case this adds up to $\prod_{i=4}^{\lambda} \binom{i}{2} = \prod_{i=4}^{\lambda} \frac{i!}{2!(i-2)!} = \prod_{i=4}^{\lambda} \frac{i \cdot (i-1)}{2}$ merge sequences per prime module of G which gives $O((\lambda!)^2)$ executions of `get-module-pair()` per prime module in G. Finding the optimal edit set for one merge operation of two modules $M_1, M_2 \in \mathbb{P}_{\max}(G[P])$ requires checking the $2^{\lambda-2}$ combinations to add or remove edges to adjust the out$_{M_1}$- and out$_{M_2}$-neighbors w.r.t. to the remaining $\lambda - 2$ modules. Therefore, for each of the remaining modules $M \in \mathbb{P}_{\max}(G[P]) \setminus \{M_1, M_2\}$ there are either only edges or only non-edges between the vertices from M and $M_1 \cup M_2$. In summary, for a given prime module P the graph $G[P]$ can be optimally edited to a cograph in $O((\lambda!)^2 2^\lambda)$ time. Therefore, with $\Lambda = \max_P |\mathbb{P}_{\max}(G[P])|$ being the size of the largest maximal strong partition among all prime modules P of G, it follows that $h(G) \in O((\Lambda!)^2 2^\Lambda)$. We note in passing that Λ is always less than or equal to the maximum degree in the modular decomposition tree, which is also known as *modular-width* [1, 18]. Hence, the latter findings together with Lemma 5.7 imply the following

Observation 5.8. The optimal cograph editing problem parameterized by the modular-width k can be solved in $O((k!)^2 2^k |V|^2)$ time and thus, it is in FPT.

Practical heuristics for `get-module-pair()` and `get-module-pair-edit()` can be implemented to run in polynomial time. In particular, as a main result, we can observe that it is always possible to find an optimal edit set by stepwisely merging only *pairs* of modules. Based on this, we provide in the following several strategies to improve the runtime of these heuristics.

A simple greedy strategy yields a heuristic with $O(|V|^3)$ time complexity as follows: In each call of `get-module-pair()` select the pair (M_i, M_j) in $\mathcal{P}$ where the edit set that adjusts the out$_{M_i}$- and out$_{M_j}$-neighbors so that the out$_{M_i \cup M_j}$-neighborhood becomes identical in $G^\star[P_p]$ has minimum cardinality. This minimum edit set can be obtained from `get-module-pair-edit()` by adjusting only the out-neighbors of the smaller module to be identical to the out-neighbors of the larger module. The pseudocode for this heuristic is given in Algorithm 2 which is, in fact, a natural extension of the exact Algorithm 1. A detailed numerical evaluation will be discussed elsewhere.

Lemma 5.9. *Algorithm 2 outputs a cograph and has a time complexity of* $O(|V|^3)$.

Proof. First we show that Algorithm 2 constructs a cograph. To this end we show that in each iteration of the main *for*-loop (Lines 16 to 41) the corresponding prime module P_p is edited such that the resulting subgraph $G^\star[P_p]$ is a cograph and P_p is still a module of $G^\star$.

Due to the processing order of the prime modules $P_1, \dots, P_m$ constructed in Line 4, we may assume that, upon processing a prime module P_p, the induced subgraphs $G^\star[M], M \in \mathbb{P}_{\max}(G[P_p])$ are already cographs and all M are modules of $G^\star$. This holds in particular for the prime modules that do not contain any other prime module in the input graph G and which, therefore, are processed first. Hence, it suffices to show that if all $G^\star[M]$, $M \in \mathbb{P}_{\max}(G[P_p])$, are already cographs and all M are modules in $G^\star$, then executing the $p-th$ iteration of the *for*-loop results in an updated intermediate graph G' with $G'[P_p]$ being a cograph and P_p as well as all modules $M \in \mathbb{P}_{\max}(G[P_p])$ remain modules of G'.

In Line 17, we define $\mathcal{P} = \mathbb{P}_{\max}(G[P_p])$ and therefore, by assumption, all $G^\star[M]$, $M \in \mathcal{P}$ are cographs and all M are modules of $G^\star$. In particular, the two sets M_i and M_j that are chosen first (in Line 20) are already cographs. Moreover, since M_i and M_j are modules of $G^\star$ if follows that $G^\star[M_i \cup M_j]$ is either the disjoint union $G^\star[M_i] \cupdot G^\star[M_j]$ or the join $G^\star[M_i] \oplus G^\star[M_j]$ of $G^\star[M_i]$ and $G^\star[M_j]$. Thus, $G^\star[M_i \cup M_j]$ is already a cograph and none of the edges within $M_i \cup M_j$ is edited further. It remains to show that

Algorithm 2 Pairwise Module Merge Heuristic

1: **INPUT:** A graph $G = (V, E)$.
2: $G^\star \leftarrow G$;
3: $\mathrm{MDs}(G) \leftarrow$ `compute-modular-decomposition(`G`)`.
4: $P_1, \ldots, P_m$ be the prime modules of G that are partially ordered w.r.t. inclusion, i.e., $P_i \subsetneq P_j$ implies $i \leq j$.
5: $A \leftarrow$ zero initialized $|\mathrm{MDs}(G)| \times |\mathrm{MDs}(G)|$ matrix
6: $B \leftarrow$ zero initialized $|\mathrm{MDs}(G)| \times |\mathrm{MDs}(G)| \times |\mathrm{MDs}(G)|$ matrix
7: ▷Lines 8 to 15: Initialize A where the entries A_{ij} store the number $|V \setminus \{M_i \cup M_j\}|$ of vertices that need to be adjusted to merge the modules M_i and M_j. Initialize B s.t. $B_{ijk} = 1$ iff M_i and M_j have different out-neighborhoods w.r.t. M_k
8: **for** each $\{M_i, M_j, M_k\} \in \binom{\mathrm{MDs}(G)}{3}$ with M_i, M_j, M_k being children of one and the same prime module P **do**
9:     **if** $\mathrm{out}_{M_i} \cap M_k \neq \mathrm{out}_{M_j} \cap M_k$ **then** $B_{ijk}, B_{jik} \leftarrow 1$ **end if**
10:     **if** $\mathrm{out}_{M_i} \cap M_j \neq \mathrm{out}_{M_k} \cap M_j$ **then** $B_{ikj}, B_{kij} \leftarrow 1$ **end if**
11:     **if** $\mathrm{out}_{M_j} \cap M_i \neq \mathrm{out}_{M_k} \cap M_i$ **then** $B_{jki}, B_{kji} \leftarrow 1$ **end if**
12:     $A_{ij}, A_{ji} \leftarrow A_{ij} + |M_k| \cdot B_{ijk}$
13:     $A_{ik}, A_{ki} \leftarrow A_{ik} + |M_j| \cdot B_{ikj}$
14:     $A_{jk}, A_{kj} \leftarrow A_{jk} + |M_i| \cdot B_{jki}$
15: **end for**
16: **for** $p = 1, \ldots, m$ **do**
17:     $\mathcal{P} \leftarrow \mathbb{P}_{\max}(G[P_p])$
18:     **while** $|\mathcal{P}| > 1$ **do**
19:         $\theta \leftarrow \emptyset$ {θ denotes the set of (non)edges that will be edited}
20:         select two distinct modules M_i and M_j from $\mathcal{P}$ with $|M_i| \geq |M_j|$ that have a minimum value of $A_{ij} * |M_j|$.
21:         ▷Line 22 to 26: Compute the edits for adjusting the $\mathrm{out}_{M_i \cup M_j}$-neighborhood s.t. M_j has the same out-neighborhood as M_i within $G[P_p]$. Note, since P_p is a module of G, M_j and M_i have the same out-neighbors in G after editing.
22:         **if** $A_{ij} \neq 0$, i.e., $M_i \cup M_j$ is no module of $G^\star$ **then**
23:             **for** each $M_k \in \mathcal{P} \setminus \{M_i, M_j\}$ **do**
24:                 **if** $B_{ijk} = 1$ **then** $\theta \leftarrow \theta \cup \{xy \mid x \in M_j, y \in M_k\}$ **end if**
25:             **end for**
26:         **end if**
27:         ▷Line 28 to 30: Adjust in A the number of edits needed for merging the new module $M_i \cup M_j$ with some M_k
28:         **for** each $M_k \in \mathcal{P} \setminus \{M_i, M_j\}$ **do**
29:             $A_{ik}, A_{ki} \leftarrow A_{ik} - |M_j| \cdot B_{ikj}$
30:         **end for**
31:         ▷Line 32 to 34: Adjust in A the number of edits needed for merging two modules M_k and M_l
32:         **for** each $\{M_k, M_l\} \in \binom{\mathcal{P} \setminus \{M_i, M_j\}}{2}$ **do**
33:             $A_{kl}, A_{lk} \leftarrow A_{kl} + |M_j| \cdot B_{kli} - |M_j| \cdot B_{klj}$
34:         **end for**
35:         remove the j-th row and column A
36:         remove the j-th layer in all 3 dimensions of B
37:         in $\mathcal{P}$ replace M_i with $M_i \cup M_j$
38:         $\mathcal{P} \leftarrow \mathcal{P} \setminus \{M_j\}$
39:         $G^\star \leftarrow G^\star \Delta\, \theta$
40:     **end while**
41: **end for**
42: **OUTPUT:** $H = G^\star$;

applying the edits constructed in Line 24 result in the (new) merged module $M_i \cup M_j$ of $G^\star\Delta\theta$. Note, if $M_i \cup M_j$ is already a module of $G^\star$ then Lines 22 to 26 are not executed and therefore, $\theta = \emptyset$, which implies that $M_i \cup M_j$ remains a module of $G^\star\Delta\theta$. On the other hand, if $M_i \cup M_j$ is no module of $G^\star$ then the *for*-loop in Lines 12 to 26 iterates over all modules M_k in $\mathcal{P} \setminus \{M_i, M_j\}$ and adjusts the edges between M_j and M_k to be in accordance to the edges between M_i and M_k. Note that all those edits are within P_p. In particular, the $\text{out}_{M_i \cup M_j}$-neighborhood was adjusted only between vertices from M_j and vertices from $P_p \setminus (M_i \cup M_j)$. After applying these edits, $M_i \cup M_j$ is therefore a module in $G^\star[P_p]\Delta\theta$. In particular, the out_{P_p}-neighborhood has not changed and P_p is therefore a module of $G^\star$ as well as of $G^\star\Delta\theta$. Then, it follows by Lemma 3.1 that $M_i \cup M_j$ is a module in $G^\star\Delta\theta$. To see that also all $M_k \in \mathcal{P} \setminus \{M_i, M_j\}$ remain modules in $G^\star\Delta\theta$ note first that $\mathcal{P}$ is a partition of P_p and second, that only edges between M_j and M_k are edited for some $M_k \in \mathcal{P} \setminus \{M_i, M_j\}$. Moreover, if a (non)edge between M_j and M_k is edited, then all (non)edges $\{xy \mid x \in M_j, y \in M_k\}$ between M_j and M_k are edited. Thus all $M_k \in \mathcal{P} \setminus \{M_i, M_j\}$ remain modules of $G^\star[P_p]\Delta\theta$ and therefore modules $G^\star\Delta\theta$.

Now consider the prime module P_{p+1} that is processed in the next iteration of the main *for*-loop. It can be easily seen that for P_{p+1} we also have: $G^\star[M], M \in \mathbb{P}_{\max}(G[P_{p+1}])$ is a cograph and all M are modules of $G^\star$, since all prime modules of G that are subsets of P_{p+1} are already processed, and therefore, are all those M are non-prime modules of $G^\star$ and form cographs $G^\star[M]$. Hence, by the same argumentation as before, $G^\star[P_{p+1}]$ is edited to a cograph by the next execution of the main *for*-loop. Thus, after processing all prime modules of G the final graph H is a cograph.

Next, we show that Algorithm 2 has a time complexity of $O(|V|^3)$. Creating the modular decomposition in Line 3 can be done in linear time by the algorithms presented in, e.g., [13, 41, 52]. Note that "linear" in this context means linear in the number of edges, i.e., $O(|V| + |E|) \in O(|V|^2)$. Initializing the matrices A and B (Lines 8 to 15) requires time $O(|V|^3)$ since the corresponding *for*-loop iterates over every ordered set of 3 strong modules of G and there are at most $O(|V|)$ such modules. Moreover, checking if the out-neighborhoods of two modules M_i and M_j w.r.t. a third module M_k are identical (the *if*-statements in Lines 9 to 11) can be done in constant time by checking the adjacencies between three arbitrary vertices, exactly one from each of the three modules. For the remaining Lines 16 to 41 we can consider how often the inner *while*-loop (Lines 18 to 40) is executed. Therefore, note that within each execution always two modules are merged and there are $O(n)$ of those merge operations at most. This can most easily be seen by considering the matrix A which has $\text{MDs}(G)$ rows and columns at first with $|\text{MDs}(G)| < |V|$. Each row, respectively each column, of A represents a module that is possibly selected for merging. Moreover, within each iteration of the *while*-loop, the matrix A is reduced by one row, respectively one column. This leads to no more than $|V|$ many executions of the *while*-loop. Selecting the two modules M_i and M_j in Line 20 requires $O(|V^2|)$ time. Although, the *for*-loop in Lines 23 to 25 is executed $O(|V|)$ times and each partial edit set that is computed in Line 24 might contain more than $O(|V|)$ many edits, the whole edit set θ (constructed within Lines 23 to 25) contains no more than $O(|V|^2)$ edits. Thus, executing Lines 12 to 26 requires $O(|V|^2)$ time at most. Adjusting the matrix A is done in two steps. Lines 28 to 30 iterates over $O(|V|)$ many modules M_k and Lines 32 to 34 iterates over $O(|V|^2)$ many pairs of modules (M_k, M_l). Shrinking the matrices A and B in Lines 35 and 36 can technically be done in time $O(|V|)$ if we use a labeling function $l\colon \mathbb{N} \times \mathbb{N}$ to index the values within the matrices, i.e., instead of reading A_{ij} we read $A_{l(i),l(j)}$. Then we just have to relabel those indices, i.e., $l(x) \leftarrow l(x) + 1$ for all $x > j$. In that way we do not have to remove anything from A or B. Line 37 and 38 can also be done in $O(|V|)$ time and applying the edits in Line 39 requires at most $O(|V|^2)$ time. In summary, executing a single iteration of the main *for*-loop requires $O(|V|^2)$ time, which yields a total time complexity of $O(|V|^3)$. □

The heuristic as given in Algorithm 2 is deterministic and therefore lacks of a randomization component which would be helpful in order to sample solutions and construct a consensus cograph. However, randomization can be introduced easily by selecting a pair of modules M_i and M_j in line 20 with a probability inversely correlated with the value of $A_{ij} \cdot |M_j|$. Moreover, with probability $p = |M_i|/(|M_i| + |M_j|)$ the edits $\{xy \mid x \in M_j, y \in M_k\}$ can be selected in line 24 and otherwise $\{xy \mid x \in M_i, y \in M_k\}$ with probability $1 - p$.

An even simpler (but probably less accurate) heuristic with time complexity $O(|V|^2)$ can be obtained by randomly selecting the next pair of modules M_i and M_j that have to be merged. Such a procedure would not require the computation of the matrices A and B at all. Nevertheless, this $O(|V|^2)$-time heuristic requires that computing the edit set θ can be done in $O(|V|)$ time. However, this is possible if we only track the $O(|V|)$ many edits on the corresponding quotient graph $G^\star[P_p]/\mathbb{P}_{\max}(G[P_p])$ and recover the $O(|V|^2)$ many individual edits from that only once in a single post-processing step at the end.

Cograph editing heuristics based on the destruction of P4s requires $O(|V|^4)$ time merely for enumerating all P4s. Thus, using module merges as editing operation may lead to significantly faster cograph editing heuristics.

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Cayley graphs of order kp are hamiltonian for $k < 48$

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Abstract

We provide a computer-assisted proof that if G is any finite group of order kp, where $1 \leq k < 48$ and p is prime, then every connected Cayley graph on G is hamiltonian (unless $kp = 2$). As part of the proof, it is verified that every connected Cayley graph of order less than 48 is either hamiltonian connected or hamiltonian laceable (or has valence ≤ 2).

Keywords: Cayley graph, hamiltonian cycle, hamiltonian connected, hamiltonian laceable.

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1 Introduction

In a series of papers [7, 11, 12, 16], it was shown that if $1 \leq k < 32$ (with $k \neq 24$) and p is any prime number, then every connected Cayley graph on every group of order kp has a hamiltonian cycle (unless $kp = 2$). This note extends that work, by treating the previously excluded case $k = 24$, and by increasing the upper bound on k:

Theorem 1.1. *If $1 \leq k < 48$, and p is any prime number, then every connected Cayley graph on every group of order kp has a hamiltonian cycle (unless $kp = 2$).*

All of the results in the previous papers [7, 11, 12, 16] were verified by hand. However, some of the proofs are quite lengthy, so many details were probably never checked by anyone other than the authors and the referees. The present paper takes the opposite approach: many of the results have not been verified by hand, but all of the source code is available at[1]

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[1] Also available in https://arxiv.org/src/1805.00149v1/anc/.

so the results can easily be reproduced by anyone with a standard installation of the computer algebra system `GAP` [10] (including the SmallGrp package [5]) and G. Helsgaun's implementation `LKH` [14] of the Lin-Kernighan heuristic for the traveling salesperson problem. An effort was made to keep the algorithms in this paper simple, so they would be easy to verify, even though this precluded many optimizations.

In addition to extending the above-mentioned results for $k < 32$, the present work also provides an independent verification of those results, because the proofs are essentially self-contained (other than relying heavily on the correctness of extensive `GAP` computations). We also establish the following two results of independent interest:

Corollary 1.2. *If* $|G| < 144$ *(and* $|G| > 2$*), then every connected Cayley graph on* G *is hamiltonian.*

Proposition 1.3. *If* $|G| < 48$*, then every connected Cayley graph on* G *is either hamiltonian connected or hamiltonian laceable (or has valence* ≤ 2*).*

Remarks 1.4.

1. The definition of the terms "hamiltonian connected" and "hamiltonian laceable" can be found in Definition 2.5.
2. Almost all of this paper is devoted to the proof of Theorem 1.1. Corollary 1.2 and Proposition 1.3 are proved in Section 2C.
3. It is explained in Section 5 that the paper's calculations for the proof of Theorem 1.1 could be substantially shortened by accepting all of the results in the literature, rather than reproving some of them. For example, instead of treating all values of k from 1 to 47, it would suffice to consider only $k \in \{24, 32, 36, 40, 42, 45\}$ (see Lemma 5.3(1)).
4. It is natural to ask whether the conclusion of Proposition 1.3 holds for all Cayley graphs, without any restriction on the order (cf. [8, Questions 4.1 and 4.3, pp. 121–122]). This is known to be true when G is abelian [6] and for a few other (very restricted) classes of Cayley graphs [1, 2, 3, 4], but Proposition 1.3 seems to be the first exhaustive examination of this topic for Cayley graphs of small order. Further calculations reported that the conclusion of Proposition 1.3 holds for all orders less than 108, but the additional computations took several weeks and were marred by crashes and other issues, so they are not definitive.

Method of attack 1.5. For each fixed k and prime number p, there are only finitely many groups G of order kp (up to isomorphism), and each of these groups has only finitely many Cayley graphs. Assuming that kp is not too large, `LKH` can find a hamiltonian cycle in all of them. This means that (given sufficient time) a computer can deal with any finite number of primes.

Therefore, large primes are the main concern. For these, we have the helpful observation that if G is a group of order kp, where p is prime and $p > k$, then G has a unique Sylow p-subgroup (so the Sylow p-subgroup is normal), and the Sylow p-subgroup is (isomorphic to) $\mathbb{Z}_p$. This means that, after some computer calculations to eliminate the small cases (see Section 2D),

$$\text{we may assume } \mathbb{Z}_p \triangleleft G, \text{ and } p \nmid k.$$

For convenience,

$$\text{let } \overline{G} = G/\mathbb{Z}_p, \text{ so } |\overline{G}| = k.$$

Since $\mathbb{Z}_p$ is cyclic, we are in position to apply the Factor Group Lemma (Lemma 2.12): it suffices to find a hamiltonian cycle in $\mathrm{Cay}\big(\overline{G}; \overline{S}\big)$ whose voltage generates $\mathbb{Z}_p$.

There are infinitely many primes p, so a given group $\overline{G}$ of order k is the quotient of infinitely many different groups G. In order to deal simultaneously with all primes, first note that the Schur-Zassenhaus Theorem [19] tells us that G is a semidirect product: $G = \mathbb{Z}_p \rtimes_\tau \overline{G}$ (see Lemma 2.13(10)). We construct a single "universal" (infinite) semidirect product $\widetilde{G} = Z \rtimes_{\widetilde{\tau}} \overline{G}$ that has every $\mathbb{Z}_p \rtimes_\tau \overline{G}$ as a quotient. (For example, if all values of the twist homomorphism τ are ± 1, then $\widetilde{G} = \mathbb{Z} \rtimes_\tau \overline{G}$.)

In almost all cases, a computer search yields a hamiltonian cycle H in $\mathrm{Cay}\big(\overline{G}; \overline{S}\big)$, such that its voltage $\widetilde{v}$ in Z is nonzero. Then H has nontrivial voltage in $\mathbb{Z}_p$ unless p is one of the finitely many prime divisors of $\widetilde{v}$. `LKH` can verify that all of the (finitely many) Cayley graphs corresponding to these primes are hamiltonian. Fortunately, theoretical arguments can handle the few situations where the computer search was unable to find any hamiltonian cycles with nonzero voltage (see Lemma 3.1).

Contents

2 Preliminaries

Notation 2.1.

1. G is always a group of order kp, where p is prime,
2. S is a generating set of G, and
3. $\mathrm{Cay}(G; S)$ is the *Cayley graph* on G with respect to the generators S. The vertices of this graph are the elements of G, and there is an edge joining g and sg whenever $g \in G$ and $s \in S$.

Remark 2.2. Unlike most authors, we do not require S to be symmetric (i.e., closed under inverses). Instead, in our notation, $\mathrm{Cay}(G; S) = \mathrm{Cay}(G; S \cup S^{-1})$.

Hamiltonian cycles in a subgraph are also hamiltonian cycles in the ambient graph, so, in order to prove Theorem 1.1, there is no harm in making the following assumption:

Assumption 2.3. The generating set S of G is *irredundant*, in the sense that no proper subset of S generates G.

As mentioned in the introduction, the paper relies heavily on the computer algebra system GAP [10] and G. Helsgaun's implementation LKH of the Lin-Kernighan heuristic [14].

2A GAP

The Small Groups library in GAP contains all of the groups of order less than 1024, and many others [5]. The number of groups of order k is given by the function

NumberSmallGroups(k),

and each group of order k has a unique id number (from 1 to NumberSmallGroups(k)). The GAP function

SmallGroup(k, id)

constructs the group of order k with the given id number.

The GAP package grape provides tools for working with graphs. In particular, it defines the function

CayleyGraph(G, S)

that constructs the Cayley graph of the group G with respect to the generating set S.

To prove Theorem 1.1, we wish to show, for certain groups G, that all of the Cayley graphs $\mathrm{Cay}(G;S)$ are hamiltonian. With Assumption 2.3 in mind, we would like to have a list of all of the irredundant generating sets of G. However, there is no need to distinguish between Cayley graphs that are isomorphic, so we consider two generating sets to be equivalent if one can be obtained from the other by applying an automorphism of G. Furthermore, since $\mathrm{Cay}(G;S) = \mathrm{Cay}(G;S \cup S^{-1})$, we also consider two generating sets to be equivalent if one can be obtained from the other by replacing some elements by their inverses. The function

IrredUndirGenSetsUpToAut(G)

constructs a list of all of the irredundant generating sets of G, up to equivalence. It is defined in the file UndirectedGeneratingSets.gap and is adapted from the AllMinimalGeneratingSets algorithm in the masters thesis of B. Fuller [9, pp. 31–34]. (Fuller's program does not allow generators to be replaced by their inverses.)

Combining IrredUndirGenSetsUpToAut(G) with CayleyGraph(G, S) provides a list of all of the irredundant Cayley graphs on any group G.

2B Finding hamiltonian cycles with LKH and exhaustive search

G. Helsgaun's [14] implementation LKH of the Lin-Kernighan heuristic is a very powerful tool for finding hamiltonian cycles, and the function

LKH(X, AdditionalEdges, RequiredEdges)

interfaces GAP with this program. (It is defined in the file LKH.gap.) Given a graph X (in grape format), and two lists of edges, the function constructs a graph X^+ by adding the edges in AdditionalEdges to X, and asks LKH to find a hamiltonian cycle in X^+ that contains all of the edges in RequiredEdges. If $X =$ CayleyGraph(G, S), then the hamiltonian cycle is returned as a list of elements of G, in the order that they are visited by the cycle.

For example, the function

IsAllHamiltonianOfTheseOrders(OrdersToCheck)

uses LKH (together with IrredUndirGenSetsUpToAut(G) and CayleyGraph(G, S)) to verify that every Cayley graph of order k is hamiltonian, for every k in the list OrdersToCheck. (It is defined in the file `IsAllHamiltonianOfTheseOrders.gap`.)

LKH returns a single hamiltonian cycle, but we sometimes want several hamiltonian cycles, in order to find one whose voltage is nonzero. The function

HamiltonianCycles(X, RequiredEdges)

finds all of the hamiltonian cycles in X that contain all of the edges in the list RequiredEdges. (It is defined in the file `HamiltonianCycles.gap`.) However, the list of all hamiltonian cycles may be unreasonably long (and may take too long to compute), so we instead rely on two functions that provide a fairly short list of hamiltonian cycles that suffice for the task at hand:

SeveralHamCycsInCay(GBar, SBar)
SeveralHamCycsInRedundantCay(GBar, S0Bar, a)

(Both of these functions are defined in the file `SeveralHamCycsInCay.gap`.) The first provides a list of hamiltonian cycles in $\mathrm{Cay}(\overline{G}; \overline{S})$, whereas the second provides hamiltonian cycles in $\mathrm{Cay}\big(\overline{G}; \overline{S_0} \cup \{\overline{a}\}\big)$.

Remark 2.4. In order to verify the correctness of the results in this paper, it is not necessary to verify the correctness of the source code of any of the four functions that provide hamiltonian cycles. This is because the output of these functions is always checked for validity before it is used; the function

IsHamiltonianCycle(X, H, AdditionalEdges, RequiredEdges)

was written for this purpose. It verifies that H is a hamiltonian cycle in the graph X^+ that is obtained from X by adding the edges in the list AdditionalEdges, and also that H contains all of the edges in the list RequiredEdges. Our convention is that each edge $[u, v]$ in AdditionalEdges and RequiredEdges is considered to be directed, unless $[v, u]$ is also in the list, in which case the edge is undirected.

2C Some Cayley graphs that are hamiltonian connected/laceable

Definition 2.5 ([3, Definition 1.3]). Let X be a graph.

1. X is *hamiltonian connected* if X has a hamiltonian path from v to w, for all vertices v and w, such that $v \neq w$.
2. X is *hamiltonian laceable* if X is bipartite, and it has a hamiltonian path from v to w, for all vertices v and w, such that v and w are not in the same bipartition set.

Justification of Proposition 1.3. It is easy to write a GAP program that

- loops through all groups G of order < 64,
- loops through all irredundant generating sets S_0 of G, and

- uses LKH to verify that $\mathrm{Cay}(G; S_0)$ is hamiltonian connected/laceable if the valence is ≥ 3.

Cayley graphs are vertex transitive, so, for the last step, it suffices to find a hamiltonian path from the identity element e to all other elements a of G (for hamiltonian connectivity) or to all elements a of the other bipartition set (for hamiltonian laceability). To find this hamiltonian path, one can ask LKH to find a hamiltonian cycle in the graph $X \cup \{ea\}$, such that the hamiltonian path contains the edge ea. (Note that, by symmetry, there is no need to find hamiltonian paths to both of a and a^{-1}.)

However, this is not sufficient to establish Proposition 1.3. Any generating set S of G contains an irredundant generating set S_0, and it is obvious that:

- If $\mathrm{Cay}(G; S_0)$ is hamiltonian connected, then $\mathrm{Cay}(G; S)$ is hamiltonian connected.
- If $\mathrm{Cay}(G; S_0)$ is hamiltonian laceable, *and* $\mathrm{Cay}(G; S)$ is bipartite, then $\mathrm{Cay}(G; S)$ is hamiltonian laceable.

But it may be the case that $\mathrm{Cay}(G; S_0)$ is bipartite and $\mathrm{Cay}(G; S)$ is not bipartite. In this situation, the hamiltonian laceability of $\mathrm{Cay}(G; S_0)$ does not imply the required hamiltonian connectivity of $\mathrm{Cay}(G; S)$.

Therefore, in cases where $\mathrm{Cay}(G; S_0)$ is bipartite, the program also needs to verify hamiltonian connectivity for generating sets of the form $S = S_0 \cup \{g\}$, such that $\mathrm{Cay}(G; S)$ is not bipartite. (Such a set S can be called a *nonbipartite extension* of S_0.) Note: we may assume that no proper subset of S generates G and gives a nonbipartite Cayley graph. (The hamiltonian connectivity of the Cayley graph of such a subset would imply the hamiltonian connectivity of $\mathrm{Cay}(G; S)$.) Since $\mathrm{Cay}(G; S_0)$ is hamiltonian laceable, we already know there are paths from e to any vertex in the other bipartition set, so only endpoints a in the bipartition set of e need to be considered.

Furthermore, if $\mathrm{Cay}(G; S_0)$ has valence two, then it is (usually) not hamiltonian laceable. Therefore, in this case, the program should verify that $\mathrm{Cay}\big(G; S_0 \cup \{g\}\big)$ is hamiltonian connected/laceable for all $g \notin \{e\} \cup S \cup S^{-1}$ (except that we need not consider both g and g^{-1}).

The GAP program in `1-3-HamConnOrLaceable.gap` does all of this. □

When dealing with the case $k = 32$, our proof of Theorem 1.1 also applies the following known result:

Lemma 2.6 ([20]). *Every connected Cayley graph of order* 64 *is hamiltonian.*

Justification. This is a special case of the fact that all Cayley graphs of prime-power order are hamiltonian (see Theorem 5.1(6)). However, to avoid relying on the literature, one can use the function call IsAllHamiltonianOfTheseOrders([64]) to verify this via a few days of computation. (There are over 14,000 Cayley graphs to consider — most of the 267 groups of order 64 have many irredundant generating sets.) □

Proof of Corollary 1.2. Assume $|G| < 144$. It is known that every connected Cayley graph on any nontrivial 2-group is hamiltonian (see Theorem 5.1(6)), so we may assume that $|G|$ is divisible by some prime $p \geq 3$. Then $|G| = kp$, where $k = |G|/p < 144/3 = 48$, so Theorem 1.1 applies.

It might be possible to avoid appealing to Theorem 5.1(6), by using LKH to find hamiltonian cycles in all of the Cayley graphs of order 128, but this would be a massive computation, and we did not carry it out. □

2D Cases where the Sylow p-subgroup is not $\mathbb{Z}_p$ or is not normal

In all later sections of this paper, we will assume that the Sylow p-subgroup of G is isomorphic to $\mathbb{Z}_p$, and is normal in G. The following proposition deals with the finitely many groups that do not satisfy this hypothesis. (See Lemma 2.13(4) for a justification of the assumption that p is the largest prime divisor of kp.)

Proposition 2.7. *Let P be a Sylow p-subgroup of G, and assume $|G| = kp$, where p is the largest prime divisor of kp, and $k < 48$.*

1. *If $P \ncong \mathbb{Z}_p$, then every connected Cayley graph on G is hamiltonian.*
2. *If $P \cong \mathbb{Z}_p$ and $P \ntriangleleft G$, then every connected Cayley graph on G is hamiltonian.*

Justification. (1) Since the Sylow p-subgroup of G is not isomorphic to $\mathbb{Z}_p$, we know that p^2 is a divisor of $|G| = kp$, so $p \mid k$. In fact, p must be the largest prime divisor of k (since it is the largest prime divisor of kp). So p is uniquely determined by k.

It is a simple matter to write a `GAP` program that

- loops through the values of k in $\{1, \ldots, 47\}$,
- loops through all the nonabelian groups G of order kp, where p is the largest prime divisor of k,
- loops through all the irredundant generating sets S of G (up to automorphisms of G), and
- uses LKH to verify that $\mathrm{Cay}(G; S)$ is hamiltonian.

(See the file `2-7(1)-SylowSubgroupNotZp.gap`.) The calculations take several hours to complete. About half of the time is spent finding hamiltonian cycles in the Cayley graphs of order $32 \times 2 = 64$, since there are so many of them, so we separated out that part of the calculation (see Lemma 2.6).

One important modification to the algorithm deals with the problem that the original version of the program ran out of memory when trying to find the generating sets of SmallGroup(1058, 4). (This group arises for $k = 23$.) Since $1058 = 2 \times 23^2$ is of the form $2p^2$, Theorem 5.1(4) tells us that every Cayley graph on this group is hamiltonian. (In fact, this group is of "dihedral type" so it is very easy either to find all of the irredundant generating sets by hand, or to prove that every connected Cayley graph is hamiltonian.) Therefore, the program skips this group (and prints the comment that it "`is dihedral type of order 2p^2`").

(2) Let d be the number of Sylow p-subgroups of G. We know from Sylow's Theorem that d is a divisor of k, and that $d \equiv 1 \pmod p$. Also note that $d > 1$, since the Sylow subgroup $\mathbb{Z}_p$ is not normal, and therefore has conjugates. This implies $p < k$ (indeed, $p < d$ since $d \equiv 1 \pmod p$, and $d \leq k$, since d is a divisor of k). Therefore, for each k, there are only finitely many possibilities for p.

It is a simple matter to write a `GAP` program that

- loops through the values of k in $\{1, \ldots, 47\}$,
- loops through the primes p that are:
  - greater than the largest prime divisor of k,

  - less than or equal to k, and
  - such that there is a divisor d of k, with $d > 1$ and $d \equiv 1 \pmod{p}$,

- loops through all the groups G of order kp, such that a Sylow p-subgroup is not normal,
- loops through all the irredundant generating sets S of G (up to automorphisms of G), and
- uses LKH to verify that $\mathrm{Cay}(G; S)$ is hamiltonian.

(See the file `2-7(2)-SylowSubgroupNotNormal.gap`.) □

2E Notation and assumptions

Notation 2.8. In the remainder of this paper:

1. G is always a group of order kp, where $1 \leq k < 48$, and p is a prime number.
2. S is a generating set of G.
3. $^{-}\colon G \to G/\mathbb{Z}_p$ is the natural homomorphism, if it is the case that $\mathbb{Z}_p$ is the unique Sylow p-subgroup of G.

Convention 2.9. To avoid treating $k = 2$ as a special case, we will consider the graph K_2 to be hamiltonian, because it has a closed walk that visits all the vertices exactly once before returning to the starting point.

Notation 2.10. For $s_1, \ldots, s_n \in S \cup S^{-1}$, we use $(s_1, \ldots, s_n)$ to denote the walk in $\mathrm{Cay}(G; S)$ that visits (in order), the vertices

$$e,\ s_1,\ s_1 s_2,\ s_1 s_2 s_3,\ \ldots,\ s_1 s_2 \cdots s_n.$$

Definition 2.11 (cf. [13, §2.1.3, p. 61])**.** For any hamiltonian cycle $H = (\overline{s_1}, \overline{s_2}, \ldots, \overline{s_n})$ in the Cayley graph $\mathrm{Cay}(\overline{G}; \overline{S})$, we let $\mathrm{volt}_{G,S}(H) = \prod_{i=1}^{n} s_i$ be the *voltage* of H. This is an element of $\mathbb{Z}_p$.

We wish to show that $\mathrm{Cay}(G; S)$ has a hamiltonian cycle. Our main tool is the following elementary observation:

Lemma 2.12 ("Factor Group Lemma" [21, §2.2])**.** *Suppose*

- $H = (\overline{s_1}, \overline{s_2}, \ldots, \overline{s_k})$ *is a hamiltonian cycle in* $\mathrm{Cay}(\overline{G}; \overline{S})$*, and*
- $\mathrm{volt}_{G,S}(H)$ *generates* $\mathbb{Z}_p$*.*

Then $(s_1, s_2, \ldots, s_k)^p$ *is a hamiltonian cycle in* $\mathrm{Cay}(G; S)$*.*

Lemma 2.13. *To prove Theorem 1.1, we may assume:*

(1) G is not abelian.

(2) $k > 1$.

(3) If G' is any group of order $k'p'$, where $1 \leq k' < k$, and p' is any prime number, then every connected Cayley graph on G' is hamiltonian.

(4) p is strictly greater than the largest prime factor of k.

(5) *$\mathbb{Z}_p$ is a Sylow p-subgroup of G, and $\mathbb{Z}_p \triangleleft G$.*

(6) *There does not exist $s \in S$, such that $\langle s \rangle \trianglelefteq G$, and such that either*

   (a) *$s \in Z(G)$, or*

   (b) *$Z(G) \cap \langle s \rangle = \{e\}$, or*

   (c) *$|s|$ is prime.*

(7) *$S \cap \mathbb{Z}_p = \emptyset$.*

(8) *$\overline{s} \neq \overline{t}$, for all $s, t \in S \cup S^{-1}$ with $s \neq t$.*

(9) *If $s \in S$ with $|\overline{s}| = 2$, then $|s| = 2$.*

(10) *$G = \mathbb{Z}_p \rtimes_\tau \overline{G}$, where τ is a homomorphism from $\overline{G}$ to $\mathbb{Z}_p^\times$.*

Proof. (1) Showing that all connected Cayley graphs on abelian groups are hamiltonian is an easy exercise. (The Chen-Quimpo Theorem (Theorem 5.5) is a much stronger result.)

(2) If $k = 1$, then $|G| = p$, so G is abelian, contrary to (1).

(3) We may assume this by induction on k.

(4) Let p' be the largest prime factor of k, and write $|G| = k'p'$. If $p = p'$, then $|G|$ is divisible by p^2, so Proposition 2.7(1) applies. If $p < p'$, then $k > k'$, so (3) applies.

(5) If either $P \ncong \mathbb{Z}_p$ or $P \ntriangleleft G$, then Proposition 2.7 applies.

(6) For any $s \in S$, we know, from (1), that $\langle s \rangle \neq G$. In addition, we see from (3) that $\mathrm{Cay}\big(G/\langle s \rangle; S\big)$ is hamiltonian. Therefore, it is well known (and easy to prove) that if s satisfies any of the given conditions, then $\mathrm{Cay}(G; S)$ is hamiltonian [16, Lemma 2.27].

(7) This is a special case of (6c).

(8) From Proposition 1.3, we see that every edge of $\mathrm{Cay}(\overline{G}; \overline{S})$ is in a hamiltonian cycle. Therefore, if $\overline{s} = \overline{t}$ with $s \neq t$, then the existence of a hamiltonian cycle in $\mathrm{Cay}(G; S)$ is a well-known (and easy) consequence of the Factor Group Lemma (Lemma 2.12) (cf. [16, Corollary 2.11]).

(9) Since $\overline{s} = \overline{s}^{-1}$, this follows from (8) with $t = s^{-1}$.

(10) From (4), we know that $\gcd\big(|\overline{G}|, k\big) = 1$. Therefore, the desired conclusion is a consequence of the Schur-Zassenhaus Theorem [19]. □

Remark 2.14. It is immediate from (7) and (8) of Lemma 2.13 that the Cayley graphs $\mathrm{Cay}(G; S)$ and $\mathrm{Cay}(\overline{G}; \overline{S})$ have the same valence (and have no loops).

3 Irredundant generating sets of the quotient

In this section, we assume that the generating set $\overline{S}$ of $\overline{G}$ is irredundant. The assumptions stated in Notations 2.1 and 2.8 and Lemma 2.13 are also assumed to hold.

In most cases, we will find a hamiltonian cycle in $\mathrm{Cay}(\overline{G}; \overline{S})$ with nonzero voltage, so that the Factor Group Lemma (Lemma 2.12) applies. The following lemma deals with the exceptional cases in which this approach does not work.

Lemma 3.1. *Assume the generating set $\overline{S}$ of $\overline{G}$ is irredundant. Then $\mathrm{Cay}(G; S)$ has a hamiltonian cycle in each of the following situations:*

1. *$\overline{S} = \{\overline{a}, \overline{b}\}$, with $|\overline{a}| = 2$, $|\overline{b}| = 3$, and $\tau(\overline{b}) = 1$.*
2. *$\overline{G} \cong A_4$, $\overline{S} = \{\overline{a}, \overline{b}\}$, where $|\overline{a}| = |\overline{b}| = 3$, and $\overline{G}$ centralizes $\mathbb{Z}_p$.*

3. *$\overline{G} = (\mathbb{Z}_2 \times \mathbb{Z}_2) \rtimes_\tau \mathbb{Z}_m$, $\overline{S} = \{\overline{a}, \overline{b}\}$, where $\overline{a} \in \mathbb{Z}_2 \times \mathbb{Z}_2$, $|\overline{b}| = m$, $\overline{G}$ is not abelian, and $\overline{G}$ centralizes $\mathbb{Z}_p$.*
4. *$\overline{S}$ contains an element a, such that $a \in Z(\overline{G})$, $|a| = 2$, and $\tau(a) = 1$.*
5. *$\overline{S}$ contains an element a, such that a^2 has prime order, $\langle a^2 \rangle \triangleleft \overline{G}$, and $\tau(a) = -1$.*
6. *$\overline{G}$ is a dihedral group of order k (with $k > 4$), $\overline{S} = \{\overline{a}, \overline{b}\}$ with $|\overline{a}| = 2$ and $\overline{b} = k/2$, $\overline{a}$ inverts $\mathbb{Z}_p$ and $\overline{b}$ centralizes $\mathbb{Z}_p$.*
7. *$|\overline{G}| = 4q$ and $|[\overline{G}, \overline{G}]| = q$, where q is prime, and $\overline{S} = \{\overline{a}, \overline{b}\}$, where $|\overline{a}| = 4$ and $|\overline{b}| = 2$. Furthermore, $\overline{G}$ centralizes $\mathbb{Z}_p$, but $\overline{b}$ does not centralize $[\overline{G}, \overline{G}]$.*

Proof. (1) We may assume a projects trivially to $\mathbb{Z}_p$. (If a centralizes $\mathbb{Z}_p$, this follows from Lemma 2.13(9). If a does not centralize $\mathbb{Z}_p$, then it is true after conjugation by some element of $\mathbb{Z}_p$.) So b must project nontrivially. Since b centralizes $\mathbb{Z}_p$, this implies $|b| = 3p$.

Since $|\overline{a}| = 2$ and $|\overline{b}| = 3$, it is easy to see that every hamiltonian cycle in $\mathrm{Cay}(A_4; \overline{a}, \overline{b})$ is of the form $(\overline{a}, \overline{b}^{\pm 2}, \overline{a}, \overline{b}^{\pm 2}, \ldots, \overline{a}, \overline{b}^{\pm 2})$ [17, p. 238]. Hence, each right coset of $\langle \overline{b} \rangle$ appears as consecutive vertices in this cycle, so it is not difficult to see that

$$(a, b^{\pm(3p-1)}, \overline{a}, b^{\pm(3p-1)}, \ldots, a, b^{\pm(3p-1)})$$

passes through all of the vertices in each right coset of $\langle b \rangle$, and is therefore a hamiltonian cycle in $\mathrm{Cay}(G; a, b)$. See Subcase 1.1 of [23, §3] for a detailed verification of a very similar example.

(2) [16, Subcase 2.2 of Proposition 7.2]: Assume, without loss of generality, that a projects nontrivially to $\mathbb{Z}_p$, so $|a| = 3p$. Therefore $4|a| = |G|$. Since $\overline{G}$ centralizes $\mathbb{Z}_p$, we have $G \cong \mathbb{Z}_p \times A_4$. Therefore, $[G, G] \cong [A_4, A_4] \cong \mathbb{Z}_2 \times \mathbb{Z}_2$, so $|[a, b]| = 2$. It is now not difficult to verify that $\big(a^{|a|-1}, b^{-1}, a^{-(|a|-1)}, b\big)^2$ is a hamiltonian cycle. (This is a special case of a lemma of D. Jungreis and E. Friedman that can be found in [16, 2.14].)

(2) Lemma 2.13(9) tells us that the projection of a to $\mathbb{Z}_p$ is trivial. So the projection of b to $\mathbb{Z}_p$ is nontrivial. Since b centralizes $\mathbb{Z}_p$, this implies $|b| = mp = |G|/4$. Also note that $\overline{b}$ does not centralize $\overline{a}$ (since $\overline{G}$ is not abelian), so $\{e, b^{-1}ab, b^{-1}ab\,a, a\} = \mathbb{Z}_2 \times \mathbb{Z}_2$. Therefore, it is easy to see that $(b^{mp-1}, a, b^{-(mp-1)}, a)^2$ is a hamiltonian cycle in $\mathrm{Cay}(G; S)$. (This is an easy special case of the same lemma of D. Jungreis and E. Friedman that was used in (3).)

(4) Let $s \in S$ with $\overline{s} = a$. Lemma 2.13(8) (with $t = a^{-1}$) implies $|s| = 2$. Since $\tau(a) = 1$, we know that s centralizes $\mathbb{Z}_p$, so Lemma 2.13(9) implies that s has trivial projection to $\mathbb{Z}_p$ (since $p > 2$). Therefore, we have $s \in Z(G)$, which contradicts Lemma 2.13(6a).

(5) Let $s \in S$ with $\overline{s} = a$. Since $\tau(a) \neq 1$, we know that s does not centralize $\mathbb{Z}_p$, so we may assume (after conjugating by an appropriate element of $\mathbb{Z}_p$) that the projection of s to $\mathbb{Z}_p$ is trivial. This means $s = a$. Then, since $\tau(a^2) = \big(\tau(a)\big)^2 = (-1)^2 = 1$, we see that s^2 generates a subgroup of prime order that is normal in G. (Indeed, we know, by assumption, that $\langle a^2 \rangle$ is normalized by $\overline{G}$, and it centralizes $\mathbb{Z}_p$ since $\tau(s^2) = 1$.) This contradicts the conclusion of Lemma 2.13(8) (with $t = s^{-1}$, and with $\langle s^2 \rangle$ in the role of $\mathbb{Z}_p$).

(6) Since $\overline{a}$ does not centralize $\mathbb{Z}_p$, we may assume that a projects trivially to $\mathbb{Z}_p$ (after replacing S with a conjugate). Since S generates G, this implies that b projects nontrivially to $\mathbb{Z}_p$. Since $\overline{b}$ centralizes $\mathbb{Z}_p$, we conclude that $|b| = p|\overline{b}|\,p$. Also, since $a = \overline{a}$ inverts both $\overline{b}$ and $\mathbb{Z}_p$, we know that a inverts b. So G is the dihedral group of order kp, and $\{a, b\}$ is

the obvious generating set consisting of a reflection a and a rotation b. Therefore, if we let $m = \frac{1}{2}|G| - 1$, then we have the hamiltonian cycle $(a, b^m)^2$.

(7) This is a known result. Namely, since $|G| = 4pq$, this is a special case of Theorem 5.1(2). (Alternatively, we may apply Theorem 5.2(1), since $[G, G] = |[\overline{G}, \overline{G}]| = q$.) For completeness, we record a proof that is adapted from [15, Case 5.3].) We know that $|\overline{G}| = 4q$, $|[\overline{G}, \overline{G}]| = q$, and $|\overline{a}| = 4$, so we may write $\overline{G} = \mathbb{Z}_q \rtimes \mathbb{Z}_4$, with $\mathbb{Z}_q = [\overline{G}, \overline{G}]$ and $\mathbb{Z}_4 = \langle \overline{a} \rangle$. Since $\overline{b}$ has order 2 and centralizes $\mathbb{Z}_p$, we see from Lemma 2.13(9) that b projects trivially to $\mathbb{Z}_p$, so a must project nontrivially. Therefore a generates $G/\mathbb{Z}_q$, so we have $b \in a^i \mathbb{Z}_q$, for some (even) i with $0 \leq i < 4p$. (Also, we know $i \neq 0$, because $|\overline{b}| = 2$ is not a divisor of q.) Then $(b, a^{-(i-1)}, b, a^{4q-i-1})$ is a hamiltonian cycle in $\mathrm{Cay}(G/\mathbb{Z}_q; a, b)$.

If we write $b = \gamma a^i$, with $\gamma \in \mathbb{Z}_q$, then the voltage of this hamiltonian cycle is

$$ba^{-(i-1)} b a^{4q-i-1} = (\gamma a^i) a^{-(i-1)} (\gamma a^i) a^{4q-i-1} = \gamma a \gamma a^{-1}.$$

Since b does not centralize $\mathbb{Z}_q$ (and $b \in a^i \mathbb{Z}_q$ with i even), we know that a does not invert $\mathbb{Z}_q$. Therefore the voltage $\gamma a \gamma a^{-1}$ is nontrivial, so the Factor Group Lemma (Lemma 2.12) applies. □

We wish to show, for each lift of $\overline{S}$ to a generating set S of G, that some hamiltonian cycle in $\mathrm{Cay}(\overline{G}; \overline{S})$ has nonzero voltage.

Definition 3.2 ([18]). Recall that the *norm* of an algebraic number is the product of all of its Galois conjugates in $\mathbb{C}$.

Lemma 3.3 (cf. [23, Lemma 2.11]). *Assume*

- $G = \mathbb{Z}_p \rtimes_\tau \overline{G}$, *where τ is a homomorphism from $\overline{G}$ to $\mathbb{Z}_p^\times$,*
- $\zeta = \phi \circ \tau$, *where ϕ is an isomorphism from $\mathbb{Z}_p^\times$ onto the group μ_{p-1} of $(p-1)$th roots of unity in $\mathbb{C}$, so ζ is an abelian character of $\overline{G}$ (more precisely, ζ is a homomorphism from $\overline{G}$ to μ_{p-1}),*
- Z *is the subring of $\mathbb{C}$ that is generated by the $(p-1)$th roots of unity,*
- $S = \{a_1, a_2, \ldots, a_m, b_1, \ldots, b_n\} \cup B_0$ *is a generating set of G, such that*
  - *each $\overline{a_i}$ has order 2, and centralizes $\mathbb{Z}_p$,*
  - *either B_0 is empty, or B_0 consists of a single element b_0 that does not centralize $\mathbb{Z}_p$,*
- H_i *is a hamiltonian cycle in $\mathrm{Cay}(\overline{G}; \overline{S})$, for $i = 1, 2, \ldots, n$, and*
- *for $j = 1, 2, \ldots, n$, S_j is the generating set of G, such that $\overline{S_j} = \overline{S}$, and $s \in \overline{G}$ for all $s \in S_j$, except that $(1, \overline{b_j}) \in S_j$.*

If $\mathrm{Norm}\big(\det\big[\mathrm{volt}_{Z \rtimes_\zeta \overline{G}, S_j}(H_i)\big]\big)$ *is not divisible by p, then* $\mathrm{Cay}(G; S)$ *is hamiltonian.*

Proof. From Lemma 2.13(9), we know that $a_i = (0, \overline{a_i})$ for each i. Also, if B_0 has an element b, then we may assume $b = (0, \overline{b})$, after conjugating by an element of $\mathbb{Z}_p$. So $b_1, \ldots, b_n$ are the only elements of S that contribute to $\mathrm{volt}_{\mathbb{Z}_p \rtimes_\tau \overline{G}, S}(H)$. Therefore, if we write $b_j = (z_j, \overline{b_j})$, then, from the definition of $S_1, \ldots, S_n$, we have

$$\mathrm{volt}_{\mathbb{Z}_p \rtimes_\tau \overline{G}, S}(H) = \sum_{j=1}^{n} z_j \, \mathrm{volt}_{\mathbb{Z}_p \rtimes_\tau \overline{G}, S_j}(H).$$

Note that $z_1, \ldots, z_n$ cannot all be 0, since $\langle S \rangle = G$. Therefore, if $\operatorname{volt}_{\mathbb{Z}_p \rtimes_\zeta \overline{G}, S}(H_i) = 0$ for all i, then elementary linear algebra tells us that

$$\Delta_p = 0, \text{ where } \Delta_p = \det\big[\operatorname{volt}_{\mathbb{Z}_p \rtimes_\tau \overline{G}, S_j}(H_i)\big]. \qquad (*)$$

We will show that this leads to a contradiction. (So there must be a hamiltonian cycle with nonzero voltage, so the Factor Group Lemma (Lemma 2.12) applies.)

The isomorphism $\phi^{-1} \colon \mu_{p-1} \to \mathbb{Z}_p^\times$ extends to a unique ring homomorphism $\Phi \colon Z \to \mathbb{Z}_p$. Since $\Phi \circ \zeta = \tau$ (and Φ is a ring homomorphism), it is easy to see that pairing Φ with the identity map on $\overline{G}$ yields a group homomorphism $\widehat{\Phi} \colon Z \rtimes_\zeta \overline{G} \to \mathbb{Z}_p \rtimes_\tau \overline{G}$. Therefore

$$\Phi\big(\operatorname{volt}_{Z \rtimes_\zeta \overline{G}, S_j}(H)\big) = \operatorname{volt}_{\mathbb{Z}_p \rtimes_\tau \overline{G}, S_j}(H)$$

for every hamiltonian cycle H in $\operatorname{Cay}(\overline{G}; \overline{S})$. Since Φ is a ring homomorphism (and determinants are calculated simply by adding and multiplying), this implies

$$\Phi(\Delta) = \Delta_p, \text{ where } \Delta = \det\big[\operatorname{volt}_{Z \rtimes_\zeta \overline{G}, S_j}(H_i)\big].$$

The assumption that $\operatorname{Norm}(\Delta)$ is not divisible by p tells us that $\Phi\big(\operatorname{Norm}(\Delta)\big) \neq 0$. Since, by definition, $\operatorname{Norm}(\Delta)$ is the product of Δ with its other conjugates, and the ring homomorphism Φ respects multiplication, we conclude that $\Phi(\Delta) \neq 0$. In other words, $\Delta_p \neq 0$. This contradiction to $(*)$ completes the proof. □

Proposition 3.4. *If the generating set $\overline{S}$ of $\overline{G}$ is irredundant, then $\operatorname{Cay}(G; S)$ is hamiltonian.*

Justification. For each group $\overline{G}$ of order less than 48, and each irredundant generating set $\overline{S}$ of $\overline{G}$, the GAP program in the file `3-4-IrredundantSBar.gap` constructs a list SeveralHamCycsInCG of some hamiltonian cycles in $\operatorname{Cay}(\overline{G}; \overline{S})$ (by calling the function SeveralHamCycsInCay).

Now, the program considers each abelian character ζ of $\overline{G}$. If Lemma 3.1 (or some other lemma) provides a hamiltonian cycle in $\operatorname{Cay}\big(\mathbb{Z}_p \rtimes_\tau \overline{G}; S\big)$, then nothing more needs to be done. Otherwise, the program constructs the list $S_1, \ldots, S_n$ of generating sets described in Lemma 3.3, and calculates the voltage $\operatorname{volt}_{Z \rtimes_\zeta \overline{G}, S_j}(H_i)$ for each H_i in SeveralHamCycsInCG.

Now, the program calls the function FindNonzeroDet, which returns a list $i_1, \ldots, i_n$ of indices. The program then verifies that if we use $H_{i_1}, \ldots, H_{i_n}$ as the hamiltonian cycles in Lemma 3.3, then the norm of the determinant of the matrix of voltages is nonzero. Hence, Lemma 3.3 provides a hamiltonian cycle in $G = \mathbb{Z}_p \rtimes_\tau \overline{G}$ for all but the finitely many primes p that are a divisor of this norm.

To deal with these remaining primes, the program calls the function CallLKHOnLiftsOfSBar, which constructs every possible lift of $\overline{S}$ to a generating set S of G, and uses LKH to verify that $\operatorname{Cay}(G; S)$ is hamiltonian. □

Remark 3.5. It is not necessary to verify the source code of SeveralHamCycsInCay or FindNonzeroDet, because the output of both of these programs is validated before it is used.

4 Redundant generating sets of the quotient

We now assume that the generating set $\overline{S}$ of $\overline{G}$ is redundant (but S is irredundant, and the other assumptions stated in Notations 2.1 and 2.8 and Lemma 2.13 are also assumed to hold). The following well-known observation tells us that (up to an automorphism of G) every S of this type can be constructed by choosing an irredundant generating set $\overline{S_0}$ of $\overline{G}$ and an element $\overline{a}$ of $\overline{G}$, and letting $S = \big(\{0\} \times \overline{S_0}\big) \cup \{(1, \overline{a})\}$.

Lemma 4.1. *Assume the generating set $\overline{S}$ of $\overline{G}$ is redundant. Then, perhaps after conjugating by an element of $\mathbb{Z}_p$, there is an element a of $\overline{S}$, such that if we let $S_0 = S \setminus \{a\}$, then*

1. *$\overline{S_0}$ is an irredundant generating set of $\overline{G}$, and*
2. *$S_0 \subseteq \{0\} \rtimes \overline{G}$.*

Proof. By assumption, there is a proper subset S_0 of S, such that $\langle \overline{S_0} \rangle = \overline{G}$. By choosing S_0 to be of minimal cardinality, we may assume that $\overline{S_0}$ is irredundant. Since $|\langle S_0 \rangle|$ is divisible by $|\langle \overline{S_0} \rangle| = |\overline{G}| = |G|/p$, and is a proper divisor of $|G|$, we must have $|\langle S_0 \rangle| = |G|/p$. So $\langle S_0 \rangle$ is a maximal subgroup of G. Therefore, we have $\langle S_0, a \rangle = G$ for any element a of S that is not in S_0. Since S is irredundant, we conclude that $S = S_0 \cup \{a\}$.

Since $|\langle S_0 \rangle| = |G|/p$, we see from Lemma 2.13(4) that $\langle S_0 \rangle$ is a Hall subgroup of G. Then, since $\mathbb{Z}_p$ is a solvable normal complement, the Schur-Zassenhaus Theorem [19] tells us that, after passing to a conjugate, we have $\langle S_0 \rangle = \{0\} \rtimes \overline{G}$. □

Lemma 4.2. *Assume*

- $S = \big(\{0\} \times \overline{S_0}\big) \cup \{(1, \overline{a})\}$,
- *$\overline{S_0}$ is an irredundant generating set of $\overline{G}$,*
- *either* $\mathrm{Cay}(\overline{G}; \overline{S_0})$ *is not bipartite, or* $\mathrm{Cay}(\overline{G}; \overline{S})$ *is bipartite, and*
- $|S_0 \cup S_0^{-1}| \geq 3$.

Then $\mathrm{Cay}(G; S)$ *is hamiltonian.*

Proof. We know from Lemma 2.13(7) that $\overline{a} \neq \overline{e}$. Therefore, Proposition 1.3 tells us there is a hamiltonian path $(\overline{s_i})_{i=1}^{n-1}$ from $\overline{e}$ to $\overline{a}^{\,-1}$ in $\mathrm{Cay}(\overline{G}; \overline{S_0})$. So $H = \big(\overline{a}, (\overline{s_i})_{i=1}^{n-1}\big)$ is a hamiltonian cycle in $\mathrm{Cay}(\overline{G}; \overline{S})$.

Write $a = (z, \overline{a})$, with $z \in \mathbb{Z}_p \setminus \{0\}$. Since $S_0 \subseteq \{0\} \rtimes \overline{G}$, we must have $z \neq 0$, and the voltage $a s_1 s_2 \cdots s_{n-1}$ of H is z. Hence, the Factor Group Lemma (Lemma 2.12) provides a hamiltonian cycle in $\mathrm{Cay}(G; S)$. □

To complete the proof of Theorem 1.1, the following two results consider the special cases that are not covered by Lemma 4.2.

Proposition 4.3. *Assume*

- $S = \big(\{0\} \times \overline{S_0}\big) \cup \{(1, \overline{a})\}$,
- *$\overline{S_0}$ is an irredundant generating set of $\overline{G}$,*
- $\mathrm{Cay}(\overline{G}; \overline{S_0})$ *is bipartite, and*
- $\mathrm{Cay}(\overline{G}; \overline{S})$ *is not bipartite.*

Then $\mathrm{Cay}(G; S)$ *is hamiltonian.*

Justification. The GAP program in 4-3-RedundantSBar.gap:

- loops through all groups $\overline{G}$ of order less than 48,
- loops through all irredundant generating sets $\overline{S_0}$ of $\overline{G}$, such that $\mathrm{Cay}(\overline{G}; \overline{S_0})$ is bipartite,
- loops through all nonidentity elements $\overline{a}$ of $\overline{G}$, such that $\mathrm{Cay}(\overline{G}; \overline{S})$ is not bipartite, where $\overline{S} = \overline{S_0} \cup \{\overline{a}\}$,
- constructs the set $S = \big(\{0\} \times \overline{S_0}\big) \cup \{(1, \overline{a})\}$,
- makes a list of a few hamiltonian cycles in $\mathrm{Cay}(\overline{G}; \overline{S})$ (by calling the function SeveralHamCycsInRedundantCay,
- loops through all abelian characters ζ of $\overline{G}$,
- ignores this character if the condition in Lemma 2.13(9) is not violated,
- ignores this character if S is not a minimal generating set of G,
- calculates the GCD of the norms of the voltages of the hamiltonian cycles in the list, and
- uses LKH to find a hamiltonian cycle in $\mathrm{Cay}(\mathbb{Z}_p \rtimes_\tau \overline{G}; S)$ for each prime p that divides the GCD, by calling CallLKHOnLiftsOfSBar.

(The use of CallLKHOnLiftsOfSBar in the last step is overkill, because we are interested only in the one particular lift S of $\overline{S}$, but we are calling a function that checks all possible lifts. It does not seem worthwhile to write and verify another GAP program, just to eliminate this slight waste.) □

Remark 4.4. It is not necessary to verify the source code of the function SeveralHamCycsInRedundantCay, because the output of this program is validated before it is used.

Lemma 4.5. *Assume*

- $S = \big(\{0\} \times \overline{S_0}\big) \cup \{(1, \overline{a})\}$,
- $\overline{S_0}$ *is an irredundant generating set of* $\overline{G}$*, and*
- $|S_0 \cup S_0^{-1}| \leq 2$.

Then $\mathrm{Cay}(G; S)$ *is hamiltonian.*

Justification. Since $\overline{S_0}$ is a generating set of $\overline{G}$, and $\overline{a} \notin \{\overline{e}\} \cup \overline{S_0} \cup \overline{S_0}^{-1}$ (by (7) and (8) of Lemma 2.13), it is easy to see that we must have $k \geq 4$. Also note that the only groups with a 2-valent, connected Cayley graph are cyclic groups and dihedral groups, and that the 2-valent generating set of such a group is unique, up to an automorphism of the group.

Applying the same method that was used for Proposition 4.3, the GAP program in 4-5-Valence2.gap:

- loops through all values of k from 4 to 47,
- loops through the groups $\overline{G}$ of order k that have a 2-valent, connected Cayley graph, and defines $\overline{S_0}$ to be the 2-valent generating set of $\overline{G}$,

- loops through all nonidentity elements $\overline{a}$ of $\overline{G}$, such that $\overline{a} \notin \{\overline{e}\} \cup \overline{S_0} \cup \overline{S_0}^{-1}$ (except that we do not need to consider both $\overline{a}$ and $\overline{a}^{-1}$),
- constructs the generating set $S = \big(\{0\} \times \overline{S_0}\big) \cup \{(1, \overline{a})\}$ of G,
- makes a list of 20 hamiltonian cycles in $\mathrm{Cay}(\overline{G}; \overline{S})$,
- loops through all abelian characters ζ of $\overline{G}$,
- ignores this character if the condition in Lemma 2.13(9) is not violated,
- ignores this character if S is not a minimal generating set of G,
- calculates the GCD of the norms of the voltages of the hamiltonian cycles in the list, and
- uses LKH to find a hamiltonian cycle in $\mathrm{Cay}(\mathbb{Z}_p \rtimes_\tau \overline{G}; S)$ for each prime p that divides the GCD, by calling CallLKHOnLiftsOfSBar.

(As in Proposition 4.3, the use of CallLKHOnLiftsOfSBar in the last step is overkill.) □

5 Known results that can reduce the number of cases

There are several results in the literature that can be used to substantially reduce the number of Cayley graphs considered in the proof of Theorem 1.1 (but then the proof is not self-contained). The following theorem of Kutnar et al. is the main example.

Theorem 5.1 ([16, Theorem 1.2], [20])**.** *Every connected Cayley graph on G is hamiltonian if $|G|$ has any of the following forms* (*where p, q, and r are distinct primes*):

1. *kp, where $1 \leq k < 32$, with $k \neq 24$,*
2. *kpq, where $1 \leq k \leq 5$,*
3. *pqr,*
4. *kp^2, where $1 \leq k \leq 4$,*
5. *kp^3, where $1 \leq k \leq 2$,*
6. *p^k.*

The following result is also useful.

Theorem 5.2 ([15, 22, 24])**.** *Every connected Cayley graph on G has a hamiltonian cycle if either*

1. *$[G, G]$ is cyclic of prime-power order, or*
2. *$|[G, G]| = pq$, where p and q are distinct primes, and $|G|$ is odd, or*
3. *$|[G, G]| = 2p$, where p is an odd prime.*

Lemma 5.3. *To prove Theorem 1.1, one may assume:*

1. *$k \in \{24, 32, 36, 40, 42, 45\}$.*
2. *$|[\overline{G}, \overline{G}]| \geq 3$.*
3. *Either $|[\overline{G}, \overline{G}]| \geq 4$, or the twist function τ is nontrivial.*

Proof. (1) If $k < 32$ and $k \neq 24$, then Theorem 5.1(1) applies. Therefore, either k is in the specified set, or $k \in \{33, 34, 35, 37, 38, 39, 41, 43, 44, 46, 47\}$, in which case some part of Theorem 5.1 applies:

k	form of $\lvert G\rvert = kp$
33	$9p$ (if $p = 3$), $3p^2$ (if $p = 11$), or pqr
34	$2p^2$ (if $p = 17$) or $2pq$
35	$25p$ (if $p = 5$), $5p^2$ (if $p = 7$), or pqr
37	p^2 (if $p = 37$) or pq
38	$2p^2$ (if $p = 19$) or $2pq$
39	$9p$ (if $p = 3$), $3p^2$ (if $p = 13$), or pqr

k	form of $\lvert G\rvert = kp$
41	p^2 (if $p = 41$) or pq
43	p^2 (if $p = 43$) or pq
44	$4p^2$ (if $p = 11$) or $4pq$
46	$2p^2$ (if $p = 23$) or $2pq$
47	p^2 (if $p = 47$) or pq

(2) The commutator subgroup of G is a subgroup of $\mathbb{Z}_p \rtimes_\tau \overline{G}'$, so its order is a divisor of $p\,|\overline{G}'|$. Therefore, if $|[\overline{G},\overline{G}]| \le 2$, then $|[G,G]|$ is either 1, 2, p, or $2p$. (Furthermore, if $p = 2$, then τ must be trivial, so $G = \mathbb{Z}_2 \times \overline{G}$, which implies that $[G,G] = [\overline{G},\overline{G}]$.) So Theorem 5.2 establishes that every connected Cayley graph on G has a hamiltonian cycle.

(3) As in (2), if τ is trivial, then $G = \mathbb{Z}_p \times \overline{G}$, so $[G,G] = [\overline{G},\overline{G}]$. Therefore, Theorem 5.2(1) provides a hamiltonian cycle in every Cayley graph on G if $|[\overline{G},\overline{G}]|$ is prime. (In particular, if $|[\overline{G},\overline{G}]| < 4$.) □

Remark 5.4. If we apply Lemma 5.3(1), then the proof of Theorem 1.1 requires hamiltonian connectivity/laceability only for Cayley graphs of the orders listed in Lemma 5.3(1), not the full strength of Proposition 1.3.

The computations to justify Proposition 1.3 could be shortened a bit by applying the following interesting result:

Theorem 5.5 (Chen-Quimpo [6]). *Assume* $\mathrm{Cay}(G;S)$ *is a connected Cayley graph. If* G *is abelian, and the valence of* $\mathrm{Cay}(G;S)$ *is at least three, then* $\mathrm{Cay}(G;S)$ *is either hamiltonian connected or hamiltonian laceable.*

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Some remarks on Balaban and sum-Balaban index*

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Abstract

In the paper we study maximal values of Balaban and sum-Balaban index, and correct some results appearing in the literature which are only partially correct. Henceforth, we were able to solve a conjecture of M. Aouchiche, G. Caporossi and P. Hansen regarding the comparison of Balaban and Randić index. In addition, we showed that for every k and large enough n, the first k graphs of order n with the largest value of Balaban index are trees. We conclude the paper with a result about the accumulation points of sum-Balaban index.

Keywords: Topological index, Balaban index, sum-Balaban index, Randić index.

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1 Introduction

In this paper we consider simple and connected graphs. For a graph G, by $V(G)$ and $E(G)$ we denote the vertex and edge sets of G, respectively. Let $n = |V(G)|$ and $m = |E(G)|$. For vertices $u, v \in V(G)$, by $\mathrm{dist}_G(u, v)$ (or shortly just $\mathrm{dist}(u, v)$) we denote the distance from u to v in G, and by $w(u)$ we denote the *transmission* (or the *status*) of u, defined as $w(u) = \sum_{x \in V(G)} d_G(u, x)$.

Balaban index and sum-Balaban index are two of many distance-based topological indices, which are widely used in QSAR/QSPR modeling. *Balaban index* $J(G)$ of a connected graph G, defined as

$$J(G) = \frac{m}{m-n+2} \sum_{e=uv} \frac{1}{\sqrt{w(u) \cdot w(v)}},$$

was introduced in early eighties by Balaban [2, 3]. Later Balaban et al. [4] (and independently also Deng [9]) proposed a derived measure, namely the *sum-Balaban index* $\mathrm{SJ}(G)$ for a connected graph G:

$$\mathrm{SJ}(G) = \frac{m}{m-n+2} \sum_{uv \in E(G)} \frac{1}{\sqrt{w(u) + w(v)}}.$$

Although sum-Balaban index was introduced just a few years ago, several interesting results have already been published. Regarding extremal values, it was shown by Deng [9] and Xing et al. [23] that for a tree T on n vertices, $n \geq 2$,

$$\mathrm{SJ}(P_n) \leq \mathrm{SJ}(T) \leq \mathrm{SJ}(S_n) \tag{1.1}$$

with left (right, resp.) equality if and only if $T = P_n$ ($T = S_n$, resp.), where P_n is the path on n vertices and S_n is the star on n vertices. In [23] also trees with the second-largest, and third-largest (as well as the second-smallest, and third-smallest) sum-Balaban index among the n-vertex trees for $n \geq 6$ were determined. In [15] alternative proof for the above results and further ranking up to seventh maximum sum-Balaban index was presented.

In [26] the authors investigated the maximum value of sum-Balaban index for trees with a given diameter. The extremal graphs which attain the maximum sum-Balaban index among trees with given number of vertices and maximum degree, are determined in [25]. Unicyclic graphs on n vertices with the maximum value of sum-Balaban index were considered in [24], and n-vertex bicyclic graphs were studied in [6, 11].

For various upper and lower bounds on general graphs in terms of some other parameters (such as the maximum degree, number of edges, etc.) see [9] and [23], and for recent results on r-regular graphs, see [20].

Balaban index is somewhat better explored. We refer an interested reader to [13, 14, 16, 18] for recent papers, and to [19] for a survey. Despite the fact that Balaban index was introduced much earlier, some of its basic properties, such as the smallest possible value among all n-vertex graphs, are still unknown.

Balaban index was originally named as the "average distance-sum connectivity index". It is based on a Randić type formula, today called the *Randić index* [21], and known also as the *connectivity index* $R(G)$ of a graph G, defined by

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{\deg(u) \cdot \deg(v)}},$$

where $\deg(u)$ ($\deg(v)$, resp.) denotes the degree of u (v, resp.) in G. Note that in the definition of Balaban index, vertex degrees are replaced by transmissions.

With this paper we would like to contribute to better understanding of maximal values of both indices, and correct erroneous statements that appeared in the literature regarding some of these values (see Section 2). In addition, having correct results, we were able to show in Section 3 that a conjecture from [1] regarding the comparison of Balaban and Randić index holds. We conclude the paper with a result about the accumulation points of sum-Balaban index. The result is based on a proof of an upper bound for the minimum value of $\mathrm{SJ}(G)$.

2 Maximum values

The *cyclomatic number* μ of G, which is the minimum number of edges that must be removed from G in order to transform it to an acyclic graph, equals $m - n + 1$. Note that the denominator $m - n + 2$ in the definition of Balaban and sum-Balaban index can be expressed as $\mu + 1$. In this section we determine maximal values for both indices for graphs which contain at least one cycle.

Theorem 2.1. *Let G be a connected graph on n vertices with $\mu \geq 1$. Then:*

(1) $J(G)$ is maximum if and only of G is the complete graph K_n;

(2) $\mathrm{SJ}(G)$ is maximum if and only of G is the complete graph K_n.

Proof. Since G is a connected graph with $\mu \geq 1$, we have $n \geq 3$ and $m \in [n, \binom{n}{2}]$. For every $u \in V(G)$, we have $w(u) \geq n - 1$, which implies

$$J(G) \leq \frac{m^2}{(m-n+2)(n-1)}, \tag{2.1}$$

with equality if and only if $G = K_n$.

Let G be a graph on n vertices which is not complete. In order to prove that $J(G) < J(K_n) = \frac{n^2(n-1)}{2(n^2-3n+4)}$, one needs to check that for every $n \geq 3$ and $m \in [n, \binom{n}{2}]$ we have

$$\frac{m^2}{(m-n+2)(n-1)} \leq \frac{n^2(n-1)}{2(n^2-3n+4)}, \tag{2.2}$$

or equivalently

$$-2m^2(n^2-3n+4) + n^2(n-1)^2(m-n+2) \geq 0. \tag{2.3}$$

Let $f(m)$ be the left-hand side of (2.3), i.e., $f(m) = -2m^2(n^2-3n+4) + n^2(n-1)^2(m-n+2)$. Then f is quadratic in m with a negative leading coefficient. Hence, $f(m)$ is concave. Since

$$f(n) = n^2(2n-6) \geq 0 \qquad \text{and} \qquad f(\tfrac{n(n-1)}{2}) = 0,$$

we conclude that $f(m) \geq 0$ for every $m \in [n, \binom{n}{2}]$. Hence (2.3) is true, which completes the proof for Balaban index.

To prove the statement for sum-Balaban index, observe that since $w(u) \geq n - 1$, we have

$$\mathrm{SJ}(G) \leq \frac{m^2}{(m-n+2)\sqrt{2n-2}}, \tag{2.4}$$

with equality if and only if $G = K_n$.

Let G be a graph on n vertices which is not complete. In order to prove that $\mathrm{SJ}(G) < \mathrm{SJ}(K_n) = \frac{n^2(n-1)^2}{2(n^2-3n+4)\sqrt{2n-2}}$, one needs to check that for every $n \geq 3$ and $m \in [n, \binom{n}{2}]$ we have

$$\frac{m^2}{(m-n+2)\sqrt{2n-2}} \leq \frac{n^2(n-1)^2}{2(n^2-3n+4)\sqrt{2n-2}}.$$

Since the above inequality is equivalent to (2.2), the proof is complete. □

Sun [22], and Dong and Guo [10], independently studied Balaban index of trees with given number of vertices. Their results hold, however Deng [8] corrected mistakes in their proofs of the statement that for a tree T on $n \geq 2$ vertices it holds

$$J(P_n) \leq J(T) \leq J(S_n) \tag{2.5}$$

with left (right, resp.) equality if and only if $T = P_n$ ($T = S_n$, resp.).

In [10] the authors also state that for a connected graph G with n vertices

$$J(G) \leq J(S_n) = \sqrt{\frac{(n-1)^3}{2n-3}},$$

with equality if and only if $G = S_n$. It was brought to our attention that two years later (seemingly unaware of the paper by Dong and Guo), Aouchiche et al. [1] posed the conjecture, which we can state here as a theorem.

Theorem 2.2. *For any connected graph G on $n \geq 2$ vertices, we have*

$$J(G) \leq \begin{cases} J(K_n), & \text{if } n \leq 7 \\ J(S_n), & \text{if } n \geq 8. \end{cases}$$

In their proof, Dong and Guo use the assumption that $n \geq 9$ and neglect smaller cases. By Theorem 2.1 and (2.5), to complete the proof of Theorem 2.2 it suffices to compare

$$J(S_n) = \sqrt{\frac{(n-1)^3}{2n-3}} \qquad \text{and} \qquad J(K_n) = \frac{n^2(n-1)}{2(n^2-3n+4)}$$

for $n \in [3, 8]$. It turns out that $J(S_n) < J(K_n)$ if $n \in [3, 7]$, while $J(S_8) > J(K_8)$.

For sum-Balaban index we have an analogous result.

Theorem 2.3. *For any connected graph G on $n \geq 2$ vertices, we have*

$$\mathrm{SJ}(G) \leq \begin{cases} \mathrm{SJ}(K_n), & \text{if } n \leq 5 \\ \mathrm{SJ}(S_n), & \text{if } n \geq 6. \end{cases}$$

Proof. By Theorem 2.1 and (1.1), it suffices to compare

$$\mathrm{SJ}(S_n) = \frac{(n-1)^2}{\sqrt{3n-4}} \qquad \text{and} \qquad \mathrm{SJ}(K_n) = \frac{n^2(n-1)^2}{2(n^2-3n+4)\sqrt{2n-2}}.$$

By a computer one can check that

$$f(x) = \frac{1}{\sqrt{3x-4}} - \frac{x^2}{2(x^2-3x+4)\sqrt{2x-2}}$$

has only two roots on $[2, \infty)$, namely 2 (in which case $S_2 = K_2$) and 5.5543. Since $\mathrm{SJ}(S_5) - \mathrm{SJ}(K_5) < 0$ and $\mathrm{SJ}(S_6) - \mathrm{SJ}(K_6) > 0$, we conclude the result. □

In [10] the authors state a problem of characterizing graphs with the maximum (the minimum) Balaban index among k-connected (k-edge-connected) graphs on n vertices. Although the case of the minumum Balaban index may be hard to solve, Theorems 2.1 and 2.2 yield the following corollary.

Corollary 2.4. *Let G be a graph with the maximum value of Balaban index in the class of k-connected (k-edge-connected) graphs of order n. Then we have:*

(1) if $k = 1$ and, $n = 2$ or $n \geq 8$, then G is the star S_n;

(2) if $k = 1$ and $n \leq 7$, or $k \geq 2$, then G is the complete graph K_n.

Analogously, by Theorems 2.1 and 2.3 we have:

Corollary 2.5. *Let G be a graph with the maximum value of sum-Balaban index in the class of k-connected (k-edge-connected) graphs of order n. Then we have:*

(1) if $k = 1$ and, $n = 2$ or $n \geq 6$, then G is the star S_n;

(2) if $k = 1$ and $n \leq 5$, or $k \geq 2$, then G is the complete graph K_n.

By the proof of Theorem 2.1, $J(K_n) \sim \frac{n}{2}$ while for every tree T we have $J(T) \sim \frac{n^2}{\overline{w}}$, where $\overline{w}$ is the harmonic mean of $\left\{\sqrt{w(u) \cdot w(v)};\ uv \in E(G)\right\}$, i.e.

$$\overline{w} = \frac{m}{\sum\limits_{uv \in E(G)} \frac{1}{\sqrt{w(u) \cdot w(v)}}},$$

(note that $J(G) = \frac{m^2}{(m-n+2)\overline{w}}$). This means that, roughly speaking, if $\overline{w} < 2n$, then $J(T) > J(K_n)$.

Denote by $D^*_{a,b}$ a tree on $a + b$ vertices, one of which has degree a, another has degree b, and all the other vertices have degree 1. Then $D^*_{a,b}$ is the *double star*. Observe that if a tree has diameter 2, then it is a star, while if it has diameter 3, it is a double star.

Theorem 2.6. *Let a and b be positive integers such that $a, b \geq 2$, $a + b = n$ and $n \geq 9$. Then $J(D^*_{a,b}) > J(K_n)$.*

Proof. Consider the double star $D^*_{a,b}$. Let u_2 and u_3 be the vertices of degree a and b, respectively. Moreover, let u_1 (u_4, resp.) be a pendant vertex adjacent to u_2 (u_3, resp.). Since $b = n - a$, we have

$$\begin{aligned}
w(u_1) &= 1 + 2(a-1) + 3(b-1) = 3n - a - 4,\\
w(u_2) &= a + 2(b-1) = 2n - a - 2,\\
w(u_3) &= b + 2(a-1) = n + a - 2,\\
w(u_4) &= 1 + 2(b-1) + 3(a-1) = 2n + a - 4.
\end{aligned}$$

Hence,

$$\begin{aligned}
f(a) &= \sum_{uv \in E(G)} \frac{1}{\sqrt{w(u) \cdot w(v)}}\\
&= \frac{a-1}{\sqrt{(3n-a-4)(2n-a-2)}} + \frac{1}{\sqrt{(2n-a-2)(n+a-2)}}\\
&\quad + \frac{n-a-1}{\sqrt{(n+a-2)(2n+a-4)}},
\end{aligned}$$

and $J(D^*_{a,b}) = (n-1)f(a)$.

In [8], see the text before Theorem 4, it is proved that $f''(x) > 0$, which means that $f(x)$ is a convex function. Since $f(a) = f(n-a)$, $2 \le a \le n-2$, we have

$$J(D^*_{2,n-2}) > J(D^*_{3,n-3}) > \cdots > J(D^*_{\lfloor n/2\rfloor,\lceil n/2\rceil}) \ge (n-1)f(n/2).$$

If $n \ge 70$, then $(n-1)f(n/2) > \frac{n^2(n-1)^2}{2n(n-3)+8} \cdot \frac{1}{n-1} = J(K_n)$, which implies that $J(D^*_{a,b}) > J(K_n)$ in this case. The cases when $n < 70$ were checked using a computer software. □

Theorem 2.6 implies the following.

Corollary 2.7. *For every k there exists n_0 such that for every $n \ge n_0$ the first k graphs of order n with the biggest value of Balaban index are trees.*

Analogous result can be proved for sum-Balaban index:

Theorem 2.8. *Let a and b be positive integers such that $a, b \ge 2$, $a + b = n$ and $n \ge 8$. Then $\mathrm{SJ}(D^*_{a,b}) > \mathrm{SJ}(K_n)$.*

Proof. Using the values w from the proof of Theorem 2.6 we get

$$f(a) = \sum_{uv \in E(G)} \frac{1}{\sqrt{w(u) + w(v)}} = \frac{a-1}{\sqrt{5n-2a-6}} + \frac{1}{\sqrt{3n-4}} + \frac{n-a-1}{\sqrt{3n+2a-6}},$$

and $\mathrm{SJ}(D^*_{a,b}) = (n-1)f(a)$. In [23, Lemma 3.2] it is proved that

$$\mathrm{SJ}(D^*_{2,n-2}) > \mathrm{SJ}(D^*_{3,n-3}) > \cdots > \mathrm{SJ}(D^*_{\lfloor n/2\rfloor,\lceil n/2\rceil}) \ge (n-1)f(n/2).$$

Since $(n-1)f(n/2) > \frac{n^2(n-1)^2}{2(n^2-3n+4)\sqrt{2n-2}} = \mathrm{SJ}(K_n)$ if $n \ge 8$, we have $\mathrm{SJ}(D^*_{a,b}) > \mathrm{SJ}(K_n)$. □

Corollary 2.9. *For every k there exists n_0 such that for every $n \ge n_0$ the first k graphs of order n with the biggest value of sum-Balaban index are trees.*

3 Comparison with Randić index

In the class of trees, the star S_n maximizes the Balaban index [8, 10, 22] and minimizes the Randić index [5]. Hence, for every tree T we have

$$\frac{J(T)}{R(T)} \le \frac{n-1}{\sqrt{2n-3}},$$

with equality if and only if T is the star S_n. This observation was pointed out by Aouchiche et al. [1], who proposed to study an extension of this bound to the class of all connected graphs. Based on their computer experiments for $n \ge 5$ they proposed the conjecture, which turns out to be true (see Theorem 3.1). Namely, by Theorem 2.2, for $n \ge 8$, the star S_n is the graph that maximizes the Balaban index over the class of n-vertex connected graphs, and over this class of graphs S_n also minimizes the Randić index [5, 27]. Using a computer program we have checked that the result holds also for $n \in \{5, 6, 7\}$, however, for $n \in \{3, 4\}$, the quotient $\frac{J(G)}{R(G)}$ attains its maximal value for the complete graph K_n. Thus we can state the following.

Theorem 3.1. *For any connected graph G on $n \geq 2$ vertices, we have*

$$\frac{J(G)}{R(G)} \leq \begin{cases} \frac{n^2-n}{n^2-3n+4}, & \text{if } n \leq 4 \\ \frac{n-1}{\sqrt{2n-3}}, & \text{if } n \geq 5, \end{cases}$$

with equality if and only if $G = K_n$ for $n \leq 4$, and for $n \geq 5$ equality holds precisely for $G = S_n$.

Note that a similar observation can be done for the class of n-vertex connected unicyclic graphs. For this class Gao and Lu [12] proved that S_n^+ (i.e., the graph obtained from the star S_n by adding an edge between two nonadjacent vertices) has the minimum Randić index, but on the other hand it has the maximum Balaban index [7, 24]. In other words,

$$J(G) \leq J(S_n^+) = \frac{n}{2}\left(\frac{1}{2n-4} + \frac{2}{\sqrt{(2n-4)(n-1)}} + \frac{n-3}{\sqrt{(2n-3)(n-1)}}\right),$$

and

$$R(G) \geq R(S_n^+) = \frac{n-3}{\sqrt{n-1}} + \frac{2}{\sqrt{2(n-1)}} + \frac{1}{2},$$

for any connected unicyclic graph on at least 4 vertices. Thus we obtain the following result.

Theorem 3.2. *For any connected unicyclic graph G on $n \geq 4$ vertices, we have*

$$\frac{J(G)}{R(G)} \leq \frac{J(S_n^+)}{R(S_n^+)}$$

with equality if and only if $G = S_n^+$.

4 Accumulation points of sum-Balaban index

In [17] it is shown that for every nonnegative real number r there exists a sequence of graphs $\{G_{r,i}\}_{i=1}^{\infty}$ such that the number of vertices of $G_{r,i}$ tends to infinity as $i \to \infty$ and $\lim_{i\to\infty} J(G_{r,i}) = r$. Here we prove an analogous result for sum-Balaban index.

Let K_a and K'_a be two disjoint complete graphs on a vertices and let P_b be a path on b vertices. The *balanced dumbbell graph* $D_{a,b}$ is obtained from $K_a \cup P_b \cup K'_a$ by joining all vertices of K_a to one end-vertex of P_b and all vertices of K'_a to the other end-vertex of P_b. Thus, $D_{a,b}$ has $2a + b$ vertices. See Figure 1 for $D_{5,5}$.

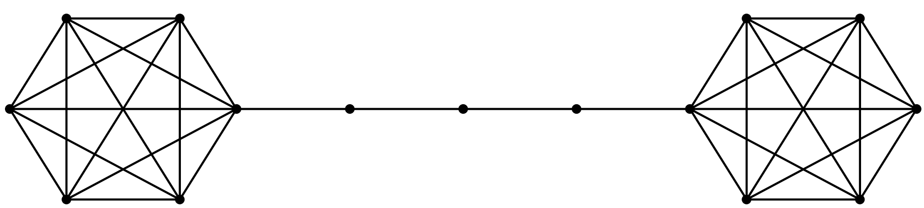

Figure 1: The graph $D_{5,5}$.

Denote $Q = \sqrt{2}\ln(1+\sqrt{2})$. Observe that $Q \doteq 1.24650$ and $1+Q+2\sqrt{Q} \doteq 4.47934$. We have the following statement.

Theorem 4.1. *Let* $r \geq 1 + Q + 2\sqrt{Q}$. *Further, let* $\{D_{a_i,b_i}\}_{i=1}^{\infty}$ *be a sequence of balanced dumbbell graphs on* $n_i = 2a_i + b_i$ *vertices such that* $n_i \to \infty$ *and*

$$\lim_{i\to\infty} \frac{a_i}{\sqrt{n_i}} = \frac{1}{\sqrt{2}}\sqrt{r - 1 - Q + \sqrt{(r-1-Q)^2 - 4Q}}.$$

Then $\lim_{i\to\infty} \mathrm{SJ}(D_{a_i,b_i}) = r$.

Proof. First observe that if $r \geq 1 + Q + 2\sqrt{Q}$ then $(r-1-Q)^2 - 4Q \geq 0$, and so $(1/\sqrt{2})\sqrt{r - 1 + Q + \sqrt{(r-1-Q)^2 - 4Q}}$ is a real number.

In [14, Equation (9)] it is proved that if $a \sim c\sqrt{n}$ for a (real) constant c, then for a balanced dumbbell graph $D_{a,b}$ on n vertices it holds

$$\mathrm{SJ}(D_{a,b}) \sim c^2 + 1 + Q + \frac{Q}{c^2}.$$

Hence, for $c = \frac{1}{\sqrt{2}}\sqrt{r - 1 - Q + \sqrt{(r-1-Q)^2 - 4Q}}$ we get

$$\begin{aligned}
\mathrm{SJ}(D_{a,b}) &\sim \frac{1}{2}\Big(r - 1 - Q + \sqrt{(r-1-Q)^2 - 4Q}\Big) + 1 + Q \\
&\qquad\qquad + \frac{2Q}{r - 1 - Q + \sqrt{(r-1-Q)^2 - 4Q}} \\
&= \frac{1}{2}\Big(r + \sqrt{(r-1-Q)^2 - 4Q} + 1 + Q \\
&\qquad\qquad + \frac{4Q}{r + \sqrt{(r-1-Q)^2 - 4Q} - 1 - Q}\Big) \\
&= \frac{1}{2} \cdot \frac{2r^2 + 2r\sqrt{(r-1-Q)^2 - 4Q} - 2r - 2rQ}{r + \sqrt{(r-1-Q)^2 - 4Q} - 1 - Q} = r.
\end{aligned}$$ □

Although we have a conjecture that for graphs G on large number of vertices

$$\mathrm{SJ}(G) \geq 1 + Q + 2\sqrt{Q}$$

(see Corollary 8 and Conjecture 9 in [14]), it is proved only that

$$\mathrm{SJ}(G) \geq 4 + o(1)$$

(see Theorem 2 in [14]). Hence, if our conjecture is false, then the problem of accumulation points of sum-Balaban index for values in interval $[4, 4.47934)$ remains open.

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On the Terwilliger algebra of a certain family of bipartite distance-regular graphs with $\Delta_2 = 0$

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Abstract

Let Γ denote a bipartite distance-regular graph with diameter $D \geq 4$ and valency $k \geq 3$. Let X denote the vertex set of Γ, and let A_i $(0 \leq i \leq D)$ denote the distance matrices of Γ. We abbreviate $A := A_1$. For $x \in X$ and for $0 \leq i \leq D$, let $\Gamma_i(x)$ denote the set of vertices in X that are distance i from vertex x.

Fix $x \in X$ and let $T = T(x)$ denote the subalgebra of $\mathrm{Mat}_X(\mathbb{C})$ generated by $A, E_0^*, E_1^*, \dots, E_D^*$, where for $0 \leq i \leq D$, E_i^* represents the projection onto the ith subconstituent of Γ with respect to x. We refer to T as the *Terwilliger algebra* of Γ with respect to x. By the *endpoint* of an irreducible T-module W we mean $\min\{i \mid E_i^* W \neq 0\}$.

In this paper we assume Γ has the property that for $2 \leq i \leq D-1$, there exist complex scalars α_i, β_i such that for all $y, z \in X$ with $\partial(x,y) = 2$, $\partial(x,z) = i$, $\partial(y,z) = i$, we have $\alpha_i + \beta_i |\Gamma_1(x) \cap \Gamma_1(y) \cap \Gamma_{i-1}(z)| = |\Gamma_{i-1}(x) \cap \Gamma_{i-1}(y) \cap \Gamma_1(z)|$.

We study the structure of irreducible T-modules of endpoint 2. Let W denote an irreducible T-module with endpoint 2, and let v denote a nonzero vector in $E_2^* W$. We show that $W = \mathrm{span}\big(\{E_i^* A_{i-2} E_2^* v \mid 2 \leq i \leq D\} \cup \{E_i^* A_{i+2} E_2^* v \mid 2 \leq i \leq D-2\}\big)$.

It turns out that, except for a particular family of bipartite distance-regular graphs with $D = 5$, this result is already known in the literature. Assume now that Γ is a member of this particular family of graphs. We show that if Γ is not almost 2-homogeneous, then up to isomorphism there exists exactly one irreducible T-module with endpoint 2 and it is not thin. We give a basis for this T-module.

Keywords: Distance-regular graphs, Terwilliger algebra, irreducible modules.

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1 Introduction

Throughout this introduction let Γ denote a bipartite distance-regular graph with diameter $D \geq 4$, valency $k \geq 3$ and path-length function ∂. Let X denote the vertex set of Γ. For $x \in X$ and $0 \leq i \leq D$, let $\Gamma_i(x)$ denote the set of vertices in X that are distance i from vertex x, and let $T = T(x)$ denote the Terwilliger algebra of Γ with respect to x (see Section 2 for formal definitions).

It is known that there exists a unique irreducible T-module with endpoint 0, and this module is thin [8, Proposition 8.4]. Moreover, Curtin showed that up to isomorphism Γ has exactly one irreducible T-module with endpoint 1, and this module is thin [4, Corollary 7.7].

We now discuss the irreducible T-modules of endpoint 2. It turns out that the structure of these modules is particularly nice if we assume that Γ has the following combinatorial property: for $2 \leq i \leq D-1$, there exist complex scalars α_i, β_i such that for all $y, z \in X$ with $\partial(x,y) = 2$, $\partial(x,z) = i$, $\partial(y,z) = i$, we have

$$\alpha_i + \beta_i |\Gamma_1(x) \cap \Gamma_1(y) \cap \Gamma_{i-1}(z)| = |\Gamma_{i-1}(x) \cap \Gamma_{i-1}(y) \cap \Gamma_1(z)|.$$

Irreducible modules of endpoint 2 of these graphs were studied extensively, see [10, 11, 12, 13, 15]. We are motivated by the fact that the above equation holds if Γ is Q-polynomial.

Assume that Γ has the above mentioned combinatorial property. We show that if W is an irreducible T-module with endpoint 2 and v is a nonzero vector in $E_2^* W$, then

$$W = \operatorname{span}\big(\{E_i^* A_{i-2} E_2^* v \mid 2 \leq i \leq D\} \cup \{E_i^* A_{i+2} E_2^* v \mid 2 \leq i \leq D-2\}\big).$$

Except for a particular family of bipartite distance-regular graphs with $D = 5$, this result is already known in the literature. To define this particular family we introduce a certain parameter Δ_2 in terms of the intersection numbers of Γ by $\Delta_2 = (k-2)(c_3-1) - (c_2-1)p^2_{22}$. It turns out that $\Delta_2 \geq 0$ and that $\Delta_2 = 0$ implies $c_2 \in \{1,2\}$ or $D \leq 5$. The above mentioned family of bipartite distance-regular graphs with $D = 5$ is exactly the family of such graphs with $\Delta_2 = 0$. Assume now that Γ is such a graph. We show that if Γ is not almost 2-homogeneous, then up to isomorphism there exists exactly one irreducible T-module with endpoint 2, and this module is not thin. We give a basis for this T-module. If Γ is almost 2-homogeneous, then the structure of irreducible T-modules with endpoint 2 is described in [7].

2 Preliminaries

In this section we review some definitions and basic results concerning distance-regular graphs. See the book of A. E. Brouwer, A. M. Cohen and A. Neumaier [2] for more background information.

Let $\mathbb{C}$ denote the complex number field and let X denote a nonempty finite set. Let $\mathrm{Mat}_X(\mathbb{C})$ denote the $\mathbb{C}$-algebra consisting of all matrices whose rows and columns are indexed by X and whose entries are in $\mathbb{C}$. Let $V = \mathbb{C}^X$ denote the vector space over $\mathbb{C}$ consisting of column vectors whose coordinates are indexed by X and whose entries are in $\mathbb{C}$. We observe $\mathrm{Mat}_X(\mathbb{C})$ acts on V by left multiplication. We call V the *standard module*. We endow V with the Hermitean inner product $\langle \, , \, \rangle$ that satisfies $\langle u, v\rangle = u^t \overline{v}$ for $u, v \in V$, where t denotes transpose and $^-$ denotes complex conjugation. Recall that

$$\langle u, Bv\rangle = \langle \overline{B}^t u, v\rangle \tag{2.1}$$

for $u, v \in V$ and $B \in \mathrm{Mat}_X(\mathbb{C})$. For $y \in X$ let $\hat{y}$ denote the element of V with a 1 in the y coordinate and 0 in all other coordinates. Note that

$$\{\hat{y} \mid y \in X\} \text{ is an orthonormal basis for } V.$$

Let $\Gamma = (X, \mathcal{R})$ denote a finite, undirected, connected graph, without loops or multiple edges, with vertex set X and edge set $\mathcal{R}$. Let ∂ denote the path-length distance function for Γ, and set $D := \max\{\partial(x,y) \mid x, y \in X\}$. We call D the *diameter* of Γ. For a vertex $x \in X$ and an integer i let $\Gamma_i(x)$ denote the set of vertices at distance i from x. For an integer $k \geq 0$ we say Γ is *regular with valency* k whenever $|\Gamma_1(x)| = k$ for all $x \in X$. We say Γ is *distance-regular* whenever for all integers h, i, j $(0 \leq h, i, j \leq D)$ and for all vertices $x, y \in X$ with $\partial(x, y) = h$, the number

$$p^h_{ij} = |\Gamma_i(x) \cap \Gamma_j(y)|$$

is independent of x and y. The p^h_{ij} are called the *intersection numbers* of Γ.

For the rest of this paper we assume Γ is distance-regular with diameter $D \geq 4$. Note that $p^h_{ij} = p^h_{ji}$ for $0 \leq h, i, j \leq D$. For convenience set $c_i := p^i_{1,i-1}$ $(1 \leq i \leq D)$, $a_i := p^i_{1i}$ $(0 \leq i \leq D)$, $b_i := p^i_{1,i+1}$ $(0 \leq i \leq D-1)$, $k_i := p^0_{ii}$ $(0 \leq i \leq D)$, and $c_0 = b_D = 0$. By the triangle inequality the following hold for $0 \leq h, i, j \leq D$: (i) $p^h_{ij} = 0$ if one of h, i, j is greater than the sum of the other two; (ii) $p^h_{ij} \neq 0$ if one of h, i, j equals the sum of the other two. In particular $c_i \neq 0$ for $1 \leq i \leq D$ and $b_i \neq 0$ for $0 \leq i \leq D-1$. We observe that Γ is regular with valency $k = k_1 = b_0$ and that

$$c_i + a_i + b_i = k \qquad (0 \leq i \leq D). \tag{2.2}$$

Note that $k_i = |\Gamma_i(x)|$ for $x \in X$ and $0 \leq i \leq D$. By [2, p. 127],

$$k_i = \frac{b_0 b_1 \cdots b_{i-1}}{c_1 c_2 \cdots c_i} \qquad (1 \leq i \leq D). \tag{2.3}$$

Recall Γ is *bipartite* whenever $a_i = 0$ for $0 \leq i \leq D$. Setting $a_i = 0$ in (2.2) we find

$$b_i + c_i = k \quad (0 \leq i \leq D). \tag{2.4}$$

The following formulae for the bipartite case will be useful.

Lemma 2.1 ([2, Lemma 4.1.7]). *Let Γ denote a bipartite distance-regular graph with diameter $D \geq 4$ and valency $k \geq 3$. Then*

$$p^i_{2i} = \frac{c_i(b_{i-1} - 1) + b_i(c_{i+1} - 1)}{c_2} \quad (1 \leq i \leq D-1), \qquad p^D_{2D} = \frac{k(b_{D-1} - 1)}{c_2}.$$

We recall the Bose-Mesner algebra of Γ. For $0 \leq i \leq D$ let A_i denote the matrix in $\mathrm{Mat}_X(\mathbb{C})$ with (x, y)-entry

$$(A_i)_{xy} = \begin{cases} 1 & \text{if } \partial(x,y) = i, \\ 0 & \text{if } \partial(x,y) \neq i \end{cases} \qquad (x, y \in X). \tag{2.5}$$

For notational convenience, we define A_i to be the zero matrix for all integers $i < 0$ or $i > D$. We call A_i the ith *distance matrix* of Γ. We abbreviate $A := A_1$ and call this the *adjacency matrix* of Γ. We observe (i) $A_0 = I$; (ii) $\sum_{i=0}^{D} A_i = J$; (iii) $\overline{A_i} = A_i$ $(0 \leq i \leq D)$; (iv) $A_i^t = A_i$ $(0 \leq i \leq D)$; (v) $A_i A_j = \sum_{h=0}^{D} p^h_{ij} A_h$ $(0 \leq i, j \leq D)$, where I (resp. J) denotes the identity matrix (resp. all 1's matrix) in $\mathrm{Mat}_X(\mathbb{C})$. Using these facts we find $A_0, A_1, \ldots, A_D$ is a basis for a commutative subalgebra M of $\mathrm{Mat}_X(\mathbb{C})$. We call M the *Bose-Mesner algebra* of Γ. It turns out that A generates M [1, p. 190].

3 Terwilliger algebra

Let Γ denote a distance-regular with diameter $D \geq 4$ and valency $k \geq 3$. We first recall the dual idempotents of Γ. To do this fix a vertex $x \in X$. We view x as a "base vertex". For $0 \leq i \leq D$ let $E_i^* = E_i^*(x)$ denote the diagonal matrix in $\mathrm{Mat}_X(\mathbb{C})$ with (y, y)-entry

$$(E_i^*)_{yy} = \begin{cases} 1 & \text{if } \partial(x,y) = i, \\ 0 & \text{if } \partial(x,y) \neq i \end{cases} \qquad (y \in X).$$

We call E_i^* the ith *dual idempotent* of Γ with respect to x [16, p. 378]. We observe (ei) $\sum_{i=0}^{D} E_i^* = I$; (eii) $\overline{E_i^*} = E_i^*$ $(0 \leq i \leq D)$; (eiii) $E_i^{*t} = E_i^*$ $(0 \leq i \leq D)$; (eiv) $E_i^* E_j^* = \delta_{ij} E_i^*$ $(0 \leq i, j \leq D)$. By these facts $E_0^*, E_1^*, \ldots, E_D^*$ form a basis for a commutative subalgebra $M^* = M^*(x)$ of $\mathrm{Mat}_X(\mathbb{C})$. We call M^* the *dual Bose-Mesner algebra* of Γ with respect to x [16, p. 378]. For $0 \leq i \leq D$ we have

$$E_i^* V = \mathrm{span}\{\widehat{y} \mid y \in X,\ \partial(x,y) = i\},$$

so $\dim E_i^* V = k_i$. We call $E_i^* V$ the ith *subconstituent of* Γ with respect to x. Note that

$$V = E_0^* V + E_1^* V + \cdots + E_D^* V \qquad \text{(orthogonal direct sum)}. \tag{3.1}$$

Moreover E_i^* is the projection from V onto $E_i^* V$ for $0 \leq i \leq D$.

We now recall the Terwilliger algebra of Γ. Let $T = T(x)$ denote the subalgebra of $\mathrm{Mat}_X(\mathbb{C})$ generated by M, M^*. We call T the *Terwilliger algebra of* Γ with respect to x [16, Definition 3.3]. Recall M is generated by A, so T is generated by A and the dual idempotents. We observe T has finite dimension. By construction T is closed under the conjugate-transpose map so T is semisimple [16, Lemma 3.4(i)].

By a *T-module* we mean a subspace W of V such that $BW \subseteq W$ for all $B \in T$. Let W denote a T-module. Then W is said to be *irreducible* whenever W is nonzero and W contains no T-modules other than 0 and W.

By [9, Corollary 6.2] any T-module is an orthogonal direct sum of irreducible T-modules. In particular the standard module V is an orthogonal direct sum of irreducible T-modules. Let W, W' denote T-modules. By an *isomorphism of T-modules* from W to W' we mean an isomorphism of vector spaces $\sigma : W \to W'$ such that $(\sigma B - B\sigma)W = 0$ for all $B \in T$. The T-modules W, W' are said to be *isomorphic* whenever there exists an isomorphism of T-modules from W to W'. By [4, Lemma 3.3] any two nonisomorphic irreducible T-modules are orthogonal. Let W denote an irreducible T-module. By [16, Lemma 3.4(iii)] W is an orthogonal direct sum of the nonvanishing spaces among $E_0^* W, E_1^* W, \ldots, E_D^* W$. By the *endpoint* of W we mean $\min\{i \mid 0 \leq i \leq D,\ E_i^* W \neq 0\}$. By the *diameter* of W we mean $|\{i \mid 0 \leq i \leq D,\ E_i^* W \neq 0\}| - 1$. We say W is *thin* whenever the dimension of $E_i^* W$ is at most 1 for $0 \leq i \leq D$.

The following matrices of $\mathrm{Mat}_X(\mathbb{C})$ will be useful later in the paper.

Definition 3.1. Let Γ denote a distance-regular with diameter $D \geq 4$ and valency $k \geq 3$. Fix $x \in X$ and let $E_i^* = E_i^*(x)$ $(0 \leq i \leq D)$ and $T = T(x)$. We define matrices $L = L(x)$, $R = R(x)$ by

$$L = \sum_{h=1}^{D} E_{h-1}^* A E_h^*, \qquad R = \sum_{h=0}^{D-1} E_{h+1}^* A E_h^*.$$

Note that $A = L+R$ [4, Lemma 4.4] and $L^t = R$. We call L and R the *lowering matrix* and the *raising matrix of* Γ with respect to x, respectively. Observe that L and R are contained in T.

Definition 3.2 ([7, Definition 3.2]). Let Γ denote a distance-regular with diameter $D \geq 4$ and valency $k \geq 3$. Fix $x \in X$. For $1 \leq i \leq D$ we define matrices $\Lambda_i = \Lambda_i(x)$ in $\mathrm{Mat}_X(\mathbb{C})$ by

$$(\Lambda_i)_{zy} = \begin{cases} |\Gamma_1(x) \cap \Gamma_1(y) \cap \Gamma_{i-1}(z)|, & \text{if } \partial(x,y) = 2, \partial(x,z) = \partial(y,z) = i, \\ 0, & \text{otherwise} \end{cases}$$

for $z, y \in X$.

4 The scalars Δ_i and γ_i

Let Γ denote a distance-regular graph with diameter $D \geq 4$ and valency $k \geq 3$. From now on we assume that Γ is bipartite. In this section we introduce certain scalars Δ_i and γ_i $(2 \leq i \leq D-1)$ which we find useful.

Definition 4.1. Let Γ denote a distance-regular with diameter $D \geq 4$ and valency $k \geq 3$. Then for $2 \leq i \leq D-1$ we define

$$\Delta_i = (b_{i-1} - 1)(c_{i+1} - 1) - (c_2 - 1)p^i_{2i}$$

and

$$\gamma_i = \frac{c_i(b_{i-1} - 1)}{p^i_{2i}}$$

(observe that $p^i_{2i} > 0$ by [3, Lemma 11]).

By [3, Theorem 12] we have $\Delta_i \geq 0$ for $2 \leq i \leq D-1$. Moreover, the scalars Δ_i and γ_i are related as follows.

Lemma 4.2 ([3, Theorem 13]). *Let* Γ *denote a distance-regular with diameter* $D \geq 4$ *and valency* $k \geq 3$ *and fix an integer* $2 \leq i \leq D-1$. *Then the following* (i),(ii) *are equivalent.*

(i) $\Delta_i = 0$.

(ii) *For all* $x, y, z \in X$ *with* $\partial(x,y) = 2$, $\partial(x,z) = i$, $\partial(y,z) = i$,

$$|\Gamma_1(x) \cap \Gamma_1(y) \cap \Gamma_{i-1}(z)| = \gamma_i.$$

If $\Delta_i = 0$ for $2 \leq i \leq D-2$, then Γ is called *almost* 2*-homogeneous*, see [7]. In this case the structure of irreducible T-modules is well understood, so we will assume that Γ is not almost 2-homogeneous. In the rest of the paper we therefore consider the following situation.

Notation 4.3. Let $\Gamma = (X, \mathcal{R})$ denote a bipartite distance-regular graph with diameter $D \geq 4$, valency $k \geq 3$ and intersection numbers b_i, c_i, which is not almost 2-homogeneous. Let A_i $(0 \leq i \leq D)$ be the distance matrices of Γ, and let V denote the standard module for Γ. We fix $x \in X$ and let $E^*_i = E^*_i(x)$ $(0 \leq i \leq D)$ and $T = T(x)$ denote the dual idempotents and the Terwilliger algebra of Γ with respect to x, respectively. We assume that for $2 \leq i \leq D-1$, there exist complex scalars α_i, β_i such that for all $y, z \in X$ with $\partial(x, y) = 2$, $\partial(x, z) = i$, $\partial(y, z) = i$, we have

$$\alpha_i + \beta_i |\Gamma_1(x) \cap \Gamma_1(y) \cap \Gamma_{i-1}(z)| = |\Gamma_{i-1}(x) \cap \Gamma_{i-1}(y) \cap \Gamma_1(z)|.$$

Let matrices $L = L(x)$, $R = R(x)$ and $\Lambda_i = \Lambda_i(x)$ $(1 \leq i \leq D)$ be as in Definitions 3.1 and 3.2. Let scalars Δ_i, γ_i $(2 \leq i \leq D-1)$ be as in Definition 4.1.

With reference to Notation 4.3, pick $2 \leq i \leq D-1$ and assume that $\Delta_i \neq 0$. By [12, Theorem 5.4] scalars α_i and β_i are uniquely determined and given by

$$\begin{aligned} \alpha_i &= \frac{c_i(c_i-1)(b_{i-1}-c_2) - c_i c_{i-1}(b_i-1)(c_2-1)}{c_2 \Delta_i}, \\ \beta_i &= \frac{c_i(c_{i+1}-c_i)(b_{i-1}-1) - b_i(c_{i+1}-1)(c_i-c_{i-1})}{c_2 \Delta_i}. \end{aligned} \tag{4.1}$$

If $\Delta_i = 0$, then scalars α_i and β_i are not uniquely determined. For example, if $\Delta_2 = 0$, then one of the possible values for α_2 and β_2 is $\alpha_2 = 0$, $\beta_2 = 1$. Note however that by Lemma 4.2 this is not the only possible solution.

5 Some products in T

With reference to Notation 4.3, in this section we compute some products of matrices of T. We start by recalling the following results.

Lemma 5.1 ([14, Lemma 6.1]). *With reference to Notation 4.3, for $0 \leq h, i, j \leq D$ and $y, z \in X$ the (y, z)-entry of $E^*_h A_i E^*_j$ is 1 if $\partial(x, y) = h$, $\partial(y, z) = i$, $\partial(x, z) = j$, and 0 otherwise.*

Lemma 5.2 ([14, Lemma 6.5]). *With reference to Notation 4.3, for $0 \leq h, i, j, r, s \leq D$ and $y, z \in X$ the (y, z)-entry of $E^*_h A_r E^*_i A_s E^*_j$ is $|\Gamma_i(x) \cap \Gamma_r(y) \cap \Gamma_s(z)|$ if $\partial(x, y) = h$, $\partial(x, z) = j$, and 0 otherwise.*

Lemma 5.3 ([7, Lemma 3.3]). *With reference to Notation 4.3, we have*

$$\Lambda_1 = E^*_1 A E^*_2, \qquad \Lambda_i = E^*_i A_{i-1} E^*_1 A E^*_2 - c_2 E^*_i A_{i-2} E^*_2 \qquad (2 \leq i \leq D).$$

In particular, $\Lambda_i \in T$ $(1 \leq i \leq D)$.

Theorem 5.4. *With reference to Notation 4.3 the following holds for $3 \leq i \leq D$:*

$$L E^*_i A_{i-2} E^*_2 = b_{i-1} E^*_{i-1} A_{i-3} E^*_2 + (c_{i-1} - \alpha_{i-1}) E^*_{i-1} A_{i-1} E^*_2 - \beta_{i-1} \Lambda_{i-1}. \tag{5.1}$$

Proof. Pick $z, y \in X$ and an integer $3 \leq i \leq D$. We show that (z, y)-entries of both sides of (5.1) agree. Note that by the property (eiv) of Section 3 and Lemma 5.2,

$$(L E^*_i A_{i-2} E^*_2)_{zy} = \begin{cases} |\Gamma_i(x) \cap \Gamma_{i-2}(y) \cap \Gamma_1(z)| & \text{if } \partial(x, y) = 2, \partial(x, z) = i-1, \\ 0 & \text{otherwise.} \end{cases} \tag{5.2}$$

It follows from (5.2), Lemma 5.1 and Definition 3.2 that the (z, y)-entries of both sides of (5.1) are 0 if $\partial(x, y) \neq 2$ or $\partial(x, z) \neq i-1$. Assume now $\partial(x, y) = 2$ and $\partial(x, z) = i-1$.

Observe that by the triangle inequality we have that $\partial(z, y) \in \{i-3, i-1, i+1\}$. We consider each of these three cases separately.

Case 1: $\partial(x, y) = 2$, $\partial(x, z) = i-1$ and $\partial(z, y) = i-3$. Note that in this case we have $(LE_i^* A_{i-2} E_2^*)_{zy} = b_{i-1}$ by (5.2). By Lemma 5.1 and Definition 3.2 the (z, y)-entries of both sides of (5.1) agree.

Case 2: $\partial(x, y) = 2$, $\partial(x, z) = i-1$ and $\partial(z, y) = i-1$. Observe that by (5.2) we have

$$\begin{aligned}(LE_i^* A_{i-2} E_2^*)_{zy} &= c_{i-1} - |\Gamma_1(z) \cap \Gamma_{i-2}(x) \cap \Gamma_{i-2}(y)| \\ &= c_{i-1} - (\alpha_{i-1} + \beta_{i-1}|\Gamma_{i-2}(z) \cap \Gamma_1(x) \cap \Gamma_1(y)|).\end{aligned}$$

By Lemma 5.1 and Definition 3.2 the (z, y)-entries of both sides of (5.1) agree.

Case 3: $\partial(x, y) = 2$, $\partial(x, z) = i-1$ and $\partial(z, y) = i+1$. By (5.2), Lemma 5.1 and Definition 3.2 the (z, y)-entries of both sides of (5.1) are 0. □

6 Irreducible T-modules with endpoint 2

With reference to Notation 4.3, let W denote an irreducible T-module with endpoint 2. In this section we find a spanning set for W.

Definition 6.1. With reference to Notation 4.3, let W denote an irreducible T-module with endpoint 2 and let v denote a nonzero vector in $E_2^* W$. For $0 \le i \le D$, define

$$v_i^+ = E_i^* A_{i-2} E_2^* v, \qquad v_i^- = E_i^* A_{i+2} E_2^* v.$$

Note that $v_2^+ = v$, $v_i^+ = 0$ if $i < 2$, and $v_i^- = 0$ if $i < 2$ or $i > D-2$.

Lemma 6.2 ([5, Corollary 9.3(i), Theorem 9.4]). *With reference to Definition 6.1, the following* (i)–(iv) *hold.*

(i) $E_i^* A_i E_2^* v = -(v_i^+ + v_i^-)$ $(2 \le i \le D)$.

(ii) $Rv_i^+ = c_{i-1} v_{i+1}^+$ $(2 \le i \le D-1)$ *and* $Rv_D^+ = 0$.

(iii) $Lv_i^- = b_{i+1} v_{i-1}^-$ $(2 \le i \le D-2)$.

(iv) $Lv_{i+1}^+ - Rv_{i-1}^- = b_i v_i^+ - c_i v_i^-$ $(1 \le i \le D-1)$.

Lemma 6.3. *With reference to Definition 6.1, the following* (i)–(iii) *hold.*

(i) $\Lambda_i v = -c_2 v_i^+$ $(2 \le i \le D)$.

(ii) $Lv_2^+ = 0$ *and*

$$Lv_i^+ = (b_{i-1} - c_{i-1} + \alpha_{i-1} + c_2\beta_{i-1}) v_{i-1}^+ - (c_{i-1} - \alpha_{i-1}) v_{i-1}^-$$

for $3 \le i \le D$.

(iii)

$$Rv_i^- = (c_2\beta_{i+1} - c_{i+1} + \alpha_{i+1}) v_{i+1}^+ + \alpha_{i+1} v_{i+1}^-$$

for $2 \le i \le D-2$.

Proof. (i) Immediate from Lemma 5.3 and Definition 6.1.

(ii) Note that $Lv_2^+ = 0$ as the endpoint of W is 2. To obtain the result for Lv_i^+ $(3 \le i \le D)$ apply (5.1) to v and use Definition 6.1, Lemma 6.2(i) and (i) above.

(iii) Immediately by (ii) above and Lemma 6.2(iv). □

Theorem 6.4. *With reference to Definition 6.1,*

$$W = \operatorname{span}\{v_2^+, v_3^+, \dots, v_D^+, v_2^-, v_3^-, \dots, v_{D-2}^-\}.$$

Proof. Denote $W' = \operatorname{span}\{v_2^+, v_3^+, \dots, v_D^+, v_2^-, v_3^-, \dots, v_{D-2}^-\}$ and note that $W' \subseteq W$. We now show that $W = W'$. Note that $E_i^* v_j^+ = \delta_{ij} v_j^+$ for $2 \leq j \leq D$ and $E_i^* v_j^- = \delta_{ij} v_j^-$ for $2 \leq j \leq D-2$. Therefore, W' is invariant under the action of E_i^* for $0 \leq i \leq D$. Observe also that W' is invariant under the action of L by Lemma 6.2(iii) and Lemma 6.3(ii), and also invariant under the action of R by Lemma 6.2(ii) and Lemma 6.3(iii). As $A = R + L$, W' is invariant under the action of A. As T is generated by A and E_i^* $(0 \leq i \leq D)$, this implies that W' is a T-module. Recall that W is irreducible and that W' contains a nonzero vector v. It follows that $W = W'$. □

Corollary 6.5. *With reference to Definition 6.1, we have*

$$\dim\left(E_{D-1}^* W\right) \leq 1, \qquad \dim\left(E_D^* W\right) \leq 1.$$

Proof. Immediately from Theorem 6.4. □

As already mentioned, the result from Theorem 6.4 is already known in the literature, except for the case $D = 5$ and $\Delta_2 = 0$, see [11, 12, 15]. In the rest of the paper we study this case in detail. If $D = 5$ and $\Delta_2 = \Delta_3 = 0$, then Γ is almost 2-homogeneous, contradicting our assumption in Notation 4.3. Therefore, we have that $\Delta_3 \neq 0$.

7 Case $\Delta_2 = 0$ and $\Delta_3 \neq 0$

With reference to Notation 4.3, in this section we study graphs with $\Delta_2 = 0$ and $\Delta_3 \neq 0$. We first have the following observation.

Lemma 7.1. *With reference to Definition 6.1, assume that $\Delta_2 = 0$ and $\Delta_3 \neq 0$. Then the following* (i), (ii) *hold.*

(i)
$$c_3 = \frac{(c_2^2 - c_2 + 1)k - c_2(c_2 + 1)}{k + c_2^2 - 3c_2}.$$

(ii)
$$\alpha_3 = 0, \qquad \beta_3 = \frac{c_2(k-2)}{k + c_2^2 - 3c_2}.$$

Proof. (i) Solve $\Delta_2 = 0$ for c_3. Note that $k + c_2^2 - 3c_2 = (c_2 - 1)(c_2 - 2) + k - 2 > 0$ as $k \geq 3$.

(ii) Use Definition 4.1, (4.1) and (i) above. □

Lemma 7.2. *With reference to Definition 6.1, assume that $\Delta_2 = 0$ and $\Delta_3 \neq 0$. Then*

$$E_2^* A_2 E_2^* v = -\frac{c_2(k-2)}{k + c_2^2 - 3c_2} v.$$

Proof. Let $\Gamma_2^2 = \Gamma_2^2(x)$ denote the graph with vertex set $\widetilde{X} = \Gamma_2(x)$ and edge set $\widetilde{R} = \{yz \,|\, y, z \in \widetilde{X}, \partial(y, z) = 2\}$. The graph Γ_2^2 has exactly k_2 vertices and it is regular with valency p^2_{22} ([6, Lemma 3.2]). Let $\widetilde{A}$ denote the adjacency matrix of Γ_2^2. The matrix $\widetilde{A}$ is symmetric with real entries. Therefore $\widetilde{A}$ is diagonalizable with all eigenvalues real. Note that eigenvalues for $E_2^* A_2 E_2^*$ and $\widetilde{A}$ are the same.

Since $\Delta_2 = 0$, we know $E_2^* A_2 E_2^*$ has exactly one distinct eigenvalue η on $E_2^* W$ by [6, Theorem 4.11, Corollary 4.13, Lemma 5.3]. Thus, every nonzero vector in $E_2^* W$ is an eigenvector for $E_2^* A_2 E_2^*$ with eigenvalue η. By [6, Lemmas 5.4, 5.5] we find $\eta = -\frac{c_2}{\gamma_2}$. The result now follows from Definition 4.1 and Lemma 7.1(i). □

Corollary 7.3. *With reference to Definition 6.1, assume that $\Delta_2 = 0$ and $\Delta_3 \neq 0$. Then*

$$v_2^- = \frac{b_2(c_2 - 1)}{k + c_2^2 - 3c_2} v_2^+.$$

Proof. By Lemma 6.2(i) and Lemma 7.2 we have

$$-v_2^+ - v_2^- = E_2^* A_2 E_2^* v = -\frac{c_2(k-2)}{k + c_2^2 - 3c_2} v_2^+.$$

The result follows. □

Corollary 7.4. *With reference to Definition 6.1, assume that $D = 5$, $\Delta_2 = 0$ and $\Delta_3 \neq 0$. Then*

$$W = \mathrm{span}\{v_2^+, v_3^+, v_4^+, v_5^+, v_3^-\}. \tag{7.1}$$

Proof. Immediately from Theorem 6.4 and Corollary 7.3. □

Observe that by (3.1) vectors $v_2^+, v_3^+, v_4^+, v_5^+$ are linearly independent, provided they are non-zero.

8 Some scalar products

With reference to Definition 6.1, assume that $D = 5$, $\Delta_2 = 0$ and $\Delta_3 \neq 0$. Our goal for the rest of this paper is to find a basis for W. In this section we compute the norms of vectors $v_3^+, v_4^+, v_5^+, v_3^-$ in terms of the intersection numbers of Γ and $\|v\|$. Note that by [10, Lemma 6.4] we have $\Delta_4 \neq 0$ as well. The assumptions of [10, Lemma 6.4] are somehow different from assumptions of Notation 4.3. However, the proof of [10, Lemma 6.4] works just fine also under assumptions of Notation 4.3.

Lemma 8.1. *With reference to Definition 6.1, assume that $\Delta_2 = 0$ and $\Delta_3 \neq 0$. Then*

$$\|v_3^+\|^2 = \frac{b_2(b_2 - c_2)}{k + c_2^2 - 3c_2} \|v\|^2.$$

In particular, if $D \geq 5$ then $v_3^+ \neq 0$.

Proof. By Lemma 6.2(ii), (2.1) and Definition 3.1 we have

$$\|v_3^+\|^2 = \langle v_3^+, v_3^+ \rangle = \langle R v_2^+, v_3^+ \rangle = \langle v_2^+, L v_3^+ \rangle.$$

The result now follows from Lemma 6.3(ii), Corollary 7.3 and since $\alpha_2 = 0$, $\beta_2 = 1$. Now assume that $v_3^+ = 0$. Observe that this implies $b_2 = c_2$. If $D \geq 5$ then by [2, Proposition 4.1.6](i),(ii) we have $c_2 \leq c_3 \leq b_2$, and so $c_2 = c_3$. But then $c_2 = 1$ by Lemma 7.1(i), and so $k = b_2 + c_2 = 2$, a contradiction. □

Lemma 8.2. *With reference to Definition 6.1, assume that* $\Delta_2 = 0$ *and* $\Delta_3 \neq 0$. *Then*

$$\langle v_3^+, v_3^- \rangle = \frac{b_2 b_4 (c_2 - 1)}{k + c_2^2 - 3c_2} \|v\|^2.$$

Proof. By Lemma 6.2(ii), (2.1) and Definition 3.1 we have

$$\langle v_3^+, v_3^- \rangle = \langle R v_2^+, v_3^- \rangle = \langle v_2^+, L v_3^- \rangle.$$

The result now follows from Lemma 6.2(iii) and Corollary 7.3. □

Lemma 8.3. *With reference to Definition 6.1, assume that* $D = 5$, $\Delta_2 = 0$ *and* $\Delta_3 \neq 0$. *Then*

$$\|v_4^+\|^2 = \frac{b_2((b_3 - 1)b_2 - c_3(c_2 - 1)b_4)}{c_2(k + c_2^2 - 3c_2)} \|v\|^2.$$

In particular, $v_4^+ = 0$ *if and only if* $c_2 \neq 1$ *and* $b_4 = b_2(b_3 - 1)/(c_3(c_2 - 1))$.

Proof. By Lemma 6.2(ii), (2.1) and Definition 3.1 we have

$$\langle v_4^+, v_4^+ \rangle = \frac{1}{c_2} \langle R v_3^+, v_4^+ \rangle = \frac{1}{c_2} \langle v_3^+, L v_4^+ \rangle.$$

The formula for $\|v_4^+\|^2$ now follows from Lemma 6.3(ii), Lemma 7.1, Lemma 8.1 and Lemma 8.2.

It is clear that $v_4^+ = 0$ if $c_2 \neq 1$ and $b_4 = b_2(b_3 - 1)/(c_3(c_2 - 1))$. Therefore assume now that $v_4^+ = 0$. It follows that $(b_3 - 1)b_2 = c_3(c_2 - 1)b_4$. If $c_2 = 1$, then also $b_3 = 1$ and $c_3 = 1$ by Lemma 7.1(i). But then $k = c_3 + b_3 = 2$, a contradiction. Therefore $c_2 \neq 1$ and the result follows. □

Lemma 8.4. *With reference to Definition 6.1, assume that* $D = 5$, $\Delta_2 = 0$ *and* $\Delta_3 \neq 0$. *Then*

$$\|v_3^-\|^2 = \left(\frac{(c_2 - 1)(c_4 - 1)b_2}{k + c_2^2 - 3c_2} + \frac{(k - 1)\Delta_3}{b_2 - 1} \right) \frac{b_2 b_4 \|v\|^2}{c_2(kc_2 - k - c_2) + b_2}.$$

Proof. By Lemma 6.2(iv), (2.1) and Definition 3.1 we have

$$c_3 \langle v_3^-, v_3^- \rangle = b_3 \langle v_3^+, v_3^- \rangle + \langle R v_2^-, v_3^- \rangle - \langle v_4^+, R v_3^- \rangle.$$

The result now follows from Lemmas 6.3(iii), 7.1, 8.2 and 8.3, Corollary 7.3 and (4.1). □

Corollary 8.5. *With reference to Definition 6.1, assume that* $D = 5$, $\Delta_2 = 0$ *and* $\Delta_3 \neq 0$. *Then the following* (i), (ii) *hold.*

(i) $v_3^- \neq 0$.

(ii) v_3^+, v_3^- *are linearly independent.*

Proof. (i) Note that $(c_2-1)(c_4-1)b_2/(k+c_2^2-3c_2) \geq 0$ and that $(k-1)\Delta_3/(b_2-1) > 0$ by [3, Theorem 12]. Moreover, it is easy to see that $c_2(kc_2 - k - c_2) + b_2 > 0$. The result follows.

(ii) Assume on the contrary that v_3^+, v_3^- are linearly dependent. Let

$$B = \begin{pmatrix} \langle v_3^+, v_3^+ \rangle & \langle v_3^+, v_3^- \rangle \\ \langle v_3^-, v_3^+ \rangle & \langle v_3^-, v_3^- \rangle \end{pmatrix}$$

and note that $\det(B) = 0$. Using Lemmas 8.1, 8.2 and 8.4 one could easily see that the only factor of $\det(B)$ which could be zero is

$$c_4k - c_2^3k + 2c_2^2k - 2c_2k + c_2^3c_4 - 2c_2^2c_4 - c_2c_4 + 2c_2^2.$$

Solving this for c_4 and then computing Δ_3 using Definition 4.1, we obtain $\Delta_3 = 0$, a contradiction. This shows that v_3^+, v_3^- are linearly independent. □

Lemma 8.6. *With reference to Definition 6.1, assume that* $D = 5$, $\Delta_2 = 0$ *and* $\Delta_3 \neq 0$. *Then*

$$\|v_5^+\|^2 = \frac{b_4 - c_4 + \alpha_4 + c_2\beta_4}{c_3}\|v_4^+\|^2.$$

In particular, $v_5^+ = 0$ *if and only if* $v_4^+ = 0$ *or* $b_4 - c_4 + \alpha_4 + c_2\beta_4 = 0$.

Proof. By Lemma 6.2(ii), (2.1) and Definition 3.1 we have

$$\langle v_5^+, v_5^+ \rangle = \frac{1}{c_3}\langle Rv_4^+, v_5^+ \rangle = \frac{1}{c_3}\langle v_4^+, Lv_5^+ \rangle.$$

The result now follows from Lemma 6.3(ii). □

9 A basis

With reference to Definition 6.1, assume that $D = 5$, $\Delta_2 = 0$ and $\Delta_3 \neq 0$. In this section we display a basis for W. We will also show that, up to isomorphism, Γ has a unique irreducible T-module with endpoint 2.

Theorem 9.1. *With reference to Definition 6.1, assume that* $D = 5$, $\Delta_2 = 0$ *and* $\Delta_3 \neq 0$. *Then the following* (i)–(iii) *hold.*

(i) *If* $v_5^+ \neq 0$, *then the following is a basis for* W*:*

$$v_i^+ \ (2 \leq i \leq 5), \qquad v_3^-. \tag{9.1}$$

(ii) *If* $v_4^+ \neq 0$ *and* $v_5^+ = 0$, *then the following is a basis for* W*:*

$$v_i^+ \ (2 \leq i \leq 4), \qquad v_3^-. \tag{9.2}$$

(iii) *If* $v_4^+ = 0$, *then the following is a basis for* W*:*

$$v_i^+ \ (2 \leq i \leq 3), \qquad v_3^-. \tag{9.3}$$

In particular, W *is not thin.*

Proof. Note that by (7.1), W is spanned by vectors v_i^+ $(2 \le i \le 5)$ and v_3^-. Vector $v_2^+ = v$ is nonzero by definition. Vectors v_3^+ and v_3^- are nonzero by Lemma 8.1 and Corollary 8.5(i), respectively. We prove part (i) of the theorem. Proofs of parts (ii) and (iii) are similar.

If $v_5^+ \neq 0$, then $v_4^+ \neq 0$ by Lemma 8.6. Vectors v_i^+ $(2 \le i \le 5)$ and v_3^- are linearly independent by (3.1) and Corollary 8.5(ii). This shows that (9.1) is a basis for W. As $\dim(E_2^*(W)) = 2$, W is not thin. The result follows. □

Theorem 9.2. *With reference to Definition 6.1, assume that $D = 5$, $\Delta_2 = 0$ and $\Delta_3 \neq 0$. Then Γ has, up to isomorphism, exactly one irreducible T-module with endpoint 2.*

Proof. Let U denote an irreducible T-module with endpoint 2, different from W. Fix nonzero $u \in E_2^* U$, and for $2 \le i \le 5$ define

$$u_i^+ = E_i^* A_{i-2} E_2^* u$$

and let $u_3^- = E_3^* A_5 E_2^* u$. It follows from the results of Section 8 and Theorem 9.1 that u_2^+, u_3^+, u_3^- are nonzero and that nonzero vectors in the set $\{u_i^+ \mid 2 \le i \le 5\} \cup \{u_3^-\}$ form a basis for U. Furthermore, it follows from Lemma 8.3 and Lemma 8.6 that u_4^+ (u_5^+, respectively) is nonzero if and only if v_4^+ (v_5^+, respectively) is nonzero.

Let $\sigma : W \to U$ be defined by $\sigma(v_i^+) = u_i^+$ $(2 \le i \le 5)$ and $\sigma(v_3^-) = u_3^-$. It follows from the comments above that σ is a vector space isomorphism from W to U. We show that σ is a T-module isomorphism. Since A generates M and $E_0^*, E_1^*, \ldots, E_5^*$ is a basis for M^*, it suffices to show that σ commutes with each of $A, E_0^*, E_1^*, \ldots, E_5^*$. Using the fact that $E_i^* E_j^* = \delta_{ij} E_i^*$ and the definition of σ we immediately find that σ commutes with each of $E_0^*, E_1^*, \ldots, E_5^*$. Recall that $A = R + L$. It follows from Lemma 6.2, Lemma 6.3 and Corollary 7.3 that σ commutes with A. The result follows. □

We would like to emphasize that together with the results in [10, 12, 15], Theorems 9.1 and 9.2 imply the following characterization.

Theorem 9.3. *Let $\Gamma = (X, \mathcal{R})$ denote a bipartite distance-regular graph with diameter $D \ge 4$ and valency $k \ge 3$. Assume Γ is not almost 2-homogeneous. We fix $x \in X$ and let $E_i^* = E_i^*(x)$ $(0 \le i \le D)$ and $T = T(x)$ denote the dual idempotents and the Terwilliger algebra of Γ with respect to x, respectively. Then the following* (i), (ii) *are equivalent.*

(i) *Γ has, up to isomorphism, exactly one irreducible T-module W with endpoint 2, and W is non-thin with $\dim(E_2^* W) = 1$, $\dim(E_{D-1}^* W) \le 1$ and $\dim(E_i^* W) \le 2$ for $3 \le i \le D$.*

(ii) *$\Delta_2 = 0$, and there exist complex scalars α_i, β_i $(2 \le i \le D-1)$ such that*

$$|\Gamma_{i-1}(x) \cap \Gamma_{i-1}(y) \cap \Gamma_1(z)| = \alpha_i + \beta_i |\Gamma_1(x) \cap \Gamma_1(y) \cap \Gamma_{i-1}(z)| \tag{9.4}$$

for all $y \in \Gamma_2(x)$ and $z \in \Gamma_i(x) \cap \Gamma_i(y)$.

With reference to Definition 6.1, assume that $\Delta_2 = 0$ and $\Delta_3 \neq 0$. It is known that this implies $c_2 \in \{1, 2\}$, or $D \le 5$, see [12, Theorem 4.4]. If $c_2 \in \{1, 2\}$, then the structure of irreducible T-modules with endpoint 2 was studied in detail in [12, 15]. Therefore, we are mainly interested in the case $c_2 \ge 3$. We have to mention however that we are not aware of any of such a graph. Using a computer program we found intersection arrays

$\{b_0, b_1, b_2, b_3, b_4; c_1, c_2, c_3, c_4, c_5\}$ up to valency $k = 20000$, which satisfy the following conditions: $c_2 \geq 3$, $\Delta_2 = 0$, $\Delta_3 > 0$, $\Delta_4 > 0$, $\gamma_2 \in \mathbb{N}$, $p^2_{22} \in \mathbb{N}$. None of them passed the feasibility condition $p^1_{ij} \in \mathbb{N} \cup \{0\}$, see the table below.

intersection arrays	feasibility condition
(58, 57, 49, 21, 1; 1, 9, 37, 57, 58)	$p^1_{23} = 1102/3 \notin \mathbb{N}$
(112, 111, 100, 45, 4; 1, 12, 67, 108, 112)	$p^1_{34} = 103600/67 \notin \mathbb{N}$
(186, 185, 161, 35, 1; 1, 25, 151, 185, 186)	$p^1_{23} = 6882/5 \notin \mathbb{N}$
(274, 273, 256, 120, 10; 1, 18, 154, 264, 274)	$p^1_{23} = 12467/3 \notin \mathbb{N}$
(274, 273, 256, 120, 1; 1, 18, 154, 273, 274)	$p^1_{23} = 12467/3 \notin \mathbb{N}$
(1192, 1191, 1156, 561, 28; 1, 36, 631, 1164, 1192)	$p^1_{23} = 118306/3 \notin \mathbb{N}$
(3236, 3235, 3136, 760, 1; 1, 100, 2476, 3235, 3236)	$p^1_{23} = 523423/5 \notin \mathbb{N}$

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Smart elements in combinatorial group testing problems with more defectives*

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Abstract

In combinatorial group testing problems Questioner needs to find a defective element $x \in [n]$ by testing subsets of $[n]$. In [18] the authors introduced a new model, where each element knows the answer for those queries that contain it and each element should be able to identify the defective one.

In this article we continue to investigate this kind of models with more defective elements. We also consider related models inspired by secret sharing models, where the elements should share information among them to find out the defectives. Finally the adaptive versions of the different models are also investigated.

Keywords: Combinatorial group testing, defectives, cancellative.

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1 Introduction

In the most basic *model* of *combinatorial group testing* Questioner needs to find a special element x of $\{1, 2, \dots, n\}$ $(=: [n])$ by asking minimal number of *queries* (or *group tests* or *pools*) of type "does $x \in F \subset [n]$?". Special elements are usually called *defective* (or *positive*). For every combinatorial group testing problem there are at least two main approaches: whether it is *adaptive (or sequential)* or *non-adaptive (or oblivious)*. In the adaptive scenario Questioner asks queries depending on the answers for the previously asked queries, however in the non-adaptive version Questioner needs to pose all the queries

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at the beginning. We call the *complexity* of a specific combinatorial group testing problem the number of the queries needed to ask by Questioner in the worst case during an optimal strategy.

Combinatorial group testing problems were first considered during the World War II by Dorfman [10] in the context of mass blood testing. Since then group testing techniques have had many different applications, for example in fault diagnosis in optical networks [20], in quality control in product testing [26] or failure detection in wireless sensor networks [23]. In this article we will mainly discuss non-adaptive models. The interested reader can find many variants and generalizations of the basic non-adaptive model and also many applications in the book [11].

1.1 Description of the new model

In [18] the authors introduced new combinatorial group testing models, inspired by the results of Tapolcai et al. [30, 29].

The main novel ingredient of these combinatorial group testing models is that the elements are smart and they distrust the Questioner, thus they want to control the tests they are involved in. So the following extra condition was introduced: **each element knows the answer for those queries that contain it**, and the goal: each element should be able to identify the defective one.

Motivated by secret sharing schemes (see e.g. [2]), the following variant was also considered: the elements can work together and share their knowledge. In this case we require certain sets of elements to be able to identify the defective, while we require other sets to be unable to identify the defective element. We emphasize that the way the data is transmitted does not play a role here. Information can not be distributed between different groups.

We mention here some other motivation to introduce these models: it is often mentioned in the group testing literature that an advantage of testing pools together is that it increases privacy. However, systematical research on this property has only started recently, see e.g. [1, 5, 16]. These papers focus on cryptographic versions of the problem. Here we deal with a simple combinatorial version, where privacy only means that an unauthorized participant cannot completely detect the defective element(s). In [18] the authors considered models with one defective element. The main aim of this article is to continue these investigations with more defectives.

1.2 Simple combinatorial models with d defectives

A well-studied generalization of the basic model is the following. There are exactly d defective elements, a query corresponds to a set F, and the answer shows if there is at least one defective elements in F or not.

About Questioner's strategy we remark that - as he should find all the defectives - the asked queries should form a *d-separating family* (see the next section for a definition) in the non-adaptive case, so for the minimum number of tests the known lower bound is $\Omega(\frac{d^2}{\log d}\log n)$, while the best upper bound construction yields $O(d^2 \log n)$ (see e.g. [14, 25]). It is one of the major open problems in the theory of combinatorial group testing models to close the gap between the previous upper and lower bound.

In the adaptive case there is a multiplicative constant factor between the information theoretic lower bound and the best existing algorithm. The known best lower bound is $d \log \frac{n}{d}$, while the upper bound is $O(d \log n)$.

1.3 Structure of the paper

We organize the paper as follows: in Section 2 we introduce some properties and related results about families of sets, that we will need later. In Section 3 we introduce the non-adaptive models that we investigate, while in Section 4 we prove the main results. In Section 5 we look at the adaptive scenario, and we finish the article with remarks and open questions in Section 6.

We also mention that in this article we use standard asymptotic notation.

2 Finite set theory background

Our topic is connected to several areas of finite set theory. In this section we introduce some notions on families of subsets and known results about them, that we will use during the proofs.

In this article we use the notation of $2^{[n]}$ for the power set of $[n]$ and for any $\mathcal{F} \subset 2^{[n]}$, $a \in [n]$ we use $\mathcal{F}_a := \{F \in \mathcal{F} : a \in F\}$. The *complement* of a family $\mathcal{F} \subset 2^n$ is $\overline{\mathcal{F}} := \{[n] \setminus F : F \in \mathcal{F}\}$, while the *dual* of a family $\mathcal{F} \subset 2^n$ is $\mathcal{F}' := \{\mathcal{F}_a : a \in [n]\}$. It is defined on the underlying set $\mathcal{F}$ and has cardinality at most n. For a family $\mathcal{F} \subset 2^{[n]}$ and $d \geq 1$ let $\mathcal{F}^d := \{\cup_{i=1}^d F_i : F_i \in \mathcal{F},\ F_i \neq F_j \text{ for } i \neq j\}$.

Now we introduce some notions about families of subsets of $[n]$.

Definition 2.1. We say that $\mathcal{F} \subset 2^{[n]}$ is:

(1) **intersection closed** if $F, G \in \mathcal{F}$ implies $F \cap G \in \mathcal{F}$.

(2) **Sperner** if there are no two different $F_1, F_2 \in \mathcal{F}$ with $F_1 \subset F_2$.

(3) **cancellative** if for any three $F_1, F_2, F_3 \in \mathcal{F}$ we have

$$F_1 \cup F_2 = F_1 \cup F_3 \Rightarrow F_2 = F_3.$$

(4) **intersection cancellative** if for any three $F_1, F_2, F_3 \in \mathcal{F}$ we have

$$F_1 \cap F_2 = F_1 \cap F_3 \Rightarrow F_2 = F_3.$$

(5) **d-separating** for some $1 \leq d \leq n-1$ positive integer, if for any two different $X_1, X_2 \subset [n]$ with $|X_1| = |X_2| = d$ there is $F \in \mathcal{F}$ with:

$$F \cap X_1 \neq \emptyset \text{ and } F \cap X_2 = \emptyset, \text{ or}$$

$$F \cap X_2 \neq \emptyset \text{ and } F \cap X_1 = \emptyset.$$

(6) **d-union-free** for some $d \geq 1$ if for different $F_1, \ldots, F_d \in \mathcal{F}$ and different $G_1, \ldots, G_d \in \mathcal{F}$

$$\bigcup_{i=1}^{d} F_i = \bigcup_{i=1}^{d} G_i$$

implies $\{F_1, \ldots, F_d\} = \{G_1, \ldots, G_d\}$.

(7) **d-cover-free** for some $d \geq 1$ positive integer if there are no $(d+1)$ different $F_1, F_2, ..., F_{d+1} \in \mathcal{F}$ with

$$F_{d+1} \subset \bigcup_{i=1}^{d} F_i.$$

(8) **(r,d)-cover-free** for some $r, d \geq 1$ positive integers if there are no $(d+r)$ different $F_1, F_2, ..., F_{d+r} \in \mathcal{F}$ with

$$\bigcap_{i=d+1}^{d+r} F_i \subset \bigcup_{i=1}^{d} F_i.$$

Before defining the last notion, we need some introduction. We will generalize a graph property, so it is more comfortable to use the word hypergraph instead of family of subsets of $[n]$ (where $\mathcal{F}$ is the set of the hyperedges and $[n]$ is the set of vertices of the hypergraph). There are several ways to define cycles in hypergraphs. Here we use one due to Berge [4]. A *Berge-cycle* in a hypergraph of length k (a Berge-C_k) consists of k different hyperedges $E_1, \ldots, E_k$ and k different vertices $x_1, \ldots x_k$ such that E_i contains x_i and x_{i+1} for $1 \leq i \leq k$ (modulo k, so E_k contains x_k and x_1). Note that for a 2-uniform hypergraph (that is a graph) this notion is the same as the 'usual' cycle in a graph. The *Berge-girth* (that we call just *girth* in this article) of a hypergraph $\mathcal{H}$ is the smallest length of a cycle in $\mathcal{H}$ (that is ∞ if there is no cycle in $\mathcal{H}$). A hypergraph is d-regular if every vertex is contained in exactly d hyperedges, r-uniform if every hyperedge has size r and linear if any two hyperedges intersect in at most one vertex.

2.1 Some known results about these notions that we will use later

• The notion cancellative was first introduced by Frankl and Füredi in [17].

Fact 2.2. *$\mathcal{F} \subset 2^{[n]}$ is intersection cancellative if and only if $\overline{\mathcal{F}}$ is cancellative.*

• The notion of separating family in the context of combinatorial search theory was introduced and first studied by Rényi in [24]. The following fact is rather trivial, so we omit its proof.

Fact 2.3. *Suppose $\mathcal{F}_n \subset 2^{[n]}$ is a minimal separating family. Then we have:*

$$|\mathcal{F}_n| \leq \lceil \log_2 n \rceil.$$

Fact 2.4. *$\mathcal{F} \subset 2^{[n]}$ finds d defectives if and only if $\mathcal{F}$ is d-separating. The dual of a d-separating family is d-union-free.*

• The notion of d-union-free families was introduced by Hwang and T. Sós in [21] under the name of *d-Sidon* families. They proved the following:

Theorem 2.5 (Hwang, T. Sós, [21, Theorem 3])**.** *There exists a d-union-free family $\mathcal{F}_n \subset 2^{[n]}$ with:*

$$\frac{1}{2}(1 + \frac{1}{(4d)^2})^n \leq |\mathcal{F}_n|.$$

• The notion of d-cover-free families was introduced by Kautz and Singleton in [22]. Note that a d-cover-free family is also d-union-free. They proved the following lower bound.

Theorem 2.6 (Kautz, Singleton, [22]). *There exists a d-cover-free family $\mathcal{F}_n \subset 2^{[n]}$ with:*

$$\Omega(\frac{1}{d^2}) = \frac{\log_2 |\mathcal{F}_n|}{n}.$$

D'yachkov and Rykov proved the following upper bound on the size of d-cover-free families:

Theorem 2.7 (D'yachkov, Rykov, [14]). *Suppose that $\mathcal{F}_n \subset 2^{[n]}$ is a d-cover-free family. Then we have:*

$$\frac{\log_2 |\mathcal{F}_n|}{n} \leq \frac{2\log_2 d}{d^2}(1 + o(1)).$$

• The notion of (r, d)-cover-free families were introduced by D'yachkov, Macula, Torney and Vilenkin in [12]. They showed that a result by Stinson, Wei and Zhu [28] implies the following:

Theorem 2.8. *If the dual of $\mathcal{F}_n \subset 2^{[n]}$ is (r, d)-cover-free, then we have:*

$$|\mathcal{F}_n| = \Omega_{d,r}(\log_2 n).$$

• Ellis and Linial [15] studied regular uniform linear hypergraphs with large girth. They mention that a result of Cooper, Frieze, Molloy and Reed [6] implies that for any $d \geq 2$, $r, g \geq 3$ and sufficiently large n, if r divides n, then there is an r-uniform, d-regular, n-vertex linear hypergraph with girth at least g. Moreover the argument can be adapted to show the same statement in the case r divides dn.

Theorem 2.9. *Let $d \geq 2$, $r, g \geq 3$, n large enough and r divides dn. Then there exists a linear, d-regular, r-uniform hypergraph with girth at least g on n vertices.*

3 Models

In this section we start our investigations and give a systematic study of models with the extra property that each element knows the answers for those queries that contain it.

In all the models in this section an input set $[n]$ is given, and d of them are defectives ($d \leq n$). We are dealing with non-adaptive models, so Questioner needs to construct a family $\mathcal{F} \subset 2^{[n]}$. A set F correspond to a query of the following type: 'is there any defective element in $F \subset [n]$?'. In each model we assume that knowing all the answers is enough information for Questioner to find the defective elements, i.e. $\mathcal{F}$ is d-separating. Note that this immediately implies a lower bound of $\Omega_d(\log_2 n)$ on the size of the query family in each model. We mention whenever the query family satisfies another property that could improve the factor depending only on d, but calculating the factors is outside the scope of this paper.

The main difference between the following models is what we want the elements to find out. Using only the information available to them, i.e. the answers to the queries containing them, we can require that they find out something about the defective elements, or oppositely, that they cannot find out something.

When we say that an element x *knows the defective elements*, we mean that the query family satisfies the following property: no matter what the defective element is, after the answers x can find out the defective ones, i.e. the subfamily $\mathcal{F}_x$ is d-separating. In the opposite when we say that x *does not know any of the defective elements*, we mean that the query family satisfies the following property: no matter what the defective elements are, after the answers x cannot identify any defective element. Equivalently, for any $D \subset [n]$, $y \in D$ with $|D| = d$ there is a $D' \subset [n]$ with $|D'| = d$, $y \notin D'$, such that the same members of $\mathcal{F}_x$ intersect D and D'.

Another variant of this problem is when elements can share information among them. It is possible that in some model some element can not find out the defective, however if we pick two elements and they share their information among them, they can find the defective elements. We consider these kind of models.

We also assume that in each model the elements know the setup of the problem, i.e. that n elements are given and exactly d of them are defectives. We use the expression that a family *solves* a model if it satisfies the property that describes the model.

In each of the following models we first give a property describing what the elements should know, and then we examine if there is a query set that solves that specific model or state results about the cardinality of such query sets. Then we consider models where we require some information to remain hidden from the elements. Finally we mix these types of properties.

In this section we assume that there are exactly $d \geq 2$ defective elements (and every element knows that). We consider models analogous to the ones introduced in [18].

3.1 Model 1_d

Probably the most natural model is the following:

Property. All elements find out if they are defective.

We note that some cryptographic problems concerning this model were investigated in [1], where the authors observed that the dual of a d-cover-free family solves this model. Here we show that only such families solve this model.

Theorem 3.1. *$\mathcal{F}$ solves Model 1_d if and only if its dual is d-cover-free.*

We prove this theorem in Section 4. By Theorem 3.1, Theorem 2.6 and Theorem 2.7 we have:

Corollary 3.2. *If $\mathcal{F}_n \subset 2^{[n]}$ solves Model 1_d and has minimum cardinality, then we have:*

$$\Omega(\frac{d^2}{\log_2 d} \log_2 n) = |\mathcal{F}_n| = O(d^2 \log_2 n).$$

3.2 Model 2_d

Another natural model is when the elements should find out everything.

Property. Every element finds all the defectives.

It is obvious that no $\mathcal{F}$ can solve Model 2_d if $1 < d < n$: a defective element cannot gather any information about the other elements, as it gets only YES answers.

3.3 Model $2'_d$

As defective elements cannot gather any information about the other elements, in the next model we only require non-defective elements to find the defective ones.

Property. Every non-defective element finds all the defectives.

Theorem 3.3. *Suppose $\mathcal{F}_n$ solves Model $2'_d$ and has minimum cardinality. Then we have*

$$|\mathcal{F}_n| = \Theta_d(\log_2 n).$$

Proof. We claim that the solution is the dual of a d-cover-free family, and the dual of a $(2, d)$-cover-free family is always a solution. This together with Theorem 2.7 and Theorem 2.8 implies the statement.

Suppose that the dual is not d-cover-free. Then there are $F_1, F_2, ..., F_{d+1} \in \mathcal{F}$ with $F_{d+1} \subset \cup_{i=1}^{d} F_i$. For the corresponding elements in the primal version we have x_{d+1} such that any set $F \in \mathcal{F}$ contains one of the other elements $x_1, \dots, x_d$. Thus if $x_1, \dots, x_d$ are the defectives, x_{d+1} receives only YES answers, thus cannot distinguish this case from the case x_{d+1} and any $d-1$ other elements are the defectives.

On the other hand let us assume $\mathcal{F}$ is the dual of a $(2, d)$-cover-free family. Then for every non-defective elements x, y there is a set $F \in \mathcal{F}$ such that F contains both x and y, but none of the defective elements, thus x finds out that y is not defective, $\mathcal{F}$ solves Model $2'_d$. Indeed, there is an element in the intersection of the duals of x and y that is not contained by the duals of the defective elements by the $(2, d)$-cover-free property. That element is the dual of a set $F \in \mathcal{F}$ that has the desired properties. □

3.4 Model $2''_d$

The fact that defective elements cannot gather any information about the other elements shows that even $d-1$ elements together cannot always find the defectives. However, if d elements share information, then either they are all the defectives and they do not need to gather information about the other elements, or at least one of them is not a defective, and then there is a solution by Model $2'_d$.

Property. d elements together know who the defective elements are.

Theorem 3.4. *$\mathcal{F}_n$ solves Model $2''_d$ if and only if its dual $\mathcal{G}$ is d-union-free and $\mathcal{G}^d$ is Sperner and intersection-cancellative.*

We prove this theorem in Section 4. Note that we know the maximum possible size of a Sperner and intersection cancellative family (by results of Frankl and Füredi [17] and Tolhuizen [31]), but we do not know if that construction can be written as $\mathcal{G}^d$ for a d-union-free family $\mathcal{G}$.

Theorem 3.5. *Suppose $\mathcal{F}_n$ solves Model $2''_d$ and has minimum cardinality. Then we have*

$$|\mathcal{F}_n| = \Theta_d(\log_2 n).$$

Proof. It is easy to see that if a family solves both Model 1_d and Model $2'_d$, then it also solves Model $2''_d$. As we have seen in the proof of Theorem 3.3, a solution for Model $2'_d$ is the dual of a d-cover-free family, thus it also solves Model 1_d by Theorem 3.1. This implies the upper bound. □

3.5 Model 3_d

Let us now examine the case when we require that elements do *not* find the defective. Note that as always, we assume that knowing all the answers is enough to find the defective element.

Property. No element knows any of the defective ones.

Note that for $d = 1$ there is a solution for Model 2_d and there is no solution for Model 3_d [18]. For $d \geq 2$ the situation is just the opposite: we will show that there is a solution for Model 3_d for n large enough. We will use arguments similar to the ones used in [3].

Theorem 3.6. *If $d \geq 2$, $r \geq 3$ and $n \geq dr + 2$, then an r-uniform, d-regular linear hypergraph with girth at least 5 solves Model 3_d.*

Proof. Let us consider an r-uniform, d-regular linear hypergraph $\mathcal{F}$ of girth 5. For an arbitrary element x its neighborhood consists of d disjoint sets of size $r - 1$. Also, there are more than d elements not in its neighborhood. It is easy to see that by $r \geq 3$ x cannot identify any defective elements.

On the other hand, if we know all the answers, the YES answers form stars with the defective elements in the centers. The elements that get only YES answers are the candidates for being defective. Every candidate that is not defective has to be connected to all the defectives. Two such candidate would form a Berge-C_4 with any two of the defective elements, thus there is only one additional candidate. But then it is the only one among the $d + 1$ candidates that is connected to the other candidates, otherwise we could find a Berge-C_3. □

Corollary 3.7. *If n is large enough compared to $d > 1$, then there is a solution for Model 3_d.*

Proof. If $d \geq 3$, let us choose $r = d$, then Theorem 2.9 shows that we can find such a family. If $d = 2$, then Theorem 2.9 with $r = 4$ shows we can find such a family for n even. If n is odd, we find such a family for $n + 1$, and delete an element. The resulting family is not 4-uniform, but that property is not actually needed (in fact, we used only that every set in $\mathcal{F}$ has size at least 3). □

3.6 Model 4_d

Now we start to investigate models where elements can share information among them. Let i and j be integers with $1 \leq i < j \leq n$. When we say that a set of j elements together know the defective elements, we mean that knowing the answers to all the queries containing at least one element from the set is enough to find all the defectives. Similarly, when we say that a set of i elements do not know any of the defectives, we mean that knowing the answers to all the queries intersecting the set is not enough to identify any of the defective elements.

Property. Any j elements together know the defectives, but i elements together do not know any of the defectives, for some i and j with $1 \leq i < j \leq n$.

Note that Corollary 3.7 shows that there is a solution if $d > 1$, $i = 1$ and $j = n$, where n is large enough compared to d. In fact any $n - r + 1$ elements together know the answer to all the queries, thus it is enough to assume $j \geq n - r + 1$. A more precise version of Theorem 2.9 (see [15], Theorem 5) shows that about $\frac{n^{1/6}}{d}$ can be chosen as r, which shows that j can be as small as $n - \frac{n^{1/6}}{d}$.

Proposition 3.8. *If $i \geq d$ or $j < d$, then there is no solution.*

Proof. Let us assume first we are given j elements. If all of them are defectives, they only get YES answers, and do not gather any information about the other elements.

If $i \geq d$, for a set X let $\mathcal{F}_X := \cup_{x \in X} \mathcal{F}_x$. Let us consider among the d-element sets X such that $\mathcal{F}_X$ is maximal. We claim that if the elements of X are the defectives, they can find it out by sharing information. Indeed, they get only YES answers. If they cannot be sure that they are the defective ones, then there is another d-set Y that could be the set of defectives. It means all the answers to the queries in $\mathcal{F}_X$ would still be YES if Y was the set of defectives, i.e. $\mathcal{F}_X \subseteq \mathcal{F}_Y$. By the assumption on X we have $\mathcal{F}_X = \mathcal{F}_Y$, but then the family is not d-separating. □

Proposition 3.9. *If $j = d$, then there is no solution.*

Proof. If x receives only YES answers, he cannot find out he is defective, thus there is a set $D = \{y_1, \ldots, y_d\}$ no containing X that intersects every member of $\mathcal{F}_x$. On the other hand, if x and $y_1, \ldots, y_{d-1}$ are the defectives, they together can figure that out. In particular, they know that the set of defectives is not D, thus there is a set intersecting $\{x, y_1, \ldots, y_{d-1}\}$ but not D. Such a set would be a member of $\mathcal{F}_x$ that does not intersect D, a contradiction. □

4 Proofs

4.1 Proof of Theorem 3.1

The dual of the d-cover-free property is that for every elements $x_1, \ldots, x_{d+1}$ we cannot have that the sets that contain x_{d+1} all contain at least one of the other x_i's. Let

$$\mathcal{H}_x := \{F \setminus \{x\} : F \in \mathcal{F}_x\},$$

and $\tau(\mathcal{H}_x)$ be the size of the smallest set that intersects every member of $\mathcal{H}_x$. With these notation the following lemma finishes the proof of Theorem 3.1.

Lemma 4.1. *An element x always finds out if he is defective if and only if $\tau(\mathcal{H}_x) > d$.*

Proof. If x gets a NO answer, he learns he is not defective, thus we can assume he only gets YES answers. If $\mathcal{H}_x$ cannot be covered by at most d elements different from x, then the only way to get YES answer to every element of $\mathcal{F}_x$ is if x is defective (as defective elements cover the sets that get YES answers). On the other hand if $\mathcal{H}_x$ can be covered by at most d elements different from x, then x cannot exclude the possibility that those are the defective elements, together with arbitrary additional elements to reach d defectives. □

4.2 Proof of Theorem 3.4

Lemma 4.2. *$\mathcal{F} \subset 2^{[n]}$ solves Model $2_d''$ if and only if the following two properties hold:*

(1) for any two different d-element sets $X, Y \subset [n]$ there is $F \in \mathcal{F}$ with $F \cap X \neq \emptyset$ and $F \cap Y = \emptyset$, and

(2) for any three different d-element sets $X, Y, Z \subset [n]$ there is $F \in \mathcal{F}$ with ($F \cap X \neq \emptyset$ and $F \cap Y \neq \emptyset$ and $F \cap Z = \emptyset$) or ($F \cap X \neq \emptyset$ and $F \cap Z \neq \emptyset$ and $F \cap Y = \emptyset$).

Proof.

1. Note that the property that Questioner can find out the answer is: for any two different d-element sets $X, Y \subset [n]$ there is $F \in \mathcal{F}$ with ($F \cap X \neq \emptyset$ and $F \cap Y = \emptyset$) or ($F \cap Y \neq \emptyset$ and $F \cap X = \emptyset$). This property is contained in (1).

Let us assume now X is a set of size d.

2. If X is the set of defectives, they have to find this out. It means that for a different d-element set Y, there should be an $F \in \mathcal{F}$ with $X \cap F \neq \emptyset$ and $Y \cap F = \emptyset$.

3. If X is not the set of defectives, then another set Y is, and they have to identify Y. Thus for a third d-element set Z, there should be a set that intersects X (so they know the answer for it), and distinguishes Y and Z, i.e. it intersects exactly one of them. □

Lemma 4.3. *$\mathcal{F} \subset 2^{[n]}$ satisfies properties (1) and (2) if and only if its dual $\mathcal{G}$ is d-union-free and $\mathcal{G}^d$ is Sperner and intersection cancellative.*

Proof. The dual of (1) is the following statement:

(3) for two different subfamilies each consisting of d sets $\{F_1, \dots, F_d\}, \{G_1, \dots, G_d\} \subset \mathcal{F}$ there is $f \in [n]$ with $f \in \cup_{i=1}^d F_i \setminus \cup_{i=1}^d G_i$.

The dual of (2) is the following statement:

(4) for three different subfamilies each consisting of d sets

$$\{F_1, \dots, F_d\}, \{G_1, \dots, G_d\}, \{H_1, \dots, H_d\} \subset \mathcal{F}$$

there is $f \in [n]$ with either

$$f \in (\cup_{i=1}^d F_i \cap \cup_{i=1}^d G_i) \setminus \cup_{i=1}^d H_i, \text{ or}$$
$$f \in (\cup_{i=1}^d F_i \cap \cup_{i=1}^d H_i) \setminus \cup_{i=1}^d G_i.$$

It is easy to see that (3) is equivalent to the statement that $\mathcal{G}$ is d-union-free and $\mathcal{G}^d$ is Sperner. Now we claim that (4) means that $\mathcal{G}^d$ is intersection cancellative. Let us use the following notation:

$$F := \cup_{i=1}^d F_i, \quad G := \cup_{i=1}^d G_i, \quad H := \cup_{i=1}^d H_i.$$

Using these, the existence of f means either $F \cap G \not\subset H$ or $F \cap H \not\subset G$. Let us define three properties.

(i) $F \cap G \not\subset H$.

(ii) $F \cap H \not\subset G$.

(iii) $H \cap G \not\subset F$.

Property (2) (for these three sets in this order) means that at least one of (i) and (ii) holds. Considering the same three sets in different orders we get that also at least one of (i) and (iii) and one of (iii) and (ii) holds. It is true if and only if at least two of these three properties hold.

To finish the proof of Lemma 4.3 we prove the following:

Claim 4.4. *A family $\mathcal{H} \subset 2^{[n]}$ is intersection cancellative if and only if at least two out of (i), (ii) and (iii) hold for any three members of it.*

Proof. Let us assume $\mathcal{F}'$ is intersection cancellative and let $F, G, H \in \mathcal{H}$. Let us assume at most one, say (iii) of the three properties holds, thus (i) and (ii) do not hold. The first one implies $F \cap G \subset H$, and obviously $F \cap G \subset F$. Thus we have $F \cap G \subset F \cap H$. Similarly the second one implies $F \cap H \subset F \cap G$, hence they together imply $F \cap H = F \cap G$, which contradicts the intersection cancellative property and our assumption that F, G, H are three different sets.

Let us assume now that $\mathcal{H}$ is not intersection cancellative, thus we have $F \cap G = F \cap H$. This implies both $F \cap G \subset H$ and $F \cap H \subset G$, thus at most one of (i), (ii) and (iii) can hold. □

We are done with the proof of Theorem 3.4. □

5 Adaptive scenario

A natural idea is to consider the adaptive versions of these problems. Here we assume the Questioner knows all the earlier answers, and then he can choose the next query. He can find the defective, and then use further queries to share some information with the elements. However, there are two versions of this problem. The elements might know the algorithm, and use the order of the queries to gain information, or they only receive the answers to the queries at the end in no particular order.

For example in Model 2_d in the second version we require that for every element x the family $\mathcal{F}_x$ with the answers is enough to find all the defectives, i.e. for two distinct sets D, D' of size d there is a query that contains x and intersects only one of D and D'. It is still obviously not solvable, as every defective element only gets YES answers and no information about the others. However, in the first version Questioner may start with a d-separating family, then ask the set of defectives and then the set of non-defectives. This way every element has to look only at the last query that contains it. If the answer to that is YES, then it is the set of defectives, if the answer is NO, it is the set of non-defectives. In both cases the defectives are identified.

From now on we consider only the second version, i.e. the elements receive the answer to the queries containing them at the end of the algorithm in no particular order, and they only know the underlying set and the number of defectives. It is still possible for the Questioner to find the defective, and then share some information using further queries.

Let $t^a(d, n)$ denote the number of queries in the fastest adaptive algorithm that finds the d defective (we mentioned some inequalities on $t^a(d, n)$ in the introduction), then $t^a(d, n)$ is a lower bound in every model. On the other hand $t^a(d, n) + d + 1$ queries are enough in Model 1_d, $t^a(d, n) + 1$ queries are enough in Model $2'_d$ and $t^a(d, n) + d + 1$ queries are enough in Model $2''_d$: first Questioner finds the d defectives, then ask them as singletons, and/or the set of non-defectives.

Let us consider now Model 3_d. By Corollary 3.7 there is a solution for n large enough, but that solution is linear in n. On the other hand it can be seen easily that for $n = d + 1$ there is no solution even adaptively. Here we give a faster algorithm.

Theorem 5.1. *There is an adaptive algorithm that solves Model 3_d and uses at most $2d \log_2 n + 5d$ queries if n is large enough.*

Proof. Questioner starts with asking a query Q of size $\lfloor n/2 \rfloor$ and its complement. Then in the next round he asks two complementing subsets of size differing by at most one in every query that was answered YES (say Q_1 and Q_2 with $Q_1 \cup Q_2 = Q$). He repeats this in every round except if the subset has size at most 5, he stops and does not ask that subset as a query. Since he asks disjoint sets in every round, he gets at most d YES answers, thus there are at most $2d$ queries in the next round. There are obviously at most $\log_2 n$ rounds. After that we have a family $\mathcal{D}$ of at most d sets of size at least 3 and at most 5, each containing at least one defective element. Let $A := \{a_1, \dots, a_l\}$ be their union ($l \leq 5d$), we also know that every defective is in A. Let $D_i \in \mathcal{D}$ be the set that contains a_i. As n is large enough, we can assume that there were two disjoint queries B and C that were answered NO and have size at least $5d$. Let $b_1, \dots, b_{5d}$ be distinct elements of B and $c_1, \dots, c_{5d}$ be distinct elements of C. Then Questioner also asks the queries $\{a_i, b_i, c_i\}$ for $i \leq l$.

As we know b_i and c_i are not defective, Questioner finds out if a_i is defective for every i. On the other hand, if a_i is defective, every query Q that contains a_i also contains either other elements of D_i or contains b_i, thus a_i cannot be sure he is defective. If a_i is not defective, then all he knows is that another element of D_i is defective, but there are more than one such elements. Any other element x appears in a query Q_1 that got answer NO. At that point when this NO answer arrives, x might knows that the answer was YES to a larger set Q that contains x. $Q \setminus Q_1$ has size at least 3, thus x does not know at this point which one is defective. If $x \notin B \cup C$, then he does not appear in any queries later, thus cannot find any defectives. If $x = b_i$ or $x = c_i$ for some i, he can get additional information about only one element of $Q \setminus Q_1$, thus there are two candidates remaining, again, x cannot find any defectives. Finally, if the answer to $\{a_i, b_i, c_i\}$ is YES, then b_i does not know if a_i or c_i is defective. $\square$

It is easy to see that Model 4_d still cannot be solved if $i \geq d$ or $j < d$. Indeed, the defectives still get only YES answers, thus less than d of them cannot have any idea about the remaining defectives. On the other hand we will show that there are possible answers such that the defectives together will find out they are the defectives, showing $i \geq d$ is impossible. Let us assume that every answer is YES, unless it is impossible. If Questioner finds out that D is the set of defectives, it means that for every other set D' of size d there was a query at some point that intersected exactly one of D and D'. At that point YES was a possible answer, thus the answer to that query was YES. Hence it intersected D and was disjoint from D'. Then an element of D knows D' is not the set of defectives, and this holds for every set $D' \neq D$ of size d.

6 Remarks

We finish this article with some possible directions that can be investigated:

• In some of the above models we proved that there is a family that solves the model, but did not say anything about its possible size.

• In case of Model 4_d our results can only be considered as the starting point of the investigations. In particular, it would be interesting to see if i can go above 1. It is tempting to try to extend the proof of Theorem 3.6 to this case, and use a linear hypergraph of large girth. However, it does not work even for $i = 2$. The property that the defectives can be identified forces the elements to be contained in many hyperedges, while the property that no 2 elements can identify any of the defectives forces the opposite.

If the query hypergraph is linear and d-separating, it is easy to see that for two elements contained by the same query there must be at least d other sets containing the two elements. This implies almost every element has to be contained in more than $(d+1)/2$ queries.

On the other hand let us consider two elements x, y that are not contained in the same hyperedge. The large girth of the query hypergraph implies that there is at most one other element z contained in a hyperedge Q together with x and another hyperedge together with y (if there is no such z, then let Q be an arbitrary query containing x). Let us assume the answer to Q is NO, and the answer to every other query containing x or y is YES. Then x and y together know that x is not defective. If they cannot identify y as a defective, there cannot be more than d hyperedges containing x or y besides Q. This implies almost every element has to be contained in at most $(d+1)/2$ queries.

• In [18] the authors considered the abstract version of the model introduced by Tapolcai et al. [29, 30]. Here we extended our models to the case of more defectives. It would be interesting to see if their model can be extended similarly.

• It is a phenomenon in combinatorial group testing that in most of the models the adaptive version actually means two round version of the problem (see e.g. [8]) Recently there was some interest in the r round (or multi-stage) versions of combinatorial group testing problems, where this phenomenon does not hold (see e.g. [7, 19]). It would be interesting to investigate these models in this context.

• One can consider a variant of these models, where instead of requiring that the elements find all (or none) of the defective elements, we require that they identify at least i and/or at most j of them.

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On 2-skeleta of hypercubes

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Abstract

It is shown that the 2-skeleton of the odd-d-dimensional hypercube can be decomposed into s_d spheres and τ_d tori, where $s_d = (d-1)2^{d-4}$ and τ_d is asymptotically in the range $(64/9)2^{d-7}$ to $(d-1)(d-3)2^{d-7}$.

Keywords: Cube decomposition, even-degree 2*-complex, generalized book.*

Math. Subj. Class. (2020): 57M20, 57M15, 05C45

1 Introduction

A *decomposition* of a graph is an edge-disjoint family of subgraphs such that each edge of the graph is in exactly one of the subgraphs. In recent decades, research on decomposition of graphs into cycles of varying lengths has been carried out for various graphs, including hypercubes.

The symbol "$\times$" denotes Cartesian product of topological spaces.

It is natural to try to extend decomposition (and other frameworks) from graphs to 2-complexes. We do that for *the* 2*-skeleton of the* d*-dimensional hypercube*: the 2-complex Q_d^2 obtained from the d-dimensional hypercube *graph* Q_d by attaching a topological 2-cell $[0,1] \times [0,1]$ to each Q_2-subgraph of Q_d in the natural way, and the decompositions are into spheres and tori.

A necessary condition to decompose a 2-complex into surfaces is that the complex be *even*: each edge belongs to a positive even number of 2-cells. But the condition isn't sufficient; e.g., a surface can intersect itself like the Klein bottle in 3-space. Note Q_d^2 is even iff $d \geq 3$ is odd.

The next section contains definitions, a precise statement of the results, and the proofs. The paper concludes with a brief discussion.

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2 Definitions, theorems, and proofs

In this section, we define complexes in a more general sense and give a product $\mathcal{K} \,\Box\, \mathcal{L}$ of 2-complexes (analogous to the Cartesian product of graphs).

A 2-*cell* is any space homeomorphic to the standard unit disk in the plane. A 2-*complex* is a graph together with a non-empty family of closed 2-cells which are attached by homeomorphisms from their boundaries to some of the cycles in the graph. The *degree* of an edge is the number of 2-cells which contain it; a complex is *even* iff all its edges have positive even degree.

If $\mathcal{K}$ is a complex, we write $\mathcal{K}^{(r)}$ for the set of r-cells, $0 \le r \le 2$, where the vertices and edges, resp., are the 0- and 1-cells. The *box-product* of two 2-complexes $\mathcal{K}$ and $\mathcal{L}$ is the 2-complex $\mathcal{M} := \mathcal{K} \,\Box\, \mathcal{L}$, where for $k = 0, 1, 2$

$$Y \in \mathcal{M}^{(k)} \iff Y = A \times B,\ A \in \mathcal{K}^{(i)},\ B \in \mathcal{L}^{(j)},\ i + j = k; \tag{2.1}$$

we call Y *of type* (i, j) in this case. It is easy to check that for all $d \ge 2$,

$$Q_d^2 = Q_{d-2}^2 \,\Box\, Q_2^2. \tag{2.2}$$

E.g., the 2-cells of $Q_4^2 = Q_2^2 \,\Box\, Q_2^2$ consist of four of type $(0, 2)$, four of type $(2, 0)$, and 16 of type $(1, 1)$. The box product of even complexes is even.

A *decomposition* of a 2-complex $\mathcal{K}$ is a set of 2-complexes whose union is $\mathcal{K}$ such that every 2-cell in $\mathcal{K}$ is in exactly one of the components.

An r-*factor* of a graph is a spanning r-regular subgraph and a factorization of a graph G is an edge-disjoint family of factors whose union is G. The following result is due to El-Zanati and Vanden Eynden [3, Theorem 7].

Theorem A. *A Let $d \ge 3$ be odd and suppose $2 \le r \le d$. Then there is a 1-factor F of Q_d such that $Q_d - F$ has a factorization into s-cycles with $s = 2^r$.*

A complex is a *sphere* or *torus* if it is homeomorphic to a sphere or torus. If a complex is isomorphic to K, we call it a K-complex.

Theorem 2.1. *For d odd ≥ 5, Q_d^2 has a decomposition into s_d spheres and t_d tori, where the spheres are Q_3^2, each torus is $C_4 \times C_\ell$ for some $\ell = 2^r$, r odd, $3 \le r \le d-2$, and*

$$s_d = (d-1)2^{d-4} \quad \textit{and} \quad t_d = \Big(2^{d-1} - (3/2)(d-3) - 4\Big)/9. \tag{2.3}$$

Theorem 2.2. *For d odd ≥ 5, Q_d^2 has a decomposition into s_d spheres and T_d tori, where each sphere equals ∂Q_3, each torus is $C_4 \times C_4$, and*

$$T_d = (d-1)(d-3)2^{d-7}. \tag{2.4}$$

For $d = 5, 7, 9$, $s_d = 8, 48, 256$, $t_d = 1, 6, 27$, and $T_d = 2, 24, 192$, respectively.

Proof of Theorem 2.1. By Theorem A, with $r = d-2$, Q_{d-2} can be factored into Hamiltonian cycles and a 1-factor F. We proceed by induction.

For the basis case $d = 5$, by equation (2.2), $Q_5^2 = Q_3^2 \,\Box\, Q_2^2$ As Q_3^2 is a sphere, the union of all 2-cells of type $(2, 0)$ in Q_5^2 is a set of four disjoint spheres. If F is the 1-factor in Q_3, then $F \,\Box\, \partial(Q_2^2)$, is the union of four disjoint cylinders formed by 16 2-cells of type

$(1,1)$, while there are eight 2-cells of type $(0,2)$ which constitute the tops and bottoms of the cylinders, giving a total of 8 spheres in the decomposition of Q_5^2. Finally, if H is the Hamiltonian cycle in $Q_3 - F$, then the 2-cells in $H \,\Box\, \partial(Q_2^2)$, each of type $(1,1)$, determine a torus of the form $C_4 \times C_8$. Thus, $s_5 = 8$ and $t_5 = 1$.

Noting that $s_3 = 1$, for the induction step, we again use equation (2.2) and the above argument to see that for $d \geq 5$, $s_d = 4s_{d-2} + 2^{d-3}$ and it is straightforward to check that $s_d = (d-1)2^{d-4}$ satisfies the recursion. Indeed, for $d \geq 5$

$$4(d-3)2^{d-6} + 2 \cdot 2^{d-4} = (d-1)2^{d-4}.$$

Similarly, as $(d-3)/2$ is the number of Hamiltonian cycles in the factorization of $Q_{d-2} - F$, we find that $t_d = 4t_{d-2} + (d-3)/2$, and for d odd ≥ 5, one easily checks that

$$4\Big(2^{d-3} - (3/2)(d-5) - 4\Big)/9 + (d-3)/2 = \Big(2^{d-1} - (3/2)(d-3) - 4\Big)/9,$$

which proves the theorem as the recursively added tori are of the form $C_4 \times C_\ell$, for ℓ the number of vertices in odd hypercubes of dimensions $< d$. $\square$

For instance, writing $\mathcal{T}_k$ for $C_k \times C_4$, the 6 tori for Q_7^2 are 4 copies of $\mathcal{T}_8$ and 2 copies of $\mathcal{T}_{32}$. For Q_9^2, there are 16 copies of $\mathcal{T}_8$, 8 of $\mathcal{T}_{32}$, and 3 of $\mathcal{T}_{128}$.

Using Theorem A with $r = 2$, one proves Theorem 2.2.

3 Conclusion

The decomposition of the odd-dimensional hypercube 2-complex into spheres and tori is an example of decomposing an even complex into surfaces, as proposed in [4]. We believe that similar decompositions are possible for even 2-complexes related to complete graphs (i.e., the simplex).

Decomposition into surfaces may allow improved display for graphs and 2-complexes embeddable in hypercubes. For instance, embedding the graph Q_d in a surface requires genus $1 + (d-4)2^{d-3}$ (e.g., [5, p. 119]) and such an embedding does not include all of the 2-complex. In contrast, a set of spheres and tori with 1-dimensional intersections suffice for the complex.

The problem of finding such representations has been considered by L. De Floriani and colleagues in a series of papers, e.g., [1, 2]. Two types of singularities 0-dimensional ("pinch points") and 1-dimensional (where several disks share a common line) are shown in Figures 3 and 1, respectively, of [1]. Their work, however, concentrates on simplicial complexes, rather than the cubical complexes considered here, and they don't consider the issue of topological complexity.

Our hypercube decompositions, which are face-disjoint unions of spheres and tori, are examples of *generalized books* in the sense of Overbay [6, 7].

If decompositions include surfaces with boundary, then every 2-complex has a decomposition. Indeed, if $\mathcal{K}$ is a 2-complex, then take a genus embedding of the underlying graph, and put each 2-cell, not corresponding to a region of the embedding, onto a separate disk.

That Q_d^2 ($d \geq 5$ odd) is decomposable into closed surfaces follows from Euler's theorem using induction as above. Indeed, removing any 1-factor from Q_{d-2} leaves a $(d-3)$-regular graph, which must be decomposable into cycles. Using [3] instead gives the least and greatest numbers of tori.

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Hereditary polyhedra with planar regular faces*

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In memory of Norman Johnson, our friend and colleague.

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Abstract

A skeletal polyhedron in Euclidean 3-space is called hereditary if the symmetries of each face extend to symmetries of the entire polyhedron. In this paper we describe the finite hereditary skeletal polyhedra which have regular convex polygons or regular star-polygons as faces.

Keywords: Symmetries of polyhedra, geometric polyhedral, uniform polyhedra.

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1 Introduction

In the design of polyhedral structures with high symmetry it is quite natural to proceed from a highly symmetric structure of lower rank (or dimension) and ask for the symmetries of the lower rank structure to be preserved for the entire structure. The entire structure then inherits the symmetries of the lower rank structure. For example, the Platonic solids and

*Special thanks go to Peter McMullen for pointing out the omission of a known uniform polyhedron from the list in an earlier version of the manuscript. We did know about the polyhedron but a bit of absentmindedness had caused us to forget to include it. His forthcoming paper [13] will describe an alternative approach to the enumeration presented here, and will also deal with the case of skew faces. We would also like to thank Tomaž Pisanski and the anonymous referee for helpful comments which have improved the paper.

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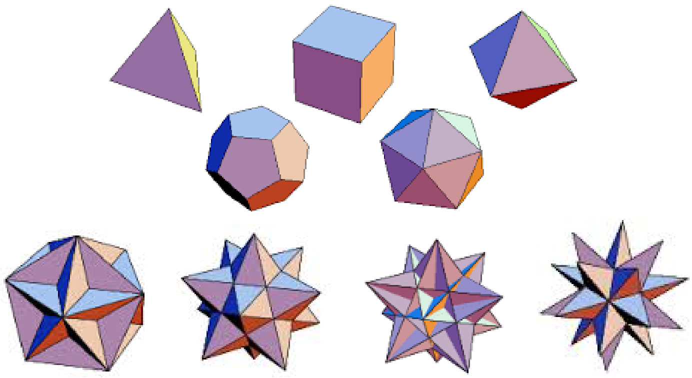

Figure 1: The finite regular polyhedra with planar faces (the five Platonic solids and the four Kepler-Poinsot polyhedra).

the Kepler-Poinsot polyhedra shown in Figure 1 have the property that each symmetry of each face extends to the entire figure (see [1]).

In this paper we study finite hereditary geometric polyhedra in $\mathbb{E}^3$ with planar regular faces. Here a polyhedron is viewed as a finite geometric graph with a distinguished class of polygonal cycles, called faces, such that two faces meet at each edge. A polyhedron is hereditary if each symmetry of each face extends to a symmetry of the polyhedron. For instance, all of the eighteen finite regular polyhedra in $\mathbb{E}^3$ are hereditary. Recall that these polyhedra consist of the nine *classical regular polyhedra*, that is, the Platonic solids and the Kepler-Poinsot polyhedra, and their Petrie duals (see [4, 5, 6, 15] or [16, Ch. 7E]). Hereditary polyhedra with regular faces are highly-symmetric polyhedra and have maximal local symmetry (with respect to faces).

For hereditary polyhedra, the regularity assumption on the faces has strong implications for the geometry and enables us to say a great deal about them. Our main result is the following theorem.

Theorem 1.1. *The finite hereditary polyhedra with planar regular faces in* $\mathbb{E}^3$ *are*

(a) *the nine classical regular polyhedra (Platonic solids and Kepler-Poinsot polyhedra),*

(b) *the medials of the eighteen finite regular polyhedra,*

(c) *the great ditrigonal icosidodecahedron* $(5 \cdot 3)^3$*,*

(d) *the small ditrigonal icosidodecahedron* $(\frac{5}{2} \cdot 3)^3$*, and*

(e) *the ditrigonal dodecadodecahedron* $(5 \cdot \frac{5}{2})^3$.

Theorem 1.1 might give the false impression that there are $9 + 18 + 3 = 30$ finite hereditary polyhedra with planar regular faces in $\mathbb{E}^3$. However, some polyhedra are counted more than once in the theorem, since pairs of dual finite regular polyhedra have the same medials, and the regular octahedron also occurs as the medial of the regular tetrahedron. The exact number of polyhedra turns out to be 25, not 30.

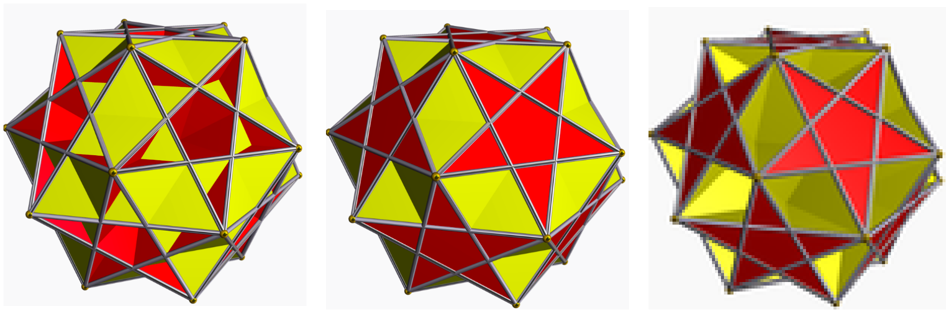

Figure 2: The great ditrigonal icosidodecahedron $(5 \cdot 3)^3$ (left), small ditrigonal icosidodecahedron $(\frac{5}{2} \cdot 3)^3$ (middle), and ditrigonal dodecadodecahedron $(5 \cdot \frac{5}{2})^3$ (right).

Theorem 1.2. *Up to similarity, there are precisely 25 finite hereditary polyhedra with planar regular faces in* $\mathbb{E}^3$.

We list these polyhedra and some of their properties in Table 1 at the end of the paper.

Figure 2 shows the three exceptional polyhedra listed in parts (c), (d), and (e) of Theorem 1.1. The Petrie duals of the classical regular polyhedra are hereditary (in fact, regular) polyhedra but have skew faces and therefore do not occur in the list of Theorem 1.1.

Historically, polyhedra with regular faces have attracted a lot of attention (for example, see [12]). Usually these figures were convex polyhedra or star-polyhedra. This paper is dedicated to the late Norman Johnson who has greatly contributed to our understanding of the geometry, combinatorics, and algebra of polyhedra and more general polyhedral structures (see Johnson [11, 10]).

2 Basic notions and facts

A (finite) *polygon*, or more specifically a *p-gon* (with $p \geqslant 3$), consists of a sequence $v_1, v_2, \ldots, v_p$ of p distinct points in $\mathbb{E}^3$, as well as of the line segments $[v_i, v_{i+1}]$ for $i = 1, \ldots, p$ (with indices considered mod p). The points are the *vertices* and the line segments are the *edges* of the polygon. A polygon is *planar* if its vertices (and edges) lie in a plane; otherwise the polygon is *skew*, or *non-planar*.

An incident vertex-edge pair of a polygon F is called a *flag* (or sometimes an *arc*) of F. A polygon F is said to be *regular* if its symmetry group $G(F)$ is transitive on the flags of F. Recall that the (geometric) *symmetry group* of a figure is the group of all isometries of the ambient space that leave the figure invariant; its elements are the *symmetries* of the figure. Thus a planar polygon has a planar symmetry group.

A planar regular polygon with p vertices is necessarily (the graph consisting of the vertices and edges of) a regular convex p-gon, denoted $\{p\}$, or a regular star polygon, denoted $\{\frac{p}{d}\}$, with $(p, d) = 1$ (see [1]). Recall that the vertices of $\{\frac{p}{d}\}$ are the same as those of $\{p\}$, and that its edges successively connect vertices d steps apart on $\{p\}$, beginning at the first vertex (say) of $\{p\}$. The symmetry group of a planar regular p-gon, the (planar) dihedral group D_p of order $2p$, by definition consists of 2-dimensional isometries, and is generated by two reflections (in lines). When the p-gon is viewed as lying in a plane of $\mathbb{E}^3$, these reflections extend in an obvious way to plane reflections generating a reflection group in $\mathbb{E}^3$ isomorphic to D_p. We call this group the *trivial extension* of D_p to $\mathbb{E}^3$, and by abuse of terminology and notation we also call this extension the dihedral group D_p.

A skew regular p-gon must have an even number of vertices p. Its symmetry group is generated by a plane reflection (interchanging the edges at a vertex) and a half-turn (about the midpoint of an edge containing that vertex), and again is isomorphic to D_p; note that in this case the product of the two generators is a rotatory reflection (the composition of a rotation, and a reflection in a plane perpendicular to the rotation axis).

A (finite *skeletal*) *polyhedron* P in $\mathbb{E}^3$ consists of a finite set of distinct points, called *vertices*, a set of line segments connecting vertices, called *edges*, and a set of polygons made up of edges, called *faces*, with the following three properties.

- The graph formed by the vertices and edges of P, called the *edge graph* (or 1-*skeleton*) of P, is connected.
- The vertex-figure at each vertex of P is connected. By the *vertex-figure* of P at a vertex v, denoted P/v, we mean the graph whose vertices are the neighbors of v in the edge graph of P and whose edges are the line segments (u, w), where (u, v) and (v, w) are edges of a common face of P.
- Each edge of P belongs to exactly two faces of P.

Note that a polyhedron is a geometric realization in $\mathbb{E}^3$, in the sense of [16, Ch. 5], of a finite abstract polyhedron and its respective map on a closed surface.

A skeletal polyhedron P is called *planar-faced* or *skew-faced* respectively, if all faces of P are planar or some faces of P are skew. We call a polyhedron P *regular-faced* if each face of P is a regular polygon (and thus is a polygon with maximum possible symmetry).

The symmetry group of a (finite) polyhedron P is a finite group of isometries of $\mathbb{E}^3$ and thus fixes the centroid of the vertex set of P, which we call the *center* of P. Throughout we assume that the center of P lies at o, the origin of $\mathbb{E}^3$. We call a face of P *central* if the center of P is the centroid of the vertex-set of the face. If a central face is planar then its ambient plane passes through the center of P. A *non-central* face of P is a face of P which is not central.

A polyhedron P is said to be (*geometrically*) *hereditary* if the symmetry group $G(F)$ of each face F of P can be viewed as a subgroup of the symmetry group $G(P)$ of P, or more informally, if each symmetry of each face F of P extends to a symmetry of P. (Note that the abstract polyhedron underlying a geometrically hereditary polyhedron P with regular faces is also combinatorially hereditary, in the sense that the combinatorial automorphism group of each face extends to a subgroup of the automorphism group of P. Combinatorially hereditary abstract polyhedra were shown in [17] to be regular or 2-orbit of type 2_{01}; see also [8] and [9].)

For a face F of a hereditary polyhedron P we let $G_P(F)$ denote the subgroup of $G(P)$ consisting of the symmetries of P which extend symmetries of F.

If a face F of a hereditary polyhedron P is skew, then each symmetry of F already is 3-dimensional and thus the extended symmetry is the symmetry itself; that is, $G_P(F) = G(F)$. Note that a regular skew face of a hereditary polyhedron must necessarily be central, since o and the center of the face must be invariant under the symmetries of the face.

However, this is different for planar faces. If a planar face F of P is non-central, then the extensions of the symmetries of F to symmetries of P still are unique, since o must be invariant; in this case, if F is a regular p-gon and $G(F) = D_p$ is identified with its trivial extension to $\mathbb{E}^3$, then $G_P(F) = G(F) = D_p$. If a planar face F of P is central, however, then the symmetries of F may occur in P in one of two ways; in fact, if F admits a reflection symmetry in a line l (through o), then this planar symmetry of F may occur either as a reflection in a plane through l perpendicular to the plane of F or as a half-turn about l. We later see that, for a regular-faced hereditary polyhedron with planar faces, each symmetry of a central face F has a unique extension to P (so reflective symmetries of F can not extend to both a plane reflection and a half-turn). The geometry of the group $G_P(F)$ then depends on the nature of these extensions but is still isomorphic to $G(F)$.

An incident vertex-edge-face triple of a polyhedron P is called a *flag* of P. A polyhedron P is (*geometrically*) *regular* if its symmetry group $G(P)$ is transitive on the flags of P. Regular polyhedra are hereditary regular-faced polyhedra.

An incident vertex-edge pair of a polyhedron P is called an *arc* of P. We say that P is *vertex-*, *edge-*, or *arc-transitive* if $G(P)$ acts transitively on the vertices, edges, or arcs of P, respectively. Clearly, if P is arc-transitive, then P is vertex-transitive and edge-transitive. For a vertex v of P, let $G_v(P)$ denote the stabilizer of v in $G(P)$.

Proposition 2.1. *Let P be a (finite) hereditary polyhedron with regular faces in $\mathbb{E}^3$. Then P is arc-transitive. In particular, the vertex-figures are mutually equivalent under $G(P)$, and the stabilizer $G_v(P)$ of a vertex v of P in $G(P)$ acts transitively on the vertices of the vertex-figure P/v at v. Moreover, the vertex-figures are planar.*

Proof. The first statement follows from [17, Prop. 1]. Any two arcs of P are related via a finite sequence of arcs such that successive arcs in the sequence are arcs of a common face of P. Since the faces are regular and thus arc-transitive under their own symmetry group, and since every symmetry of a face of P extends to a symmetry of P, it follows that P is arc-transitive. Thus P is vertex-transitive and the stabilizer $G_v(P)$ of a vertex v in $G(P)$ acts transitively on the vertices of the vertex-figure P/v at v.

Moreover, the vertex-figures must be planar since P is finite. In fact, by the vertex-transitivity, the vertices of P must all lie on a sphere centered at o; and since $G_v(P)$ acts vertex-transitively on P/v, the vertices of P/v must all lie on a sphere centered at v. Thus the vertices of P/v all lie on the intersection of the two spheres, which is a circle. This shows that P/v is planar. □

It follows that every hereditary polyhedron with regular faces is a uniform polyhedron in $\mathbb{E}^3$. Recall that a *uniform* polyhedron is a vertex-transitive polyhedron with regular faces (see [1]).

The finite uniform polyhedra with *planar* faces were classified by Coxeter, Longuet-Higgins and Miller [2] in 1954. It is customary to describe these polyhedra by a *vertex-symbol* $(n_1 \cdot n_2 \cdot \ldots \cdot n_q)$ with integral or rational entries. Here q is the valency of a vertex, and the entries $n_1, \ldots, n_q$ represent the faces that surround a vertex, in cyclic order, such that the face corresponding to n_i has Schläfli symbol $\{n_i\}$ for $i = 1, \ldots, q$ (thus the face is a convex regular n_i-gon if n_i is an integer, or a regular star-polygon $\{n_i\}$ if n_i is a fraction). For example, the small ditrigonal icosidodecahedron occurring in Theorem 1.1 and shown in Figure 2 has vertex-symbol $(\frac{5}{2} \cdot 3 \cdot \frac{5}{2} \cdot 3 \cdot \frac{5}{2} \cdot 3)$, indicating that at each vertex three pentagrams $\{\frac{5}{2}\}$ and three triangles $\{3\}$ alternate; the symbol is abbreviated to $(\frac{5}{2} \cdot 3)^3$.

For our purposes, we further refine the vertex-symbol to indicate the presence of central faces. If a polyhedron has a central face, then the superscript "$*$" in its *refined vertex-symbol* indicates that the corresponding face type represents a *central* face of the polyhedron. For example, the symbol $(\frac{5}{2} \cdot 6^* \cdot \frac{5}{2} \cdot 6^*)$ would represent a polyhedron in which two pentagrams

$\{\frac{5}{2}\}$ and two *central* regular hexagons $\{6\}$ alternate at a vertex. Thus, a polyhedron has a central face if and only if a "$*$" occurs in its refined vertex-symbol.

No classification of the finite uniform polyhedra with skew faces is known to date, but new uniform polyhedra with skew faces have recently been found in [21, 23, 24]. See also Grünbaum [7].

Note that, for a regular-faced hereditary polyhedron with vertices of valency q, the vertex stabilizers $G_v(P)$ may not be isomorphic to D_q, even though $G_v(P)$ acts vertex-transitively on the q-gonal vertex-figure P/v at v. However, the following proposition holds.

Proposition 2.2. *Let P be a (finite) regular-faced hereditary polyhedron without central faces and with vertices of valency q. Then, for every vertex v of P, the vertex stabilizer $G_v(P)$ of v in $G(P)$ is a dihedral subgroup D_q, if q is odd, or contains a dihedral group $D_{q/2}$ which acts transitively on the q vertices of the vertex-figure P/v, if q is even. Moreover, if q is odd then P is a regular polyhedron.*

Proof. By the vertex-transitivity of P it suffices to consider the vertex stabilizer subgroup for a single vertex. So let v be a vertex of P. Since the faces are non-central, each face F of P at v contributes to $G(P)$ a unique plane reflection which leaves both F and v invariant and interchanges the two edges of F meeting at v. This holds regardless of whether F is planar or skew. These reflections for the q faces at v generate a dihedral group D_q if q is odd, or $D_{q/2}$ if q is even. Note that this subgroup of $G_v(P)$ acts vertex-transitively on P/v.

If q is odd, then the dihedral subgroup D_q of $G_v(P)$ must necessarily coincide with $G_v(P)$. Hence $G_v(P)$ must contain symmetries that swap adjacent faces of P meeting at v. Thus $G_v(P)$ must act flag-transitively on the vertex-figure P/v at v, and since P is vertex-transitive, $G(P)$ itself must act flag-transitively on P. Thus P is a regular polyhedron. □

Proposition 2.1 is telling us that the vertex-figures of hereditary regular-faced polyhedra must be congruent. The faces, however, need not be congruent (even though all are regular). On the other hand, by the edge-transitivity of P there can be at most two face orbits under $G(P)$. If indeed there are two face orbits, then the two faces of P meeting at an edge of P must lie in different face orbits under $G(P)$, and hence q must be even.

If a hereditary regular-faced polyhedron P has a central planar face, then each face adjacent to any such face must either be a non-central planar face or a skew face, as we explain in a moment. As a consequence, by the edge-transitivity of P, each edge of P must lie in a central planar face as well as in a non-central planar face or a skew face. In particular, $G(P)$ must have two face orbits, one consisting of the central planar faces and the other of the non-central planar faces or the skew faces. Further, q must be even.

Note that P cannot have a pair of adjacent central planar faces. In fact, any such pair of faces would necessarily have to lie in the same plane and share o as the center. The edge transitivity then would force the entire polyhedron P to lie in this plane, with all faces sharing the same symmetry group. However this is impossible since then all faces would have to coincide; in fact, since the faces are regular, the symmetry group of a face is entirely determined by the angle subtended at o by one of its edges.

We noted earlier that, for non-central planar faces or skew faces of a hereditary regular-faced polyhedron P, there is just one way in which a planar symmetry of a face can extend to a symmetry of P. This also remains true for the central planar faces of P, for the following reason. Suppose F is a central planar face and l is a reflection line for F in the plane that contains F. There are only two isometries of $\mathbb{E}^3$ which extend the 2-dimensional reflection in l, namely the half-turn about l and the reflection in the plane perpendicular at l to the plane of F. Now if both isometries are symmetries of P, then so is their product, which is the reflection in the plane containing F. However, this reflection cannot be a symmetry, since the image of an adjacent (non-central planar, or skew, respectively) face G of F under this reflection would yield another (non-central planar, or skew) face G' of F meeting F at the same edge as G. This is impossible. Thus each planar reflection symmetry of F extends in just one way to a symmetry of P. This forces the same to be true for the rotational symmetries of F.

We also require the following two well-known concepts for polyhedra (see [1, 16, 19]).

A *Petrie polygon* of a regular polyhedron P in $\mathbb{E}^3$ is a path along edges of P such that every two, but no three, consecutive edges belong to a face of P (see [1, 3, 19]). Every regular polyhedron P gives rise to a new structure, denoted P^π and called the *Petrie dual*, or *Petrial*, of P, which in most cases is again a polyhedron (see [16, Lemma 7B3]). For example, $\{4,3\}^\pi$, the Petrial of a cube, is a polyhedron with four hexagonal skew faces.

Given a regular polyhedron P in $\mathbb{E}^3$ the *medial* $\mathrm{Me}(P)$ is a new structure, usually a polyhedron, with faces of two kinds: the polygons with vertices at the midpoints of consecutive edges in a face of P, and the polygons with vertices at the midpoints of consecutive edges meeting at a vertex of P. The medial of a regular polyhedron may not always be a polyhedron. For example, in the blended polyhedron $\{3,6\}\#\{\,\}$ edges can cross at midpoints and hence the edge midpoints occupy the same point in $\mathbb{E}^3$ (see [16, Ch. 7E]). Thus its medial is not a polyhedron.

3 Planar-faced polyhedra with no central faces

In the next two sections, we describe and characterize the finite regular-faced hereditary polyhedra P in $\mathbb{E}^3$ all of whose faces are planar. Their vertex-figures are also planar, by Proposition 2.1. Our analysis of these polyhedra greatly depends on whether or not they have central faces.

In this section, we deal with the finite planar-faced hereditary polyhedra P with no central faces. Polyhedra with central faces are discussed in the next section.

So let P be a finite hereditary polyhedron with regular faces all of which are planar and non-central, and with vertices of valency q. Recall our standing assumption that the center of P lies at o. Then each symmetry of each face F of P is extended to P in the trivial way. Thus the subgroup $G_P(F)$ of $G(P)$ is a dihedral group, namely the trivial extension of the dihedral symmetry group $G(F)$ of F. In particular, $G(P)$ must contain many plane reflections. It follows that $G(P)$ must be the full symmetry group of a Platonic solid R (say), and that the face centers of P, being centers of rotation of a regular face, must lie on axes of rotation of R. In particular, each face F of P must have 3, 4 or 5 vertices.

As P has no central faces, we know from Proposition 2.2 that the vertex stabilizer $G_v(P)$ of a vertex v is a dihedral subgroup D_q if q is odd, or contains a dihedral subgroup $D_{q/2}$ if q is even. In particular, each vertex v of P is a center of rotational symmetry of P about an axis passing through v and o. Thus v must lie on a rotation axis of the underlying Platonic solid R and therefore coincide with a vertex, the midpoint of an edge, or the center of a face of R, up to rescaling of R. Clearly, by replacing R by its dual (if need be), we may assume that the vertices of P lie either at vertices or edge midpoints of R. Then, since $G(P) = G(R)$ and P is vertex-transitive, the vertex set of P coincides with either the full vertex set of R or the full set of edge midpoints of R.

If the vertex valency q is odd, then Proposition 2.2 is telling us that P is a regular polyhedron and that $G_v(P) = D_q$ for every vertex v of P. Thus the vertex-figures are congruent regular polygons, and by Proposition 2.1 are planar. Inspection of the list of finite regular polyhedra in $\mathbb{E}^3$ then establishes the following proposition (see [16]).

Proposition 3.1. *Let P be a (finite) hereditary polyhedron with planar regular faces, all non-central, and with vertices of odd valency. Then P is either a Platonic solid or a Kepler-Poinsot polyhedron.*

When the vertex valency q of P is even, the $(q/2)$-fold rotation about a vertex of P has order 2, 3, 4, or 5, and so $q = 4$, 6, 8, or 10. This case is more involved. The remainder of this section deals with the proof of the following proposition.

Proposition 3.2. *Let P be a (finite) hereditary polyhedron with planar regular faces, all non-central, and with vertices of even valency. Then P is the medial of a Platonic solid, the medial of a Kepler-Poinsot polyhedron, a small ditrigonal icosidodecahedron $(\frac{5}{2}\cdot 3)^3$, a great ditrigonal icosidodecahedron $(5\cdot 3)^3$, or a ditrigonal dodecadodecahedron $(5\cdot\frac{5}{2})^3$.*

Proof. The proof of Proposition 3.2 investigates the two possible placements of the vertices of P on R, with R as above, namely either at the vertices of R (Case 1) or at the edge midpoints of R (Case 2). So let the vertex valency q of P be even.

Case 1: The vertices of P lie at the vertices of R.

We first rule out the possibility that R is a tetrahedron $\{3,3\}$, a cube $\{4,3\}$, or an icosahedron $\{3,5\}$. Clearly, since $q \geqslant 4$, R cannot be $\{3,3\}$. To see that $R = \{3,5\}$ is impossible, we note that since q is even and P in this case has 5-fold rotational symmetries about its vertices, q must be 10 and the vertex-figures of P must be planar decagons; however, no ten vertices of $\{3,5\}$ lie in a common plane. Similarly, $R = \{4,3\}$ is impossible since no six vertices of $\{4,3\}$ lie in a common plane.

If $R = \{3,4\}$, then clearly $q = 4$ and the neighbors of a vertex v in P are just those in R. Since a 4-fold rotation about v must cyclically permute the faces of P at v, and since the faces are planar, the faces of P at v must necessarily be the faces of R at v. Hence $P = \{3,4\}$, which is the medial of the tetrahedron.

The case when $R = \{5,3\}$ is more complicated. By arguments as above we find that $q = 6$, and that the vertex-figure at a vertex v of P is a planar hexagon with D_3-symmetry and with vertices among those of R. It is easy to see that only two configurations for the convex hull of the vertex-figure at v are possible, as indicated by the yellow and blue polygons in Figure 3. In the first (yellow) configuration for the convex hull, the vertex-figure of P at v has as its vertices the vertices of the three pentagons of R at v that lie on edges opposite to v on these pentagons. In the second (blue) configuration for the convex hull, the vertices are the antipodes of the vertices of the hexagon in the first configuration. We next consider these two configurations in turn to show that the first leads to three hereditary polyhedra with non-central planar faces, and that the second cannot occur.

For the first configuration of the convex hull three scenarios are possible and each contributes one polyhedron.

First suppose that the vertex-figure of P at v is a convex hexagon and thus coincides with its convex hull. Then the edges opposite to v on the pentagon faces of R at v are among the edges of the vertex-figure of P at v. In P, these edges appear as the vertex-figures of pentagram faces $\{\frac{5}{2}\}$ at v inscribed in the pentagon faces of R at v. The other

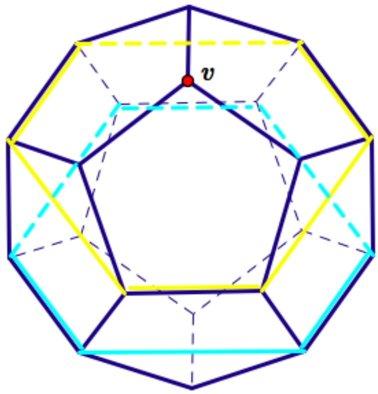

Figure 3: Configurations for the convex hull of the vertex-figure at v when P has the same vertex-set as $R = \{5,3\}$.

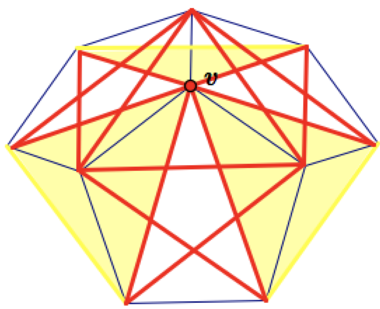

Figure 4: Faces of P at v, for the yellow (first) configuration of Figure 3 when the vertex-figure at v is a convex hexagon.

faces of P at v are equilateral triangles formed by the three vertices that are adjacent in R to a neighbour of v in R. Thus three pentagrams and three triangles alternate around v in P, as illustrated in Figure 4. The resulting polyhedron P is the uniform polyhedron $(\frac{5}{2}\cdot 3)^3$ called the small ditrigonal icosidodecahedron (see [2]).

Next suppose that (still in the first configuration for the convex hull) the vertex-figure of P at v is not a convex hexagon. In this case the vertex-figure is a non-convex hexagon of one of two kinds.

The first kind of non-convex hexagonal vertex-figure is indicated with dashed red lines in Figure 5. Here the edges opposite to v on the pentagon faces of R at v are not among the edges of the vertex-figure of P at v. The faces of P at v again are of two kinds alternating around v. There are three regular convex pentagons "cutting across" R (shown in heavy red lines in Figure 5), and there are three equilateral triangles of the same kind as before, each formed by the three vertices that are adjacent in R to a neighbour of v in R. Now P is the uniform polyhedron $(5\cdot 3)^3$ called the great ditrigonal icosidodecahedron (see [2]).

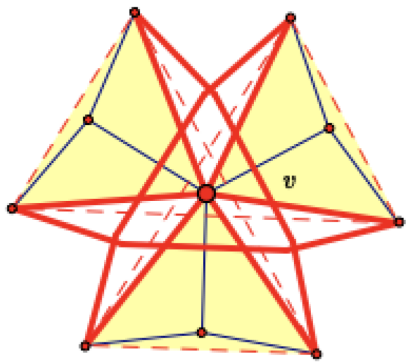

Figure 5: Faces of P at v, for the yellow (first) configuration of Figure 3 when the vertex-figure at v is a non-convex hexagon not sharing any edges with $R = \{5, 3\}$.

The second kind of non-convex hexagonal vertex-figure is indicated with dashed red lines in Figure 6. Now the edges opposite to v on the pentagon faces of R at v are edges of the vertex-figure of P at v. Again two kinds of faces of P alternate at v. There are three regular convex pentagons "cutting across" R (shown in heavy red lines in Figure 6), and there are three pentagrams inscribed in the pentagon faces of R at v. Thus P is the uniform polyhedron $(5 \cdot \frac{5}{2})^3$ called the ditrigonal dodecadodecahedron (see [2]).

The second (blue) configuration of Figure 3 for the convex hull of the vertex-figure of P at v can be ruled out as follows. As for the first configuration of Figure 3, the vertex-figure of P at v must either be a convex hexagon identical with the convex hull, or a non-convex hexagon sharing three edges with the convex hull. In either case, each edge of the vertex-figure of P at v which is an edge of the convex hull is necessarily the vertex-figure of a face of P at v, and therefore must span, together with v, the plane of this face. As this plane contains only three vertices of R, the face itself could only be a (non-regular) triangle, so P could not be regular-faced. Thus the second configuration of Figure 3 cannot occur.

This completes the enumeration of the polyhedra P for Case 1. We next investigate the second possibility for the placement of vertices of P relative to R. Recall that q is even.

Case 2: The vertices of P lie at the edge midpoints of R.

In this case necessarily $q = 4$ since now the vertices of P have only D_2-symmetry. Thus the vertex-figures are congruent planar 4-gons with D_2-symmetry. As pairs of dual Platonic solids yield the same set of edge midpoints up to similarity, it suffices to consider only the regular polyhedra $R = \{3, 3\}$, $\{3, 4\}$, and $\{5, 3\}$.

The first possibility can be ruled out immediately. If $R = \{3, 3\}$, then the (planar) faces of P must be regular triangles since R has only rotations of order 2 or 3. The vertices of P are just those of a regular octahedron, and the vertex-figures are given by equatorial squares of this octahedron. Hence P must coincide with this octahedron. But then $G(P) \neq G(R)$, which contradicts our choice of R. (Recall that the octahedron occurred as the medial of $\{3, 3\}$ in Case 1.) Thus this choice R does not contribute a polyhedron.

If $R = \{3, 4\}$, then the faces of P must be regular triangles or squares since R has only rotations of order 2, 3 or 4. Now the vertices of P are just those of a cuboctahedron

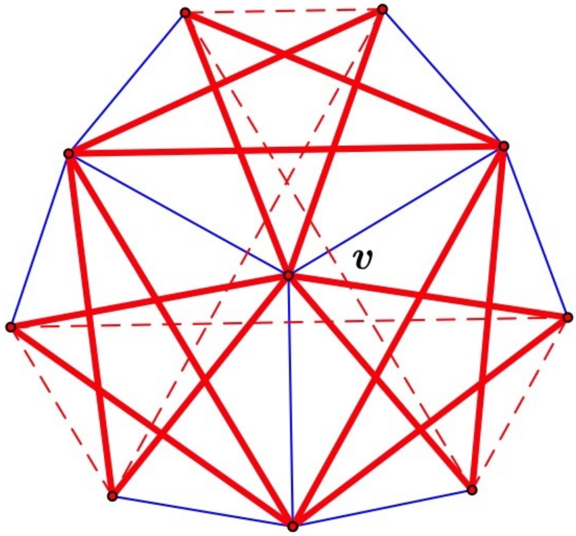

Figure 6: Faces of P at v, for the yellow (first) configuration of Figure 3 when the vertex-figure at v is a non-convex hexagon sharing edges with pentagonal faces of $R = \{5, 3\}$ at v.

$\left\{ \begin{smallmatrix} 3 \\ 4 \end{smallmatrix} \right\}$. The vertex-figure at a vertex v of P must necessarily be convex. In fact, opposite vertices of the convex hull of the vertex-figure at v cannot be joined (in a bowtie fashion) by an edge of the vertex-figure, since otherwise the planar face at v determined by this edge would need to be central, in violation to our standing assumption in this section that P has no central faces. There are only two possible configurations (shown in yellow and light blue in Figure 7) for the four neighbours of v in P.

In the first (yellow) configuration, the neighbors of v in P are the same as those of v in the cuboctahedron. In this case P must coincide with the cuboctahedron and thus be the medial of $\{3, 4\}$. In fact, the triangular faces of P at v must be just those of the cuboctahedron, and then this must also hold for the square faces.

In the second (light blue) configuration, the neighbors of v in P are the antipodal points of those in the first configuration. But this choice can be ruled out since the triangular faces at v could not be regular.

If $R = \{3, 5\}$, then the faces of P must be regular triangles, convex pentagons, or pentagrams, since R has only rotations of order 2, 3 or 5. Now the vertices of P are just those of an icosidodecahedron $\left\{ \begin{smallmatrix} 3 \\ 5 \end{smallmatrix} \right\}$.

Any triangular face of P must either be inscribed in a triangle face of R as shown in Figure 8(a), or have as its vertices the midpoints of the edges of R which emanate from the vertices of a triangle face of R but do not belong to the adjacent triangle faces (see Figure 8(b)). Clearly, not all faces of P can be triangles. Similarly, by the D_5-symmetry of the pentagonal faces of P, there can only be two possible configurations for the vertex sets of pentagonal faces of P. The convex hulls of these vertex sets are shown in Figures 8(c,d).

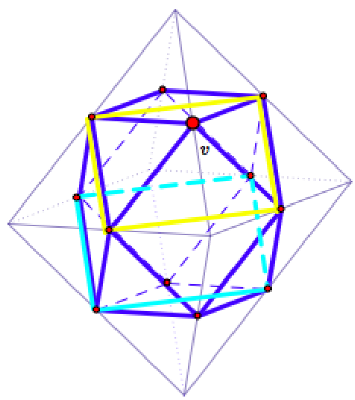

Figure 7: Possible convex hulls of the vertex-figures of P at v when the vertices of P lie at the edge midpoints of an octahedron.

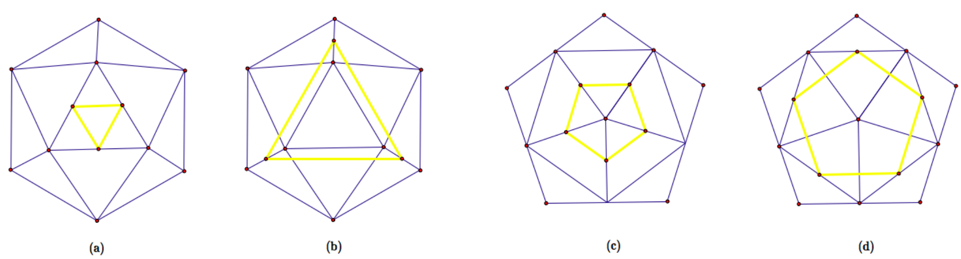

Figure 8: Possible convex hulls of the faces of P when the vertices of P lie at the edge midpoints of $\{3, 5\}$.

First suppose that P indeed has a triangular face. If the triangular faces are positioned as in Figure 8(a), then the pentagonal faces must be convex and P itself must be an icosidodecahedron, the medial of the icosahedron. On the other hand, if the triangular faces are as in Figure 8(b), then the pentagonal faces must be pentagrams with vertex sets located as in Figure 8(d), and P itself must be $\left\{ \begin{smallmatrix} 3 \\ \frac{5}{2} \end{smallmatrix} \right\}$, the medial of the Kepler-Poinsot polyhedron $\{3, \frac{5}{2}\}$ (or its dual $\{\frac{5}{2}, 3\}$).

If P has no triangular faces, then all its faces must be convex pentagons or pentagrams. If a pentagonal face with vertices located as in Figure 8(c) occurs, then this must be a pentagram face whose adjacent faces are convex pentagon faces with vertex sets located as in Figure 8(d). Then P must be $\left\{ \begin{smallmatrix} 5 \\ \frac{5}{2} \end{smallmatrix} \right\}$, the medial of $\{5, \frac{5}{2}\}$ (or its dual $\{\frac{5}{2}, 5\}$). Lastly, we can rule out the possibility that all pentagonal faces of P have vertex sets as in Figure 8(d). In fact, otherwise all faces of P must be convex pentagons, or all faces of P must be pentagrams, in both cases with four faces meeting at a vertex. But the vertex configurations of Figure 8(d) arising from two different vertices of the icosahedron R (each corresponding to a point like the central point in the figure) can never intersect in more than one point, so adjacent faces of P cannot both be convex pentagons or pentagrams.

This settles the enumeration of the polyhedra P for Case 2, and completes the proof of Proposition 3.2. □

4 Planar-faced polyhedra with a central face

In this section, we treat the finite hereditary polyhedra P with planar regular faces some of which are central. So let P be a polyhedron of this kind. Recall from Section 2 that then each edge of P must lie in a central planar face and a non-central planar face, and that $G(P)$ must have two face orbits given by the central faces respectively the non-central faces of P. Moreover, the vertex valency q is even and the vertex-figures are planar.

First observe that the reflections in the perpendicular bisectors of edges of P are symmetries of P. In fact, the planar symmetry group of the non-central face at a given edge, trivially extended to a subgroup of $G(P)$, is generated by plane reflections and in particular contains the reflection in the perpendicular bisector of this edge.

Next we need to analyze the way in which the planar symmetries of central faces F that interchange the two edges of F at a vertex of F appear in $G(P)$. It turns out that there can only be two possible scenarios: either all such symmetries appear as plane reflections, or all appear as half-turns. In particular we will see that the first scenario will not occur.

The goal of this section is to prove the following proposition.

Proposition 4.1. *Let P be a (finite) hereditary polyhedron with regular planar faces, including some central faces. Then P is the medial of the Petrie dual of either a Platonic solid or a Kepler-Poinsot polyhedron.*

Proof. The proof investigates the two possible ways (Cases 1 and 2 below, respectively) in which the planar reflective symmetries of a central face are extended to symmetries of P, namely either all as plane reflections or one half as plane reflections (interchanging the two vertices of an edge) and the other half as half-turns (interchanging the two edges at a vertex). The behavior is uniform across all central faces, since any two central faces are equivalent under $G(P)$. If the reflective symmetries of all central faces are extended to P by plane reflections, then the reflective symmetries of all faces of P are extended to P by plane reflections, since we know this to be true for the non-central faces.

Now suppose P is a finite hereditary polyhedron with regular planar faces, including some central faces.

Case 1: The planar reflective symmetries of central faces are extended to P by plane reflections.

We show that this case does not occur; in other words, there are no polyhedra with central faces in which all reflective symmetries of all faces are extended by plane reflections.

Suppose that P is a polyhedron with central faces such that all planar reflective symmetries of all faces are extended to P by plane reflections. Then all subgroups of $G(P)$ extending planar symmetry groups of faces of P are generated by plane reflections. Again, as in Section 3, the vertices of P must lie at the vertices or the edge midpoints of a Platonic solid R with $G(R) = G(P)$.

The case $R = \{3, 3\}$ can be eliminated as follows. In this case the vertices of P could only be the six edge midpoints of R, since otherwise P could not have a central face. Then the central faces of P could only be given by the three equatorial squares of the octahedron formed by these six vertices, and the non-central faces by four alternate triangle faces of this octahedron. Thus P would have to be $\mathrm{Me}(\{3, 3\}^\pi)$, the medial of the Petrial of $\{3, 3\}$. However, the planar reflective symmetries of the central faces of $\mathrm{Me}(\{3, 3\}^\pi)$ that interchange the edges at a vertex are not extended to $\mathrm{Me}(\{3, 3\}^\pi)$ by plane reflections, so in the present context this polyhedron must be rejected by our case assumption. Note, however, that $\mathrm{Me}(\{3, 3\}^\pi)$ will occur as a legitimate polyhedron in Case 2.

Now let $R = \{3, 4\}$. If the vertices of P are just those of R, then again P must be the medial of the Petrial of a tetrahedron and can be eliminated as before (or here, alternatively, because $G(P) \neq G(R)$). The case when the vertices of P are the edge midpoints of R (that is, the vertices of a cuboctahedron) can be ruled out as follows. Since a central face would need to have full dihedral symmetry, it could only be a triangle or square. There are no central triangles with D_3-symmetry spanned by vertices of a cuboctahedron, so the central faces could only be squares. However, the squares inscribed as central squares in the vertex-set of a cuboctahedron are such that each vertex of the cuboctahedron can only lie in one such square. Thus this possibility is excluded as well.

The cube $R = \{4, 3\}$ also does not contribute a polyhedron. The case of vertex placements for P at the edge-midpoints of R is the same as for $\{3, 4\}$ and can again be ruled out. The vertices of P also cannot lie at the vertices of R, since there are no central regular polygons spanned by vertices of the cube.

The two cases $R = \{3, 5\}$ and $R = \{5, 3\}$ similarly do not give a polyhedron. In fact, the central regular faces of P would have to be triangles, pentagons or pentagrams. But no such faces can be placed with full dihedral symmetry. This applies to both kinds of vertex placements for P on R.

In summary, Case 1 does not lead to a hereditary polyhedron of the desired kind.

Case 2: Some planar reflective symmetries of central faces are not extended to P by plane reflections.

We know from our previous discussion that the reflective symmetries of faces which are not extended to P by plane reflections, are just the reflective symmetries of central faces which interchange the two edges at a vertex, and that these are extended to P by half-turns. Thus the subgroups of $G(P)$ extending symmetry groups of central faces are generated by a plane reflection and a half-turn. In particular, the central faces must have an even number of vertices. The subgroups of $G(P)$ extending symmetry groups of non-central faces still are generated by two plane reflections.

We show that $q = 4$ and that the vertices of P must lie on axes of 2-fold rotation. Suppose v is a vertex, F a central face at v, and G a non-central face at v adjacent to F. Let r_F and r_G respectively denote the extended symmetries of the faces F and G that interchange the edges at v. Then it is clear that the product $r_F r_G$ has order $q/2$. (Recall that q is even.) On the other hand, r_F is the half-turn about the line through o and v, and r_G is a reflection in a plane through o and v perpendicular to the plane of G. Hence, since the rotation axes of r_F lies in the reflection plane of r_G, the product $r_F r_G$ must be a reflection in the plane which is perpendicular to the reflection plane of r_G and meets this plane in the rotation axis of r_F. Thus $q = 4$, and there are just two central faces and two non-central faces meeting in alternating fashion at v. If F' and G' respectively are the central and non-central faces of P at v distinct from F and G, and $r_{F'}$ and $r_{G'}$ are the extended symmetries of F' and G' defined in the same way as r_F and r_G for F and G, then necessarily $r_{F'} = r_F$ and $r_{G'} = r_G$, and $r_F r_G$ interchanges F and F', and G and G'.

It follows as before that the vertices of P must lie at the vertices or edge midpoints of a Platonic solid R with $G(R) = G(P)$. Clearly, by what we just said, the vertices of P could only lie at vertices of R if $R = \{3, 4\}$ or $\{4, 3\}$ (but below these possibilities will be ruled out as well).

If $R = \{3, 3\}$ then vertex placements for P at the edge midpoints of R are possible precisely for the reason that they were ruled out under Case 1. In fact, the resulting polyhedron is $\mathrm{Me}(\{3, 3\}^\pi)$, the medial of the Petrie dual of $\{3, 3\}$, also known as the tetrahemihexahedron (see [2]). In $\mathrm{Me}(\{3, 3\}^\pi)$, the planar symmetries of the central faces that interchange the edges at a vertex indeed are extended by half-turns, not plane reflections. Thus $R = \{3, 3\}$ contributes $\mathrm{Me}(\{3, 3\}^\pi)$.

Now let $R = \{3, 4\}$. In this case the vertex placements for P at the vertices of R can be ruled out, since the only possible candidate for a polyhedron, $\mathrm{Me}(\{3, 3\}^\pi)$, has a smaller symmetry group than R. This polyhedron occurred in the previous case for R. On the other hand, the vertex placements for P at the edge midpoints of R lead to two possible polyhedra, as we can see as follows. First note that, under the assumption of Case 2, the only possible central faces are the equatorial hexagons of the cuboctahedron determined by the edge midpoints of R, or triangles with vertices among those of an equatorial hexagon. The latter are excluded since the central faces must have an even number of vertices. Thus the central faces are the equatorial hexagons of the cuboctahedron. The non-central faces must necessarily be triangles or squares, as only these have dihedral symmetry. In either case the non-central faces must be faces of the cuboctahedron. If the non-central faces are triangles, then P is the medial of the Petrie dual of a cube, $\mathrm{Me}(\{4, 3\}^\pi)$, also called the octahemioctahedron [2]. If the non-central faces are squares, then P is the medial of the Petrie dual of the octahedron, $\mathrm{Me}(\{3, 4\}^\pi)$, also called the cubohemioctahedron [2].

For $R = \{4, 3\}$, the polyhedron P cannot have its vertices at the vertices of R, since a central face could not be regular. On the other hand, by duality, the vertex placements for P at the edge-midpoints of R result in the same two polyhedra as in the previous case.

Now let $R = \{3, 5\}$. Suppose the vertices of P lie at the edge midpoints of R. The central faces all must have 2-fold, 3-fold, or 5-fold rotational symmetry, as well as an even number of vertices, and thus must be squares, hexagons, or decagons. Squares can be ruled out immediately. In fact, although a square can be placed as a central square with its vertices at edge midpoints of R, this cannot be done in such a way that all symmetries of

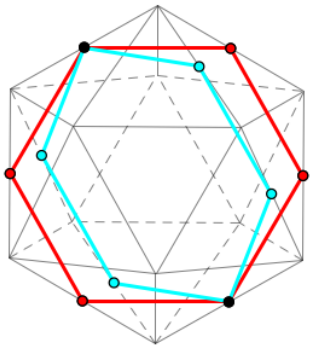

Figure 9: Central hexagonal faces with vertices at edge midpoints of an icosahedron.

the square extend to symmetries of P (or equivalently, R), so P could not be hereditary.

On the other hand, hexagonal central faces indeed can occur. Figure 9 shows how the vertices of a central regular hexagon can be placed at the edge midpoints of R, in such a way that the half-turns about the edges of R that contain a vertex of this hexagon map the hexagon to itself. Each pair of antipodal vertices of this hexagon also lies in another central hexagon of the same kind. These two hexagons are interchanged by the reflection in the plane spanned by the pair of antipodal edges of R determining the common vertices of the hexagons. Note that the six edges of R whose midpoints are the vertices of any such hexagon form a regular skew hexagon centered at o; this is a 2-zigzag of R (see [16, p. 196]). At each vertex v of P, two central hexagonal faces and two non-central faces meet in an alternating fashion. The angle at v between an edge of a central hexagon at v, and an edge of the other central hexagon at v, is either $2\pi/5$ or $3\pi/5$ (see again Figure 9). Thus, in between the two central hexagons meeting at v can fit only two regular convex pentagons or two regular pentagrams. If the pentagonal faces are convex, then P is $\mathrm{Me}(\{\frac{5}{2}, 5\}^\pi)$, the medial of the Petrie dual of the regular star polyhedron $\{\frac{5}{2}, 5\}$, with vertex-symbol $(5 \cdot 6^*)^2$, also called the great dodecahemi-icosahedron [2]. If the pentagonal faces are pentagrams, then P is $\mathrm{Me}(\{5, \frac{5}{2}\}^\pi)$, the medial of the Petrie dual of the regular star polyhedron $\{5, \frac{5}{2}\}$, with vertex-symbol $(\frac{5}{2} \cdot 6^*)^2$, called the small dodecahemi-icosahedron [2].

There are also four hereditary polyhedra P where the central faces are regular decagons (and the vertices still are at the edge midpoints of R). Their central faces are regular convex decagons $\{10\}$ or regular star decagons $\{\frac{10}{3}\}$, with each central face lying in a plane perpendicular to a 5-fold rotation axis of R.

If the central faces of P are convex decagons, then each pair of antipodal vertices of a central decagon also lies in another central decagon of the same kind, as shown in Figure 10. This only leaves room at a vertex for non-central faces which are regular triangles or regular convex pentagons. If the non-central faces are triangles, then P is $\mathrm{Me}(\{5, 3\}^\pi)$, the medial of the Petrie dual of a dodecahedron, with vertex-symbol $(3 \cdot 10^*)^2$, known as the small icosihemidodecahedron [2]. If the non-central faces are convex pentagons, then P is $\mathrm{Me}(\{3, 5\}^\pi)$, the medial of the Petrie dual of an icosahedron, with vertex-symbol $(5 \cdot 10^*)^2$, called the small dodecahemidodecahedron [2].

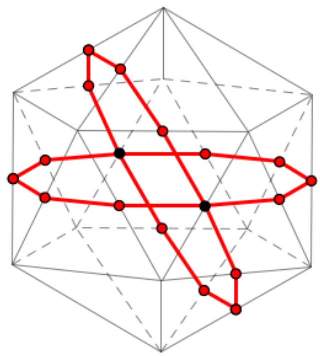

Figure 10: Central decagonal faces with vertices at edge midpoints of an icosahedron.

On the other hand, if the central faces of P are star decagons $\{\frac{10}{3}\}$, which we may picture as inscribed in a regular decagon of the kind shown in Figure 10, then the non-central faces must either be regular triangles or regular pentagrams $\{\frac{5}{2}\}$. If the non-central faces are triangles, then P is a great icosihemidodecahedron [2], $\mathrm{Me}(\{\frac{5}{2},3\}^{\pi})$, the medial of the Petrie dual of $\{\frac{5}{2},3\}$, with vertex-symbol $(3\cdot(\frac{10}{3})^{*})^{2}$. If the non-central faces are pentagrams, then P is a great dodecahemidodecahedron [2], $\mathrm{Me}(\{3,\frac{5}{2}\}^{\pi})$, the medial of the Petrie dual of $\{3,\frac{5}{2}\}$, with vertex-symbol $(\frac{5}{2}\cdot(\frac{10}{3})^{*})^{2}$.

Finally, appealing to duality, for $R=\{5,3\}$ the vertex placements for P at the edge midpoints of R produce the same four polyhedra as in the previous case.

This settles the enumeration of the polyhedra in Case 2. Now the proof of Proposition 4.1 is complete. □

The final step of the proof of Theorem 1.1 consists of drawing together Propositions 3.1 and 4.1. Propositions 3.1 describes the finite polyhedra with no central planar face, while Propositions 4.1 deals with the polyhedra that have central planar faces. This leads to the desired result.

5 The enumeration

As pointed out earlier, several polyhedra listed in Theorem 1.1 are counted more than once in the theorem. For example, each pair of dual finite regular polyhedra gives the same medial. The Platonic solids and Kepler-Poinsot polyhedra each have a geometric dual which is also regular, but their Petrie duals do not. The Petrie duals of course have combinatorial duals, but these are not realizable as regular geometric polyhedra in $\mathbb{E}^3$. Leaving aside the octahedron, which is already counted in the list of Platonic solids but also occurs as the medial of the tetrahedron, we therefore can obtain at most 4+9=13 different medials (other than the octahedron) from regular polyhedra. This then leaves at most 25 possible polyhedra.

Inspection of the 25 polyhedra shows that these are indeed different, that is, mutually geometrically non-similar. The arguments are based on a comparison of the vertex-symbols as well as on the existence and nature of central faces (if any).

In Table 1, we list the 25 polyhedra along with the refined vertex-symbols, symmetry groups, and relevant internal references. Recall that the superscript π denotes the Petrie-dual, and that the superscript "$*$" in a vertex-symbol means that the corresponding face type represents a *central* face of the polyhedron. For example, the medial of the Petrie dual of the Kepler-Poinsot polyhedron $\{\frac{5}{2},3\}$, denoted $\mathrm{Me}(\{\frac{5}{2},3\}^{\pi})$, has vertex-symbol $(3\cdot(\frac{10}{3})^{*})^{2}$, indicating that two regular triangles $\{3\}$ and two *central* regular star-decagons $\{\frac{10}{3}\}$ alternate at a vertex. A vertex-symbol only contains a superscript "$*$" if the polyhedron has a central face. The next to last column lists the symmetry groups, with $[p,q]$ denoting the symmetry group of the Platonic solids $\{p,q\}$. The last column of the table gives the internal reference where the corresponding polyhedron is described or derived; for example, 4.1/C2 means "Proposition 4.1, Case 2 of its proof".

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Polyhedra	Description	Vertex-symbol	Group	Proposition/ Case
Platonic	$\{3,3\}$	$(3)^3$	$[3,3]$	3.1
	$\{3,4\} = \mathrm{Me}(\{3,3\})$	$(3)^4$	$[3,4]$	3.2/C1
	$\{4,3\}$	$(4)^3$	$[3,4]$	3.1
	$\{3,5\}$	$(3)^5$	$[3,5]$	3.1
	$\{5,3\}$	$(5)^3$	$[3,5]$	3.1
Kepler-Poinsot	$\{3,\frac{5}{2}\}$	$(3)^5$	$[3,5]$	3.1
	$\{\frac{5}{2},3\}$	$(\frac{5}{2})^3$	$[3,5]$	3.1
	$\{5,\frac{5}{2}\}$	$(5)^5$	$[3,5]$	3.1
	$\{\frac{5}{2},5\}$	$(\frac{5}{2})^5$	$[3,5]$	3.1
Medials	$\mathrm{Me}(\{3,4\}) = \mathrm{Me}(\{4,3\})$	$(3\cdot 4)^2$	$[3,4]$	3.2/C2
	$\mathrm{Me}(\{3,5\}) = \mathrm{Me}(\{5,3\})$	$(3\cdot 5)^2$	$[3,5]$	3.2/C2
	$\mathrm{Me}(\{3,\frac{5}{2}\}) = \mathrm{Me}(\{\frac{5}{2},3\})$	$(3\cdot \frac{5}{2})^2$	$[3,5]$	3.2/C2
	$\mathrm{Me}(\{5,\frac{5}{2}\}) = \mathrm{Me}(\{\frac{5}{2},5\})$	$(5\cdot \frac{5}{2})^2$	$[3,5]$	3.2/C2
	$\mathrm{Me}(\{3,3\}^\pi)$	$(3\cdot 4^*)^2$	$[3,3]$	4.1/C2
	$\mathrm{Me}(\{3,4\}^\pi)$	$(4\cdot 6^*)^2$	$[3,4]$	4.1/C2
	$\mathrm{Me}(\{4,3\}^\pi)$	$(3\cdot 6^*)^2$	$[3,4]$	4.1/C2
	$\mathrm{Me}(\{3,5\}^\pi)$	$(5\cdot 10^*)^2$	$[3,5]$	4.1/C2
	$\mathrm{Me}(\{5,3\}^\pi)$	$(3\cdot 10^*)^2$	$[3,5]$	4.1/C2
	$\mathrm{Me}(\{3,\frac{5}{2}\}^\pi)$	$(\frac{5}{2}\cdot (\frac{10}{3})^*)^2$	$[3,5]$	4.1/C2
	$\mathrm{Me}(\{\frac{5}{2},3\}^\pi)$	$(3\cdot (\frac{10}{3})^*)^2$	$[3,5]$	4.1/C2
	$\mathrm{Me}(\{5,\frac{5}{2}\}^\pi)$	$(\frac{5}{2}\cdot 6^*)^2$	$[3,5]$	4.1/C2
	$\mathrm{Me}(\{\frac{5}{2},5\}^\pi)$	$(5\cdot 6^*)^2$	$[3,5]$	4.1/C2
Exceptional		$(3\cdot 5)^2$	$[3,5]$	3.2/C1
		$(3\cdot \frac{5}{2})^2$	$[3,5]$	3.2/C1
		$(5\cdot \frac{5}{2})^2$	$[3,5]$	3.2/C1

Table 1: The 25 finite hereditary polyhedra with planar regular faces in $\mathbb{E}^3$.

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On median and quartile sets of ordered random variables*

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Abstract

We give new results about the set of all medians, the set of all first quartiles and the set of all third quartiles of a finite dataset. We also give new and interesting results about relationships between these sets. We also use these results to provide an elementary correctness proof of the Langford's doubling method.

Keywords: Statistics, probability, median, first quartile, third quartile, median set, first quartile set, third quartile set.

Math. Subj. Class. (2020): 62-07, 60E05, 60-08, 60A05, 62A01

1 Introduction

Quantiles play a fundamental role in statistics: they are the critical values used in hypothesis testing and interval estimation. Often they are the characteristics of distributions we usually wish to estimate. The use of quantiles as primary measure of performance has

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gained prominence, particularly in microeconomic, financial and environmental analysis and others. Quartiles (i.e 0.25, 0.50, and 0,75 quantiles) are used in elementary statistics very early, c.f. for drawing box and whisker plots.

Whereas there is no dispute that the median of an ordered dataset is either the middle element or the arithmetic mean of the two middle elements (when the number of elements is even), the situation is seemingly much more complicated when quartiles are considered. There are many well-known formulas and algorithms that give certain values, claiming for these values to be medians (or quartiles) for a given statistical data (for examples see [5]). However, the trouble begins when realizing that different formulas (or algorithms) may give different values. Many authors or users of such formulas or algorithms go even further by taking the value obtained by such a formula or an algorithm to be the definition of the median or the first quartile or the third quartile of a given data. As a result, going through the literature, one may find it very difficult to find and then choose an appropriate definition (formula, algorithm) of a median or a quartile to use it for the statistical analysis of a given data. In [2, 5] provide references and comparison of several methods for computing the quartiles of a finite data set that appear in the literature and in software. While it is well known that these methods do not always give the same results, Langford writes that the *"situation is far worse than most realize "* [5]. Although the differences tend to be small, Langford further answered the question *"Why worry? The differences are small so who cares? "* with words of [1]:

> *"Before we go into any details, let us point out that the numerical differences between answers produced by the different methods are not necessarily large; indeed, they may be very small. Yet if quartiles are used, say to establish criteria for making decisions, the method of their calculation becomes of critical concern. For instance, if sales quotas are established from historical data, and salespersons in the highest quarter of the quota are to receive bonuses, while those in the lowest quarter are to be fired, establishing these boundaries is of interest to both employer and employee. In addition, computer-software users are sometimes unaware of the fact that different methods can provide different answers to their problems, and they may not know which method of calculating quartiles is actually provided by their software."*

Langford [5] also proposes a method that is consistent with the CDF (cumulative distribution function). The method is slightly more complicated than some other methods used, however it is not too much involved and there are equivalent methods that can be used in the classroom [10, 9]. Indeed, the discussion about quartiles in teaching elementary statistics is considerable, c.f. [10, 1, 4, 5, 9]. In short, some of the elementary methods are based on the idea that a quartile is a median of the lower, or the upper half of the dataset. The question arises what is the half of dataset when it has an odd number of elements. Langford naturally answers with the idea of doubling the dataset thus assuring the even number of elements, while the quantile values remain the same.

On the positive side, it seems that all methods have one thing in common: they all expect the following to hold:

1. the median to be such a value $m \in \mathbb{R}$, for which at least half of the data is less or equal to m and at least half of the data is greater or equal to m,
2. the first quartile to be such a value $q_1 \in \mathbb{R}$, for which at least quarter of the data is less or equal to q_1 and at least three quarters of the data is greater or equal to q_1,

3. the third quartile to be such a value $q_3 \in \mathbb{R}$, for which at least three quarters of the data is less or equal to q_3 and at least quarter of the data is greater or equal to q_3.

We will use this fact as a motivation to define the median set, the first quartile set, and the third quartile set of a given data.

The main contribution of this paper is the idea to redefine the median, and the quartiles, and possibly more general, the quantiles as sets (intervals) instead of the usual consideration of this notions as reals. We indicate that in this way we may avoid the dispute caused by various methods, algorithms, and even definitions of quartiles. We also show that some methods for computing the quartiles do not extend to quartile sets, and provide an elementary method that can be used to compute the quartile sets.

The rest of the paper is organized as follows. The set of all medians $M(X)$ of X is defined in Section 3, and in Section 4, the set of all first quartiles $Q_1(X)$ of X and the set of all third quartiles $Q_3(X)$ of X are defined. Main results about relationships among these sets are provided in Section 5. In Section 6, we recall some well known methods for computing of quartiles and show that one of them, the Langford's doubling method can be used to compute the quartile sets.

2 Preliminaries

Here we introduce some basic notions that we use in the paper. Suppose that we have a finite ordered m-tuple $(y_1, y_2, y_3, \ldots, y_m) \in \mathbb{R}^m$ of some data such that $y_1 < y_2 < y_3 < \ldots < y_m$, together with the m-tuple of their frequencies $(k_1, k_2, k_3, \ldots, k_m) \in \mathbb{N}^m$. This means that the datum y_i occurs k_i-times for each $i \in \{1, 2, 3, \ldots, m\}$. Let $k_1 + k_2 + k_3 + \ldots + k_m = n$. Then the random variable Y defined by

$$Y \sim \begin{pmatrix} y_1 & y_2 & y_3 & \cdots & y_m \\ \frac{k_1}{n} & \frac{k_2}{n} & \frac{k_3}{n} & \cdots & \frac{k_m}{n} \end{pmatrix},$$

where $\frac{k_i}{n}$ is the probability $P(Y = y_i)$ for each $i \in \{1, 2, 3, \ldots, m\}$, represents these data.

One may represent the above data equivalently, using the random variable X in the following way

$$X \sim \begin{pmatrix} x_1 & x_2 & x_3 & \cdots & x_n \\ \frac{1}{n} & \frac{1}{n} & \frac{1}{n} & \cdots & \frac{1}{n} \end{pmatrix},$$

where $x_1 \le x_2 \le x_3 \le \ldots \le x_n$ and

$$x_1 = x_2 = x_3 = \ldots = x_{k_1} = y_1,$$

$$x_{k_1+1} = x_{k_1+2} = x_{k_1+3} = \ldots = x_{k_1+k_2} = y_2,$$

$$x_{k_1+k_2+1} = x_{k_1+k_2+2} = x_{k_1+k_2+3} = \ldots = x_{k_1+k_2+k_3} = y_3,$$

$$\vdots$$

$$x_{k_1+k_2+\ldots+k_{m-1}+1} = x_{k_1+k_2+\ldots+k_{m-1}+2} = x_{k_1+k_2+\ldots+k_{m-1}+3} = \ldots = x_n = y_m.$$

In this article, we will present data using such random variable X. We will call such a random variable X an ordered random variable.

Using this notation, we define the set of all medians $M(X)$ of X, the set of all first quartiles $Q_1(X)$ of X, and the set of all third quartiles $Q_3(X)$ of X in the following sections.

3 The median set of a random variable

We begin the section by giving the definition of a median and the median set of an ordered random variable.

Definition 3.1. Let X be an ordered random variable, given by

$$X \sim \begin{pmatrix} x_1 & x_2 & x_3 & \cdots & x_n \\ \frac{1}{n} & \frac{1}{n} & \frac{1}{n} & \cdots & \frac{1}{n} \end{pmatrix},$$

and let x be any real number. We say that x is a *median* of X, if

$$P(X \leq x) \geq \frac{1}{2} \quad \text{and} \quad P(X \geq x) \geq \frac{1}{2}.$$

We call the set

$$M(X) = \{x \in \mathbb{R} \mid x \text{ is a median of } X\}$$

the *median set* of the random variable X.

In the following proposition we give an explicit description of the median set $M(X)$ for any ordered random variable X.

Proposition 3.2. *Let X be an ordered random variable, given by*

$$X \sim \begin{pmatrix} x_1 & x_2 & x_3 & \cdots & x_n \\ \frac{1}{n} & \frac{1}{n} & \frac{1}{n} & \cdots & \frac{1}{n} \end{pmatrix}.$$

Then

$$M(X) = \begin{cases} \{x_k\} & \text{if } n = 2k-1 \text{ for some positive integer } k, \\ [x_k, x_{k+1}] & \text{if } n = 2k \text{ for some positive integer } k. \end{cases}$$

Proof. We consider the following two possible cases.

CASE 1: $n = 2k - 1$ for some positive integer k. Since

$$P(X \leq x_k) = k \cdot \frac{1}{n} = \frac{n+1}{2} \cdot \frac{1}{n} = \frac{1}{2} + \frac{1}{2n} \geq \frac{1}{2}$$

and

$$P(X \geq x_k) = k \cdot \frac{1}{n} = \frac{n+1}{2} \cdot \frac{1}{n} = \frac{1}{2} + \frac{1}{2n} \geq \frac{1}{2},$$

it follows that $x_k \in M(X)$. Next, let $x < x_k$. Since

$$P(X \leq x) \leq P(x \leq x_{k-1}) = (k-1) \cdot \frac{1}{n} = \frac{n-1}{2} \cdot \frac{1}{n} = \frac{1}{2} - \frac{1}{2n} < \frac{1}{2},$$

therefore $x \notin M(X)$. Finally, let $x > x_k$. Since

$$P(X \geq x) \leq P(x \geq x_{k+1}) = (k-1) \cdot \frac{1}{n} = \frac{n-1}{2} \cdot \frac{1}{n} = \frac{1}{2} - \frac{1}{2n} < \frac{1}{2},$$

it follows that $x \notin M(X)$.

CASE 2: $n = 2k$ for some positive integer k and let $x \in [x_k, x_{k+1}]$. Since

$$P(X \leq x) \geq P(X \leq x_k) = k \cdot \frac{1}{n} = \frac{n}{2} \cdot \frac{1}{n} = \frac{1}{2} \geq \frac{1}{2}$$

and

$$P(X \geq x) \geq P(X \geq x_{k+1}) = k \cdot \frac{1}{n} = \frac{n}{2} \cdot \frac{1}{n} = \frac{1}{2} \geq \frac{1}{2},$$

it follows that $x \in M(X)$ for any $x \in [x_k, x_{k+1}]$. Next, let $x < x_k$. Since

$$P(X \leq x) \leq P(x \leq x_{k-1}) = (k-1) \cdot \frac{1}{n} = \frac{n-2}{2} \cdot \frac{1}{n} = \frac{1}{2} - \frac{1}{n} < \frac{1}{2},$$

therefore $x \notin M(X)$. Finally, let $x > x_{k+1}$. Since

$$P(X \geq x) \leq P(x \geq x_{k+2}) = (n-k+1) \cdot \frac{1}{n} = \frac{n-2}{2} \cdot \frac{1}{n} = \frac{1}{2} - \frac{1}{n} < \frac{1}{2},$$

therefore $x \notin M(X)$. □

Note that for any ordered random variable X,

$$X \sim \begin{pmatrix} x_1 & x_2 & x_3 & \cdots & x_n \\ \frac{1}{n} & \frac{1}{n} & \frac{1}{n} & \cdots & \frac{1}{n} \end{pmatrix},$$

the following holds:

1. the median set $M(X)$ is nonempty,
2. the median set $M(X)$ is bounded and closed in $\mathbb{R}$,
3. $\max(M(X)) = \begin{cases} x_k & \text{if } n = 2k-1 \text{ for some positive integer } k, \\ x_{k+1} & \text{if } n = 2k \text{ for some positive integer } k. \end{cases}$
4. $\min(M(X)) = \begin{cases} x_k & \text{if } n = 2k-1 \text{ for some positive integer } k, \\ x_k & \text{if } n = 2k \text{ for some positive integer } k. \end{cases}$
5. $M(X) \cap \{x_1, x_2, x_3, \ldots, x_n\} =$
$$= \begin{cases} \{x_k\} & \text{if } n = 2k-1 \text{ for some positive integer } k, \\ \{x_k, x_{k+1}\} & \text{if } n = 2k \text{ for some positive integer } k. \end{cases}$$

Clearly, the statements (1) and (2) above imply

Fact 3.3. *The median set $M(X)$ is either a singleton (one real number) or a closed interval.*

We call the maximum $\max(M(X))$ of $M(X)$ the *upper median* of X and we will always denote it by m^1; we call the minimum $\min(M(X))$ of $M(X)$ the *lower median* of X and we will always denote it by m^0. The median

$$m^{\frac{1}{2}} = \frac{\min(M(X)) + \max(M(X))}{2} = \begin{cases} x_k & \text{if } n = 2k-1 \text{ for some positive integer } k, \\ \frac{x_k + x_{k+1}}{2} & \text{if } n = 2k \text{ for some positive integer } k \end{cases}$$

will be called the *middle median* of X or the *canonical value* of median of X.

4 The first and the third quartile sets of a random variable

We begin this section by giving the definition of a first and a third quartile as well as the first quartile and the third quartile set of an ordered random variable.

Definition 4.1. Let X be an ordered random variable, given by

$$X \sim \begin{pmatrix} x_1 & x_2 & x_3 & \cdots & x_n \\ \frac{1}{n} & \frac{1}{n} & \frac{1}{n} & \cdots & \frac{1}{n} \end{pmatrix},$$

and let x be any real number. We say that x is

1. a *first quartile* of X, if

$$P(X \le x) \ge \frac{1}{4} \quad \text{and} \quad P(X \ge x) \ge \frac{3}{4}.$$

2. a *third quartile* of X, if

$$P(X \le x) \ge \frac{3}{4} \quad \text{and} \quad P(X \ge x) \ge \frac{1}{4}.$$

We call the set

$$Q_1(X) = \{x \in \mathbb{R} \mid x \text{ is a first quartile of } X\}$$

the *first quartile set* of the random variable X and the set

$$Q_3(X) = \{x \in \mathbb{R} \mid x \text{ is a third quartile of } X\}$$

the *third quartile set* of the random variable X.

In the following proposition we give an explicit description of the sets $Q_1(X)$ and $Q_2(X)$ for any ordered random variable X.

Proposition 4.2. *Let X be an ordered random variable, given by*

$$X \sim \begin{pmatrix} x_1 & x_2 & x_3 & \cdots & x_n \\ \frac{1}{n} & \frac{1}{n} & \frac{1}{n} & \cdots & \frac{1}{n} \end{pmatrix}.$$

Then

$$Q_1(X) = \begin{cases} [x_k, x_{k+1}] & \text{if } n = 4k \text{ for some positive integer } k, \\ \{x_{k+1}\} & \text{if } n = 4k+1 \text{ for some non-negative integer } k, \\ \{x_{k+1}\} & \text{if } n = 4k+2 \text{ for some non-negative integer } k, \\ \{x_{k+1}\} & \text{if } n = 4k+3 \text{ for some non-negative integer } k \end{cases}$$

and

$$Q_3(X) = \begin{cases} [x_{3k}, x_{3k+1}] & \text{if } n = 4k \text{ for some positive integer } k, \\ \{x_{3k+1}\} & \text{if } n = 4k+1 \text{ for some non-negative integer } k, \\ \{x_{3k+2}\} & \text{if } n = 4k+2 \text{ for some non-negative integer } k, \\ \{x_{3k+3}\} & \text{if } n = 4k+3 \text{ for some non-negative integer } k. \end{cases}$$

Proof. We consider the following four possible cases.

CASE 1: $n = 4k$ for some positive integer k.

First we find all such $\ell \in \{1, 2, 3, \dots, n\}$ that $x_\ell \in Q_1(X)$. Suppose that $\ell \in \{1, 2, 3, \dots, n\}$ is such an integer that $x_\ell \in Q_1(X)$. Then

- $\frac{\ell}{4k} \geq \frac{1}{4}$ holds and
$$\frac{\ell}{4k} \geq \frac{1}{4} \iff \ell \geq k,$$
- $\frac{4k - \ell + 1}{4k} \geq \frac{3}{4}$ holds and
$$\frac{4k - \ell + 1}{4k} \geq \frac{3}{4} \iff \ell \leq k + 1.$$

Therefore,
$$x_\ell \in Q_1(X) \iff \ell \in \{k, k + 1\}.$$
Therefore, it can easily be seen that $Q_1(X) = [x_k, x_{k+1}]$.

Next we find all such $\ell \in \{1, 2, 3, \dots, n\}$ that $x_\ell \in Q_3(X)$. Suppose that $\ell \in \{1, 2, 3, \dots, n\}$ is such an integer that $x_\ell \in Q_3(X)$. Then

- $\frac{\ell}{4k} \geq \frac{3}{4}$ holds and
$$\frac{\ell}{4k} \geq \frac{3}{4} \iff \ell \geq 3k,$$
- $\frac{4k - \ell + 1}{4k} \geq \frac{1}{4}$ holds and
$$\frac{4k - \ell + 1}{4k} \geq \frac{1}{4} \iff \ell \leq 3k + 1.$$

Therefore,
$$x_\ell \in Q_3(X) \iff \ell \in \{3k, 3k + 1\}.$$
Therefore, it can easily be seen that $Q_3(X) = [x_{3k}, x_{3k+1}]$.

CASE 2: $n = 4k + 1$ for some non-negative integer k.

First we find all such $\ell \in \{1, 2, 3, \dots, n\}$ that $x_\ell \in Q_1(X)$. Suppose that $\ell \in \{1, 2, 3, \dots, n\}$ is such an integer that $x_\ell \in Q_1(X)$. Then

- $\frac{\ell}{4k+1} \geq \frac{1}{4}$ holds and
$$\frac{\ell}{4k+1} \geq \frac{1}{4} \iff \ell \geq k + \frac{1}{4},$$
- $\frac{4k + 1 - \ell + 1}{4k + 1} \geq \frac{3}{4}$ holds and
$$\frac{4k - \ell + 2}{4k + 1} \geq \frac{3}{4} \iff \ell \leq k + \frac{5}{4}.$$

Therefore,

$$x_\ell \in Q_1(X) \iff \ell = k+1.$$

Therefore, it can easily be seen that $Q_1(X) = \{x_{k+1}\}$.

Next we find all such $\ell \in \{1,2,3,\dots,n\}$ that $x_\ell \in Q_3(X)$. Suppose that $\ell \in \{1,2,3,\dots,n\}$ is such an integer that $x_\ell \in Q_3(X)$. Then

- $\frac{\ell}{4k+1} \geq \frac{3}{4}$ holds and

$$\frac{\ell}{4k+1} \geq \frac{3}{4} \iff \ell \geq 3k + \frac{3}{4},$$

- $\frac{4k+1-\ell+1}{4k+1} \geq \frac{1}{4}$ holds and

$$\frac{4k-\ell+2}{4k+1} \geq \frac{1}{4} \iff \ell \leq 3k + \frac{7}{4}.$$

Therefore,

$$x_\ell \in Q_3(X) \iff \ell = 3k+1.$$

Therefore, it can easily be seen that $Q_3(X) = \{x_{3k+1}\}$.

CASE 3: $n = 4k+2$ for some non-negative integer k.

First we find all such $\ell \in \{1,2,3,\dots,n\}$ that $x_\ell \in Q_1(X)$. Suppose that $\ell \in \{1,2,3,\dots,n\}$ is such an integer that $x_\ell \in Q_1(X)$. Then

- $\frac{\ell}{4k+2} \geq \frac{1}{4}$ holds and

$$\frac{\ell}{4k+2} \geq \frac{1}{4} \iff \ell \geq k + \frac{1}{2},$$

- $\frac{4k+2-\ell+1}{4k+2} \geq \frac{3}{4}$ holds and

$$\frac{4k-\ell+3}{4k+2} \geq \frac{3}{4} \iff \ell \leq k + \frac{3}{2}.$$

Therefore,

$$x_\ell \in Q_1(X) \iff \ell = k+1.$$

Therefore, it can easily be seen that $Q_1(X) = \{x_{k+1}\}$.

Next we find all such $\ell \in \{1,2,3,\dots,n\}$ that $x_\ell \in Q_3(X)$. Suppose that $\ell \in \{1,2,3,\dots,n\}$ is such an integer that $x_\ell \in Q_3(X)$. Then

- $\frac{\ell}{4k+2} \geq \frac{3}{4}$ holds and

$$\frac{\ell}{4k+2} \geq \frac{3}{4} \iff \ell \geq 3k + \frac{3}{2},$$

- $\dfrac{4k+2-\ell+1}{4k+2} \geq \dfrac{1}{4}$ holds and

$$\frac{4k-\ell+3}{4k+2} \geq \frac{1}{4} \iff \ell \leq 3k+\frac{5}{2}.$$

Therefore,

$$x_\ell \in Q_3(X) \iff \ell = 3k+2.$$

Therefore, it can easily be seen that $Q_3(X) = \{x_{3k+2}\}$.

CASE 4: $n = 4k+3$ for some non-negative integer k.

First we find all such $\ell \in \{1,2,3,\ldots,n\}$ that $x_\ell \in Q_1(X)$. Suppose that $\ell \in \{1,2,3,\ldots,n\}$ is such an integer that $x_\ell \in Q_1(X)$. Then

- $\dfrac{\ell}{4k+3} \geq \dfrac{1}{4}$ holds and

$$\frac{\ell}{4k+3} \geq \frac{1}{4} \iff \ell \geq k+\frac{3}{4},$$

- $\dfrac{4k+3-\ell+1}{4k+3} \geq \dfrac{3}{4}$ holds and

$$\frac{4k-\ell+4}{4k+3} \geq \frac{3}{4} \iff \ell \leq k+\frac{7}{4}.$$

Therefore,

$$x_\ell \in Q_1(X) \iff \ell = k+1.$$

Therefore, it can easily be seen that $Q_1(X) = \{x_{k+1}\}$.

Finally, we find all such $\ell \in \{1,2,3,\ldots,n\}$ that $x_\ell \in Q_3(X)$. Suppose that $\ell \in \{1,2,3,\ldots,n\}$ is such an integer that $x_\ell \in Q_3(X)$. Then

- $\dfrac{\ell}{4k+3} \geq \dfrac{3}{4}$ holds and

$$\frac{\ell}{4k+3} \geq \frac{3}{4} \iff \ell \geq 3k+\frac{9}{4},$$

- $\dfrac{4k+3-\ell+1}{4k+3} \geq \dfrac{1}{4}$ holds and

$$\frac{4k-\ell+4}{4k+3} \geq \frac{1}{4} \iff \ell \leq 3k+\frac{13}{4}.$$

Therefore,

$$x_\ell \in Q_3(X) \iff \ell = 3k+3.$$

Therefore, it can easily be seen that $Q_3(X) = \{x_{3k+3}\}$. □

Note that for any ordered random variable X,

$$X \sim \begin{pmatrix} x_1 & x_2 & x_3 & \cdots & x_n \\ \frac{1}{n} & \frac{1}{n} & \frac{1}{n} & \cdots & \frac{1}{n} \end{pmatrix},$$

the following holds:

1. the sets $Q_1(X)$ and $Q_3(X)$ are both nonempty,
2. the sets $Q_1(X)$ and $Q_3(X)$ are both bounded and closed in $\mathbb{R}$,
3. $\max(Q_1(X)) = \begin{cases} x_{k+1} & \text{if } n = 4k \text{ for some positive integer } k, \\ x_{k+1} & \text{if } n = 4k+1 \text{ for some non-negative integer } k, \\ x_{k+1} & \text{if } n = 4k+2 \text{ for some non-negative integer } k, \\ x_{k+1} & \text{if } n = 4k+3 \text{ for some non-negative integer } k \end{cases}$
4. $\min(Q_1(X)) = \begin{cases} x_{k} & \text{if } n = 4k \text{ for some positive integer } k, \\ x_{k+1} & \text{if } n = 4k+1 \text{ for some non-negative integer } k, \\ x_{k+1} & \text{if } n = 4k+2 \text{ for some non-negative integer } k, \\ x_{k+1} & \text{if } n = 4k+3 \text{ for some non-negative integer } k \end{cases}$
5. $\max(Q_3(X)) = \begin{cases} x_{3k+1} & \text{if } n = 4k \text{ for some positive integer } k, \\ x_{3k+1} & \text{if } n = 4k+1 \text{ for some non-negative integer } k, \\ x_{3k+2} & \text{if } n = 4k+2 \text{ for some non-negative integer } k, \\ x_{3k+3} & \text{if } n = 4k+3 \text{ for some non-negative integer } k \end{cases}$
6. $\min(Q_3(X)) = \begin{cases} x_{3k} & \text{if } n = 4k \text{ for some positive integer } k, \\ x_{3k+1} & \text{if } n = 4k+1 \text{ for some non-negative integer } k, \\ x_{3k+2} & \text{if } n = 4k+2 \text{ for some non-negative integer } k, \\ x_{3k+3} & \text{if } n = 4k+3 \text{ for some non-negative integer } k \end{cases}$
7. $Q_1(X) \cap \{x_1, x_2, x_3, \ldots, x_n\} =$

$$= \begin{cases} \{x_k, x_{k+1}\} & \text{if } n = 4k \text{ for some positive integer } k, \\ \{x_{k+1}\} & \text{if } n = 4k+1 \text{ for some non-negative integer } k, \\ \{x_{k+1}\} & \text{if } n = 4k+2 \text{ for some non-negative integer } k, \\ \{x_{k+1}\} & \text{if } n = 4k+3 \text{ for some non-negative integer } k \end{cases}$$

8. $Q_3(X) \cap \{x_1, x_2, x_3, \ldots, x_n\} =$

$$= \begin{cases} \{x_{3k}, x_{3k+1}\} & \text{if } n = 4k \text{ for some positive integer } k, \\ \{x_{3k+1}\} & \text{if } n = 4k+1 \text{ for some non-negative integer } k, \\ \{x_{3k+2}\} & \text{if } n = 4k+2 \text{ for some non-negative integer } k, \\ \{x_{3k+3}\} & \text{if } n = 4k+3 \text{ for some non-negative integer } k \end{cases}$$

Similarly as for the median, we observe that

Fact 4.3. *The quartile sets $Q_1(X)$ and $Q_3(X)$ are either singletons (one real number) or closed intervals.*

We call the maximum $\max(Q_1(X))$ and the minimum $\min(Q_1(X))$ of $Q_1(X)$ the *upper first quartile* and the *lower first quartile* of X respectively, and we will denote them by q_1^1 and q_1^0 respectively. The first quartile

$$q_1^{\frac{1}{2}} = \frac{\min(Q_1(X)) + \max(Q_1(X))}{2}$$
$$= \begin{cases} \frac{x_k + x_{k+1}}{2} & \text{if } n = 4k \text{ for some positive integer } k, \\ x_{k+1} & \text{if } n = 4k+1 \text{ for some non-negative integer } k, \\ x_{k+1} & \text{if } n = 4k+2 \text{ for some non-negative integer } k, \\ x_{k+1} & \text{if } n = 4k+3 \text{ for some non-negative integer } k \end{cases}$$

will be called the *middle first quartile* of X (or, the *canonical value* of the first quartile).

We call the maximum $\max(Q_3(X))$ and the minimum $\min(Q_3(X))$ of $Q_3(X)$ the *upper third quartile* and the *lower third quartile* of X respectively, and we will always denote them by q_3^1 and q_3^0 respectively. The third quartile

$$q_3^{\frac{1}{2}} = \frac{\min(Q_3(X)) + \max(Q_3(X))}{2}$$
$$= \begin{cases} \frac{x_{3k} + x_{3k+1}}{2} & \text{if } n = 4k \text{ for some positive integer } k, \\ x_{3k+1} & \text{if } n = 4k+1 \text{ for some non-negative integer } k, \\ x_{3k+2} & \text{if } n = 4k+2 \text{ for some non-negative integer } k, \\ x_{3k+3} & \text{if } n = 4k+3 \text{ for some non-negative integer } k \end{cases}$$

will be called the *middle third quartile* of X (or, the *canonical value* of the third quartile).

5 Main results

In present section we formulate and prove our main theorems. We start with the following definition.

Definition 5.1. Let X be an ordered random variable, given by

$$X \sim \begin{pmatrix} x_1 & x_2 & x_3 & \cdots & x_n \\ \frac{1}{n} & \frac{1}{n} & \frac{1}{n} & \cdots & \frac{1}{n} \end{pmatrix}.$$

Then $2X$ is the ordered random variable, defined by

$$2X \sim \begin{pmatrix} y_1 & y_2 & y_3 & \cdots & y_{2n} \\ \frac{1}{2n} & \frac{1}{2n} & \frac{1}{2n} & \cdots & \frac{1}{2n} \end{pmatrix},$$

where $y_{2i-1} = y_{2i} = x_i$ for each $i \in \{1, 2, 3, \ldots, n\}$.

The following theorem says that the set of all medians of X may be obtained by calculating the set of all medians of $2X$.

Theorem 5.2. *Let X be an ordered random variable, given by*

$$X \sim \begin{pmatrix} x_1 & x_2 & x_3 & \cdots & x_n \\ \frac{1}{n} & \frac{1}{n} & \frac{1}{n} & \cdots & \frac{1}{n} \end{pmatrix}.$$

Then $M(X) = M(2X)$.

Proof. Let

$$2X \sim \begin{pmatrix} y_1 & y_2 & y_3 & \cdots & y_{2n} \\ \frac{1}{2n} & \frac{1}{2n} & \frac{1}{2n} & \cdots & \frac{1}{2n} \end{pmatrix},$$

We look at the following two possible cases.

CASE 1: $n = 2k - 1$ for some positive integer k.

By Proposition 3.2 and by the definition of $2X$, the following holds:

$$M(2X) = [y_{2k-1}, y_{2k}] = [x_k, x_k] = \{x_k\} = M(X).$$

CASE 2: $n = 2k$ for some positive integer k.

By Proposition 3.2 and by the definition of $2X$, the following holds:

$$M(2X) = [y_{2k}, y_{2k+1}] = [x_k, x_{k+1}] = M(X).$$

□

In the following theorem, the ordered random variable $4X$ is defined to be the ordered random variable $2(2X)$. The theorem says that the set of all first (third) quartiles of X may be obtained by calculating the set of all first (third) quartiles of $4X$.

Theorem 5.3. *Let X be an ordered random variable, given by*

$$X \sim \begin{pmatrix} x_1 & x_2 & x_3 & \cdots & x_n \\ \frac{1}{n} & \frac{1}{n} & \frac{1}{n} & \cdots & \frac{1}{n} \end{pmatrix}.$$

Then $Q_1(X) = Q_1(4X)$ and $Q_3(X) = Q_3(4X)$.

Proof. Let

$$4X \sim \begin{pmatrix} y_1 & y_2 & y_3 & \cdots & y_{4n} \\ \frac{1}{4n} & \frac{1}{4n} & \frac{1}{4n} & \cdots & \frac{1}{4n} \end{pmatrix},$$

We look at the following four possible cases.

CASE 1: $n = 4k$ for some positive integer k.

By Proposition 4.2 and by the definition of $4X$, the following holds:

$$Q_1(4X) = [y_n, y_{n+1}] = [x_k, x_{k+1}] = Q_1(X)$$

and

$$Q_3(4X) = [y_{3n}, y_{3n+1}] = [x_{3k}, x_{3k+1}] = Q_3(X).$$

CASE 2: $n = 4k + 1$ for some non-negative integer k.

By Proposition 4.2 and by the definition of $4X$, the following holds:

$$Q_1(4X) = [y_n, y_{n+1}] = [x_{k+1}, x_{k+1}] = \{x_{k+1}\} = Q_1(X)$$

and

$$Q_3(4X) = [y_{3n}, y_{3n+1}] = [x_{3k+1}, x_{3k+1}] = \{x_{3k+1}\} = Q_3(X).$$

CASE 3: $n = 4k + 2$ for some non-negative integer k.

By Proposition 4.2 and by the definition of $4X$, the following holds:

$$Q_1(4X) = [y_n, y_{n+1}] = [x_{k+1}, x_{k+1}] = \{x_{k+1}\} = Q_1(X)$$

and

$$Q_3(4X) = [y_{3n}, y_{3n+1}] = [x_{3k+2}, x_{3k+2}] = \{x_{3k+2}\} = Q_3(X).$$

CASE 4: $n = 4k + 3$ for some non-negative integer k.

By Proposition 4.2 and by the definition of $4X$, the following holds:

$$Q_1(4X) = [y_n, y_{n+1}] = [x_{k+1}, x_{k+1}] = \{x_{k+1}\} = Q_1(X)$$

and

$$Q_3(4X) = [y_{3n}, y_{3n+1}] = [x_{3k+3}, x_{3k+3}] = \{x_{3k+3}\} = Q_3(X).$$

□

In the definitions and the results that follow we try to mimic statistical methods that suggest the following well-known strategy. To find a first or a third quartile, split the data into two halves and find the medians of these halves.

Definition 5.4. Let X be an ordered random variable, given by

$$X \sim \begin{pmatrix} x_1 & x_2 & x_3 & \cdots & x_{2n} \\ \frac{1}{2n} & \frac{1}{2n} & \frac{1}{2n} & \cdots & \frac{1}{2n} \end{pmatrix}.$$

Then $\frac{1}{2}X^-$ is the ordered random variable, given by

$$\frac{1}{2}X^- \sim \begin{pmatrix} x_1 & x_2 & x_3 & \cdots & x_n \\ \frac{1}{n} & \frac{1}{n} & \frac{1}{n} & \cdots & \frac{1}{n} \end{pmatrix}$$

and $\frac{1}{2}X^+$ is the ordered random variable, given by

$$\frac{1}{2}X^+ \sim \begin{pmatrix} x_{n+1} & x_{n+2} & x_{n+3} & \cdots & x_{2n} \\ \frac{1}{n} & \frac{1}{n} & \frac{1}{n} & \cdots & \frac{1}{n} \end{pmatrix}$$

We continue with the following theorem which gives a relationship between $M(\frac{1}{2}X^-)$ and $Q_1(X)$, and $M(\frac{1}{2}X^+)$ and $Q_3(X)$.

Theorem 5.5. *Let X be an ordered random variable, given by*

$$X \sim \begin{pmatrix} x_1 & x_2 & x_3 & \cdots & x_{2n} \\ \frac{1}{2n} & \frac{1}{2n} & \frac{1}{2n} & \cdots & \frac{1}{2n} \end{pmatrix}.$$

Then $M(\frac{1}{2}X^-) = Q_1(X)$ and $M(\frac{1}{2}X^+) = Q_3(X)$.

Proof. We look at the following two possible cases.

CASE 1: $n = 2k - 1$ for some positive integer k.

By Propositions 3.2 and 4.2, and by the definition of $\frac{1}{2}X^-$ and $\frac{1}{2}X^+$, the following holds:

$$M(\frac{1}{2}X^-) = \{x_k\} = Q_1(X)$$

and

$$M(\frac{1}{2}X^+) = \{x_{n+k}\} = \{x_{3k-1}\} = Q_3(X).$$

CASE 2: $n = 2k$ for some positive integer k.

By Propositions 3.2 and 4.2, and by the definition of $\frac{1}{2}X^-$ and $\frac{1}{2}X^+$, the following holds:

$$M(\frac{1}{2}X^-) = [x_k, x_{k+1}] = Q_1(X)$$

and

$$M(\frac{1}{2}X^+) = [x_{n+k}, x_{n+k+1}] = [x_{3k}, x_{3k+1}] = Q_3(X).$$

□

Note that $\frac{1}{2}X^-$ and $\frac{1}{2}X^+$ can only be obtained if $n = 2k$ for some positive integer k. The following definition generalizes the notion of $\frac{1}{2}X^-$ and $\frac{1}{2}X^+$ to define the lower and upper parts of X in any proportion for arbitrary n.

Definition 5.6. Let X be an ordered random variable, given by

$$X \sim \begin{pmatrix} x_1 & x_2 & x_3 & \cdots & x_n \\ \frac{1}{n} & \frac{1}{n} & \frac{1}{n} & \cdots & \frac{1}{n} \end{pmatrix}$$

and let $x \in [x_1, x_n]$ be any real number. Then we define the ordered random variables L_x^c, L_x^o, U_x^c, and U_x^o by

$$L_x^c \sim \begin{cases} \begin{pmatrix} x_1 & x_2 & x_3 & \cdots & x_k \\ \frac{1}{k} & \frac{1}{k} & \frac{1}{k} & \cdots & \frac{1}{k} \end{pmatrix} & \text{if } x = x_k \text{ for some } k, \\ \begin{pmatrix} x_1 & x_2 & x_3 & \cdots & x_k \\ \frac{1}{k} & \frac{1}{k} & \frac{1}{k} & \cdots & \frac{1}{k} \end{pmatrix} & \text{if } x_k < x < x_{k+1} \text{ for some } k \end{cases}$$

$$L_x^o \sim \begin{cases} \begin{pmatrix} x_1 & x_2 & x_3 & \cdots & x_{k-1} \\ \frac{1}{k-1} & \frac{1}{k-1} & \frac{1}{k-1} & \cdots & \frac{1}{k-1} \end{pmatrix} & \text{if } x = x_k \text{ for some } k, \\ \begin{pmatrix} x_1 & x_2 & x_3 & \cdots & x_k \\ \frac{1}{k} & \frac{1}{k} & \frac{1}{k} & \cdots & \frac{1}{k} \end{pmatrix} & \text{if } x_k < x < x_{k+1} \text{ for some } k \end{cases}$$

$$U_x^c \sim \begin{cases} \begin{pmatrix} x_k & x_{k+1} & x_{k+2} & \cdots & x_n \\ \frac{1}{n-k+1} & \frac{1}{n-k+1} & \frac{1}{n-k+1} & \cdots & \frac{1}{n-k+1} \end{pmatrix} & \text{if } x = x_k \text{ for some } k, \\ \begin{pmatrix} x_{k+1} & x_{k+2} & \cdots & x_n \\ \frac{1}{n-k} & \frac{1}{n-k} & \cdots & \frac{1}{n-k} \end{pmatrix} & \text{if } x_k < x < x_{k+1} \text{ for some } k. \end{cases}$$

$$U_x^o \sim \begin{cases} \begin{pmatrix} x_{k+1} & x_{k+2} & \cdots & x_n \\ \frac{1}{n-k} & \frac{1}{n-k} & \cdots & \frac{1}{n-k} \end{pmatrix} & \text{if } x = x_k \text{ for some } k, \\ \begin{pmatrix} x_{k+1} & x_{k+2} & \cdots & x_n \\ \frac{1}{n-k} & \frac{1}{n-k} & \cdots & \frac{1}{n-k} \end{pmatrix} & \text{if } x_k < x < x_{k+1} \text{ for some } k. \end{cases}$$

The sets L_x^o, L_x^c, U_x^o, and U_x^c can respectively be called open and closed lower part, and open and closed upper parts of X relative to x.

From the definitions it directly follows:

Proposition 5.7. *Let X be an ordered random variable, given by*

$$X \sim \begin{pmatrix} x_1 & x_2 & x_3 & \cdots & x_n \\ \frac{1}{n} & \frac{1}{n} & \frac{1}{n} & \cdots & \frac{1}{n} \end{pmatrix}.$$

Then

1. $L_x^c \supseteq L_x^o$, $U_x^c \supseteq U_x^o$ *for any* $x \in [x_1, x_n]$,
2. $L_x^o \cap U_x^o = \emptyset$ *for any* $x \in [x_1, x_n]$,
3. *if* $x = x_k \in X$ *then* $L_x^c \cap U_x^c = \{x\}$,
4. *if* $x \neq x_k \in X$ *then* $L_x^o \cup U_x^o = X$,
5. $L_x^c \cup U_x^c = X$ *for any* $x \in [x_1, x_n]$.

Furthermore, the following theorem holds.

Theorem 5.8. *Let X be an ordered random variable, given by*

$$X \sim \begin{pmatrix} x_1 & x_2 & x_3 & \cdots & x_n \\ \frac{1}{n} & \frac{1}{n} & \frac{1}{n} & \cdots & \frac{1}{n} \end{pmatrix}.$$

If $n = 2k$ for some k, then for any median $m \in M(X)$, $m \neq m^0$, $m \neq m^1$, we have
(1) $L_m^c = L_m^o = \frac{1}{2}X^-$ *and* $U_m^c = U_m^o = \frac{1}{2}X^+$.
(2) $M(L_m^c) = M(L_m^o) = Q_1(X)$ *and* $M(U_m^c) = M(U_m^o) = Q_3(X)$.

Proof. Statement (1) follows directly from the definitions. Statement (2) follows from (1) and Theorem 5.5. □

The situation is a bit more complicated for odd n. Recall that for odd number of elements $n = 2\ell + 1$, the median $m = x_{\ell+1}$ is an element of X.

Theorem 5.9. *Let n be an odd integer and X be an ordered random variable, given by*

$$X \sim \begin{pmatrix} x_1 & x_2 & x_3 & \cdots & x_n \\ \frac{1}{n} & \frac{1}{n} & \frac{1}{n} & \cdots & \frac{1}{n} \end{pmatrix}.$$

Then

(1) if $n = 4k+1$ then for the unique median $m = x_{2k+1}$ we have $M(L_m^c) = Q_1(X) = \{x_{k+1}\} \subseteq M(L_m^o) = [x_k, x_{k+1}]$ *and* $M(L_m^c) = Q_3(X) = \{x_{3k+1}\} \subseteq M(L_m^o) = [x_{k+1}, x_{k+2}]$.

(2) if $n = 4k+3$ then for the unique median $m = x_{2k+2}$ we have $M(L_m^o) = Q_1(X) = \{x_{k+1}\} \subseteq M(L_m^c) = [x_{k+1}, x_{k+2}]$ *and* $M(L_m^o) = Q_3(X) = \{x_{3k+3}\} \subseteq M(L_m^o) = [x_{3k+2}, x_{3k+3}]$.

Proof. The proof is straight forward. We leave it to a reader. □

Thus from Theorem 5.8 we have learned that for X with even number of elements, taking any value from the median set to divide X to obtain the lower and the upper half, and computing its median sets will provide exact values of the first and the third quartile sets.

However, by Theorem 5.9, the situation is slightly more complicated for odd n. Two cases have to be distinguished, because the quartile sets are median sets of the open halves when $n = 4k+1$ and are medians of the closed halves when $n = 4k+3$.

We conclude the section by stating and proving another interesting result not depending whether n is even or odd. It gives an algorithm how to obtain the first and the third quartile sets of any data by doubling the data first, and then obtaining the median sets of the first and the second halves of the obtained doubled data. The advantage of this method is the fact that it works perfectly in both cases — for any even and for any odd n.

Theorem 5.10. *Let X be an ordered random variable, given by*

$$X \sim \begin{pmatrix} x_1 & x_2 & x_3 & \cdots & x_n \\ \frac{1}{n} & \frac{1}{n} & \frac{1}{n} & \cdots & \frac{1}{n} \end{pmatrix}.$$

Then $M(\frac{1}{2}(2X)^-) = Q_1(X)$ and $M(\frac{1}{2}(2X)^+) = Q_3(X)$.

Proof. We distinguish the following four possible cases.

CASE 1: $n = 4k$ for some positive integer k.

By Proposition 4.2, $Q_1(X) = [x_k, x_{k+1}]$ and $Q_3(X) = [x_{3k}, x_{3k+1}]$.

In this case

$$2X \sim \begin{pmatrix} x_1 & x_1 & \cdots & x_{2k} & x_{2k} & x_{2k+1} & x_{2k+1} & \cdots & x_{n-1} & x_n & x_n \\ \frac{1}{2n} & \frac{1}{2n} & \cdots & \frac{1}{2n} & \frac{1}{2n} & \frac{1}{2n} & \frac{1}{2n} & \cdots & \frac{1}{2n} & \frac{1}{2n} & \frac{1}{2n} \end{pmatrix}.$$

By Proposition 3.2, one can easily get that $M(\frac{1}{2}(2X)^-) = [x_k, x_{k+1}] = Q_1(X)$ and $M(\frac{1}{2}(2X)^+) = [x_{3k}, x_{3k+1}] = Q_3(X)$.

CASE 2: $n = 4k+1$ for some non-negative integer k.

By Proposition 4.2, $Q_1(X) = \{x_{k+1}\}$ and $Q_3(X) = \{x_{3k+1}\}$, and by Proposition 3.2, $M(X) = \{x_{2k+1}\}$.

In this case

$$2X \sim \begin{pmatrix} x_1 & x_1 & x_2 & \cdots & x_{2k} & x_{2k+1} & x_{2k+1} & x_{2k+2} & \cdots & x_n & x_n \\ \frac{1}{2n} & \frac{1}{2n} & \frac{1}{2n} & \cdots & \frac{1}{2n} & \frac{1}{2n} & \frac{1}{2n} & \frac{1}{2n} & \cdots & \frac{1}{2n} & \frac{1}{2n} \end{pmatrix}.$$

By Proposition 3.2, $M(\frac{1}{2}(2X)^-) = \{x_{k+1}\} = Q_1(X)$ and $M(\frac{1}{2}(2X)^+) = \{x_{3k+1}\} = Q_3(X)$.

CASE 3: $n = 4k+2$ for some non-negative integer k.

By Proposition 4.2, $Q_1(X) = \{x_{k+1}\}$ and $Q_3(X) = \{x_{3k+2}\}$.

In this case

$$2X \sim \begin{pmatrix} x_1 & x_1 & x_2 & \cdots & x_{2k+1} & x_{2k+2} & \cdots & x_{n-1} & x_n & x_n \\ \frac{1}{2n} & \frac{1}{2n} & \frac{1}{2n} & \cdots & \frac{1}{2n} & \frac{1}{2n} & \cdots & \frac{1}{2n} & \frac{1}{2n} & \frac{1}{2n} \end{pmatrix}.$$

By Proposition 3.2, $M(\frac{1}{2}(2X)^-) = \{x_{k+1}\} = Q_1(X)$ and $M(\frac{1}{2}(2X)^+) = \{x_{3k+2}\} = Q_3(X)$.

CASE 4: $n = 4k + 3$ for some non-negative integer k.

By Proposition 4.2, $Q_1(X) = \{x_{k+1}\}$ and $Q_3(X) = \{x_{3k+3}\}$.

In this case

$$2X \sim \begin{pmatrix} x_1 & x_1 & x_2 & x_2 & \cdots & x_{2k+2} & x_{2k+2} & \cdots & x_n & x_n \\ \frac{1}{2n} & \frac{1}{2n} & \frac{1}{2n} & \frac{1}{2n} & \cdots & \frac{1}{2n} & \frac{1}{2n} & \cdots & \frac{1}{2n} & \frac{1}{2n} \end{pmatrix}.$$

By Proposition 3.2, $M(\frac{1}{2}(2X)^-) = \{x_{k+1}\} = Q_1(X)$ and $M(\frac{1}{2}(2X)^+) = \{x_{3k+3}\} = Q_3(X)$. □

6 On some elementary methods for computing the quartiles

The usual methods for computation of quartiles are based on the idea to split the dataset in two halves and obtain the quartiles as the medians of the halves. The obvious question arises "how to define the halves if the number of elements is odd ?". As we know it is answered differently, yielding different methods and, unfortunately, different results(!) [5]. Three methods are among the most popular, the first two being often used in elementary textbooks. The third was proposed in [5] and argued to be accessible at elementary level in [10]. All the methods below first compute the median of X and then divide X in two halves to obtain the quartiles as medians of the halves. However, when n is odd, the methods differ as follows:

- Method M1. Include the median in both halves.
- Method M2. Exclude the median in both halves.
- Method L. If $n = 4k + 1$ then include the median. If $n = 4k + 3$ then exclude the median.

Method L was suggested by Langford [5] who shows that both M1 and M2 fail to provide correct answers in some cases.

We say that a method or an algorithm for computing a first quartile of a given data is correct, if it gives a value q and $q \in Q_1(X)$. We say that a method or an algorithm for computing a third quartile of a given data is correct, if it gives a value q and $q \in Q_3(X)$.

Considering Theorem 5.9 immediately confirms that M1 and M2 are not correct. For example, for $n = 4k+3$, method M1 gives q_1 as the median of the lowest $2k+2$ elements, i.e. $\frac{1}{2}(x_{k+1} + x_{k+2})$ whereas $Q_1(X) = \{x_{k+1}\}$. Similarly, for $n = 4k + 1$, method M2 gives q_1 as the median of the lowest $2k$ elements, i.e. $\frac{1}{2}(x_k + x_{k+1})$ whereas $Q_1(X) = \{x_{k+1}\}$.

Method L however naturally extends to the general case.

Theorem 6.1. *The L method is a correct algorithm for computing the quartile sets.*

Proof. Let n be even, say $n = 2k$. Then by method L, the first quartile is the median of the set $\{x_1, x_2, \ldots, x_k\}$, and the third quartile is the median of the set $\{x_{k+1}, x_{k+2}, \ldots, x_{2k}\}$, which is correct by Theorem 5.5.

Let n be odd. If $n = 4k + 1$ then by method L, the first quartile is the median of the set $\{x_1, x_2, \ldots, x_{2k+1}\}$, and the third quartile is the median of the set $\{x_{2k+1}, x_{2k+2}, \ldots, x_{4k+1}\}$, (median included in both sets), which is correct by Theorems 5.8 and 5.9.

If $n = 4k + 3$ then by method L, the first quartile is the median of the set $\{x_1, x_2, \ldots, x_{2k+1}\}$, and the third quartile is the median of $\{x_{2k+3}, x_{2k+4}, \ldots, x_{4k+3}\}$, (median excluded from both sets), which is correct by Theorems 5.8 and 5.9. □

Another natural idea [5], equivalent to method L, can naturally be extended to a method for computing the quartile sets. Instead of asking and to answering the question whether to include or exclude the median when splitting the dataset in two halves, one can decide to give "half of the median" to each part. This can be realized by doubling the dataset and giving one copy of the median into each half. We call this the Langford's doubling method. Recall that Theorem 5.5 implies that this method works correctly for the generalized definition of quartiles.

Theorem 6.2. *The doubling method is a correct algorithm for computing the quartile sets.*

In conclusion, one may ask how some other methods for computing quartiles are related to the generalized notion of median and quartiles. For example, assuming $n = 4k$, one could ask whether a method of interest gives quartile values that are within the quartile set. This may be a good evidence that the method is sound.

Finally, we wish to note that the interval sets can be naturally associated with any quantiles, and an analogous theory may be developed.

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Sphere decompositions of hypercubes*

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Abstract

For $d \equiv 1$ or $3 \pmod 6$, the 2-skeleton of the d-dimensional hypercube is decomposed into the union of pairwise face-disjoint isomorphic 2-complexes, each a topological sphere. If $d = 5^n$, then such a decomposition can be achieved, but with non-isomorphic spheres.

Keywords: Face-disjoint union of spheres, combinatorial design, 2-skeleton of a cube.

Math. Subj. Class. (2020): 57M20, 57M15, 05C45

By Euler's theorem [9, Prop. 1.2.27], any graph (1-complex) with all vertices of even degrees is an edge-disjoint union of cycles. We say a 2-complex is **even** if every edge lies in a positive even number of (2-dimensional) faces. Is every even 2-complex a face-disjoint union of "2*-dimensional cycles*"? (A 2-complex X is a **face-disjoint** union of 2-complexes $X_1, \dots, X_n$ if $X = \bigcup_{i=1}^{n} X_i$ and each face of X is a face of exactly one X_i.)

There are (at least) two natural choices for a 2-dimensional interpretation of cycle – *sphere* or *manifold*. As even complexes include surfaces like the torus, one cannot always decompose them into face-disjoint spheres. But we show below that sphere decompositions do exist in more than two-thirds of the odd-dimensional hypercubes. For $d \equiv 1$ or 3 (mod 6), we can decompose the 2-skeleton Q_d^2 of the d-dimensional hypercube Q_d into face-disjoint copies of ∂Q_3, the boundary of a 3-cube. That is, Q_d^2 is **factored by** ∂Q_3.

In [6], when d is odd (so the 2-skeleton is even), Q_d^2 is decomposed into a face-disjoint union of tori and 3-cube boundaries. In [4] we showed that the 2-skeleton of any d-dimensional Platonic polytope is a face-disjoint union of surfaces if the 2-skeleton is even. Except for the hypercubes, all such decompositions were decompositions into spheres. (A polytope is **Platonic** if it is maximally symmetric. In dimension greater than four, the Platonic polytopes are just the cubes, simplexes, and hyperoctahedra.)

For which odd d is the 2-skeleton of the d-cube decomposable into spheres? For which d can the decomposition be a factorization? We address these questions below.

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Throughout this paper I denotes the interval $[0,1]$ and O its boundary $O = \{0,1\}$. (We use the non-standard notation O for ∂I because it will be convenient to think of an interval as being "active" (I) or "inactive" (O) in the manner indicated below.) We regard the d-cube as $Q_d = I^d \subseteq \mathbb{R}^d$. Thus the 2^d **vertices** of Q_d are the elements of O^d, which we identify with the binary strings of length d. An **edge** of Q_d is a line segment joining two vertices that differ in exactly one position (i.e., coordinate). Selecting a coordinate i from 1 to d, there are 2^{d-1} edges among the connected components of $O \times O \times \cdots \times I \times \cdots \times O$, where the sole ("active") factor I occurs in the ith position. Thus Q_d has $d2^{d-1}$ edges. The **faces** of Q_d are the squares that are the connected components of

$$O \times \cdots \times I \times \cdots \times I \times \cdots \times O,$$

where exactly two of the factors are I's and the rest are O's. Thus Q_d has $\binom{d}{2}2^{d-2}$ faces, and the boundary of each face consists of four edges. Likewise Q_d has $\binom{d}{3}2^{d-3}$ **3-facets**

$$O \times \cdots \times I \times \cdots \times I \times \cdots \times I \times \cdots \times O,$$

formed by selecting three positions for the I's. Each 3-facet is a 3-cube whose boundary consists of six faces. Similarly, Q_d has $\binom{d}{k}2^{d-k}$ k-facets for each $0 \le k \le d$, and each k-facet is a k-cube. The 2**-skeleton**, Q_d^2, of Q_d is the union of all of its faces.

Notice that each edge of Q_d belongs to $d-1$ faces, so the 2-skeleton is even if and only if d is odd. Hence Q_d^2 has no sphere decomposition if d is even.

1 Sphere decompositions in dimensions 1 and 3 (mod 6)

Here we show that if $d = 3, 7, 9, 13, 15, 19, 21, \ldots$, that is, if $d \equiv 1$ or $3 \pmod 6$, then the 2-skeleton of Q_d can be decomposed into a face-disjoint union of boundaries of 3-cubes.

We use combinatorial designs [1], [8, pp. 96–100]. Let $[d] := \{1, \ldots, d\}$. A **k-design** $S(k,d)$ on $[d]$ is a family of k-subsets of $[d]$ (called **blocks**) such that each 2-subset of $[d]$ is contained in a unique block. Though 3-designs are called *Steiner triple systems*, it was Kirkman [7] who proved that they exist if and only if $d \equiv 1$ or 3 (mod 6). Conditions that are algebraically necessary turned out to be combinatorially sufficient.

Before describing our general construction we illustrate it for Q_7. We will decompose the 2-skeleton of Q_7 into 112 pairwise face-disjoint 3-cube boundaries. The first step is to realize a Steiner triple system $S(3,7)$. Label the vertices of a 7-gon with the integers 1 through 7, as in in Figure 1. The shaded triangle on the left has vertices 1, 2 and 4, and any two of them are a distance of 1, 2 or 3 apart along the 7-gon. Rotating the triangle in multiples of $2\pi/7$ yields seven triangles, whose respective vertex sets are tallied below them. These are the blocks of $S(3,7)$ because any two vertices on the 7-gon are at distance 1, 2, or 3, and therefore they are vertices of exactly one of the triangles.

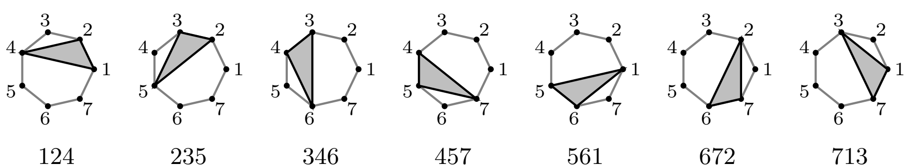

Figure 1: Construction of a Steiner triple system $S(3,7)$.

Each block of $S(3,7)$ corresponds to one of seven classes of 3-cubes in Q_7 indicated in Table 1, where an integer i belongs to the block if and only if the product is active in the ith factor. Notice that permuting the factors in a class cyclicly yields the subsequent class.

124	$I \times I \times O \times I \times O \times O \times O$
235	$O \times I \times I \times O \times I \times O \times O$
346	$O \times O \times I \times I \times O \times I \times O$
457	$O \times O \times O \times I \times I \times O \times I$
561	$I \times O \times O \times O \times I \times I \times O$
672	$O \times I \times O \times O \times O \times I \times I$
713	$I \times O \times I \times O \times O \times O \times I$

Table 1: The seven classes of 3-cubes in Q_7.

As $O = \{0,1\}$, each of the seven classes contains 16 disjoint 3-cubes, for a total of 112 3-cubes. Notice that any two cubes from the same class have empty intersection. Further, two 3-cubes from different classes are either disjoint or they intersect at an edge because by construction they have exactly one I as a common factor. We have accounted for $6 \cdot 112 = 672$ faces of Q_7, which has indeed $\binom{7}{2}2^5 = 672$ faces. We therefore have a decomposition of its 2-skeleton into pairwise face-disjoint boundaries of 3-cubes.

To visualize this, let $P : \mathbb{R}^7 \to \mathbb{R}^2$ be the projection sending the standard basis elements $\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_7$ to the vertices of a regular 7-gon, cyclically, as in Figure 1. Figure 2 (left) shows the projection P of the 16 disjoint 3-cubes in the class $I \times I \times O \times I \times O \times O \times O$ (shown bold in the figure, with other edges of Q_7 gray). There is much overlap in this figure. The right of Figure 2 shows the same projection, but with the vectors $P(\mathbf{e}_1)$, $P(\mathbf{e}_2)$ and $P(\mathbf{e}_4)$ scaled by a factor of about 0.2 in order to separate the 3-cubes. Observe that rotating Figure 2 (left) by $2\pi/7$ brings the cubes $I \times I \times O \times I \times O \times O \times O$ to the cubes $O \times I \times I \times O \times I \times O \times O$, etc.

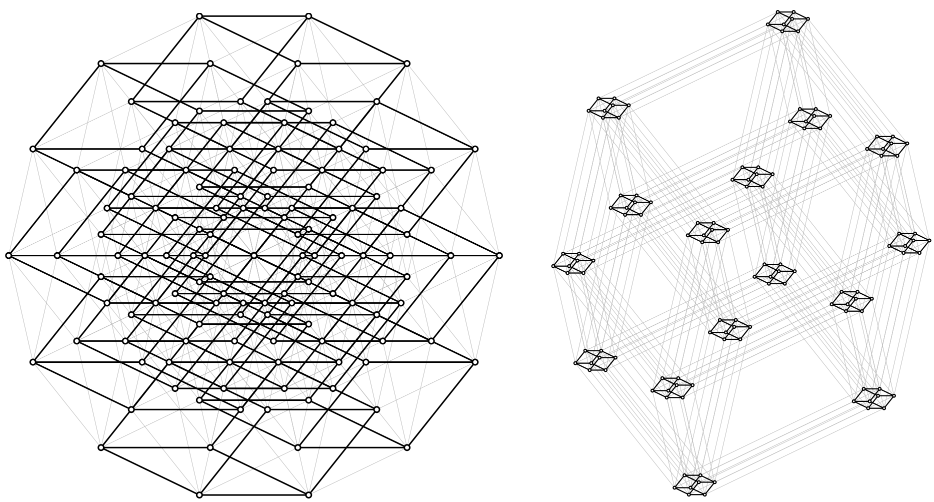

Figure 2: Two views of the sixteen 3-cubes $I \times I \times O \times I \times O \times O \times O$ (bold lines) in Q_7.

Now that we have illustrated our construction, we can prove the general result.

Theorem 1.1. *The* 2*-skeleton of* Q_d *can be decomposed into a pairwise face-disjoint union of 3-cube boundaries if and only if* $d \equiv 1$ *or* 3 $(mod\ 6)$.

Proof. Let $d \equiv 1$ or $3 \pmod 6$ and let $S(3, d)$ be a 3-design. As $[d]$ has $\binom{d}{2}$ pairs and each block of $S(3, d)$ contains $\binom{3}{2} = 3$ pairs, the number of blocks is $\frac{1}{3}\binom{d}{2} = \frac{d(d-1)}{6}$. For each block $\{i, j, k\}$ of $S(3, d)$, construct a class of 3-cubes

$$O \times \cdots \times I \times \cdots \times I \times \cdots \times I \times \cdots \times O,$$

where there is an I precisely in the ith, jth and kth factors. Such a class consists of 2^{d-3} disjoint 3-cubes. By construction, the intersection of any two 3-cubes from different classes corresponding to blocks $\{i, j, k\}$ and $\{i', j', k'\}$ is either empty, or a vertex, or an edge. Indeed, the intersection cannot be a face in any $O \times \cdots \times I \times \cdots \times I \times \cdots \times O$ because this would mean that some pair belongs to both $\{i, j, k\}$ and $\{i', j', k'\}$. Thus these 3-cubes are pairwise face-disjoint. The cubes in the $\frac{d(d-1)}{6}$ classes thus account for $6\frac{d(d-1)}{6}2^{d-3} = \binom{d}{2}2^{d-2}$ faces of Q_d, which is all of the faces of Q_d. We have thus decomposed the 2-skeleton of Q_d into a pairwise face-disjoint union of boundaries of 3-cubes.

Conversely suppose that $d \not\equiv 1$ or $3 \pmod 6$. If d is even, then Q_d^2 is not even, so it does not have a sphere decomposition. Thus assume d is odd, in which case $d \equiv 5 \pmod 6$. An easy computation shows that, in this case, the number of faces in Q_d^2 is not a multiple of 6. Hence Q_d^2 cannot be decomposed as a pairwise face-disjoint union of 3-cubes. □

Theorem 1.1 does not cover the cases $d = 5, 11, 17, 23, \ldots$, where $d \equiv 5 \pmod 6$. We do not know if all such such Q_d^2 have sphere decompositions. In the next section we find sphere decompositions when $d = 5^n$. However, these decompositions are not factorizations as they involve non-isomorphic complexes.

2 A sphere decomposition of the 5-cube

We now show that there is a sphere decomposition for Q_5^2, which is the smallest case not covered by a Steiner triple system. In fact, we will get somewhat more. Theorem 2.1 below guarantees sphere decompositions of Q_d^2 exist for arbitrarily large $d \equiv 5 \pmod 6$.

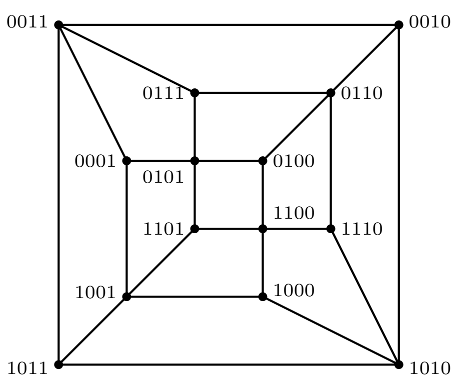

Figure 3: The 2-skeleton of the 4-cube, minus the vertices 0000 and 1111, is a sphere S.

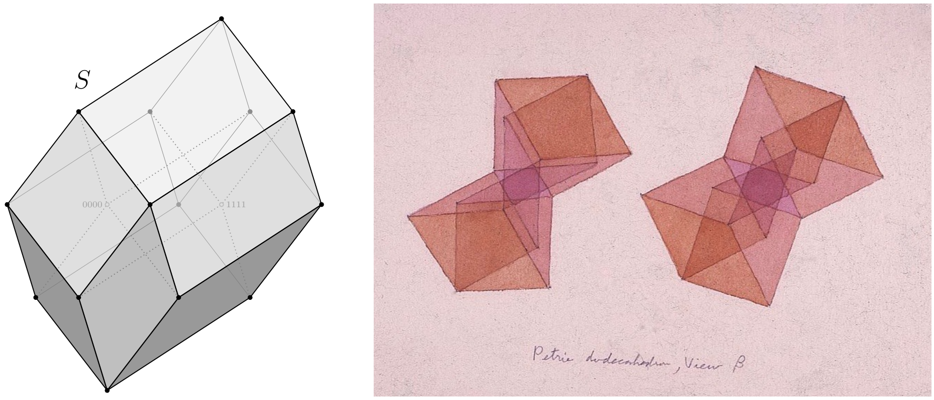

Figure 4: The rhombic dodecahedron obtained by deleting opposite vertices of Q_4^2. The watercolor (right) by David W. Brisson (1977) is a *hypersterogram* [2] showing two views differing in two degrees of parallax. Used with permission of Harriet and Erik Brisson.

Theorem 2.1. *If $d = 5^n$, then the 2-skeleton of Q_d is a face-disjoint union of spheres.*

Proof. We first treat the case $d = 5$. The case $d = 5^n$ will follow from design theory.

Our plan is to realize the 2-skeleton of Q_4 as a face-disjoint union of a sphere S and six disks $D_1, \ldots, D_6$ with edge-disjoint boundaries, then show that the 2-skeleton of Q_5 is the face-disjoint union of the eight spheres $S\times\{0\}$, $S\times\{1\}$, $\partial(D_1\times[0,1]), \cdots, \partial(D_6\times[0,1])$.

Let $S = Q_4^2 - \{0000, 1111\}$ be Q_4^2 with the antipodal vertices 0000 and 1111 removed (and with them all the edges and faces incident with them). We thus have removed two vertices, eight edges and 12 faces. What remains is a sphere S with 12 square faces. It is shown in Figure 3 embedded in the punctured sphere (plane). We note in passing that sphere S is a rhombic dodecahedron, which can be embedded in $\mathbb{R}^3$ with 12 congruent rhombic faces. (See Figure 4.)

The sphere S accounts for 12 of the 4-cube's 24 faces. The 12 missing squares are all incident with one or the other of the removed vertices 0000 and 1111. Figure 5 shows eight of these missing squares. Four of them form a disk D_1 centered at 0000 and the other four make a disk D_2 centered at 1111. These disks are pairwise face-disjoint, and their boundaries are pairwise edge-disjoint. And none of their faces are faces of S, because each face of D_1 and D_2 contains either the vertex 0000 or 1111, and neither of these vertices is in S.

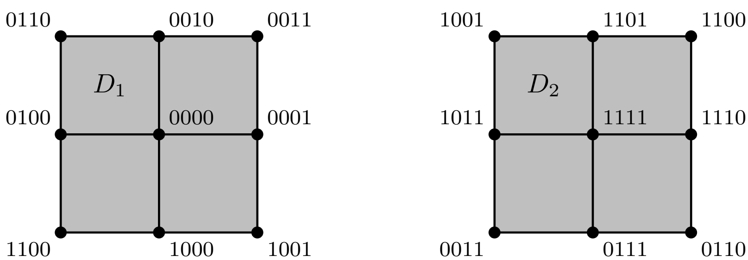

Figure 5: The disks D_1 and D_2 centered at 0000 and 1111, respectively.

So far we have accounted for 20 squares of Q_4^2, 12 of them in S, four in D_1, and four in D_2. There are just four squares in Q_4^2 that are unaccounted for. They are not hard to find, because 0000 and 1111 are each contained in *six* squares of Q_4^2 and Figure 5 shows only four squares at 0000 and 1111. Thus the four missing squares are incident with 0000 or 1111. They are shown in Figure 6, superimposed on the drawings from Figure 5. Call these four squares disks D_3, D_4, D_5 and D_6.

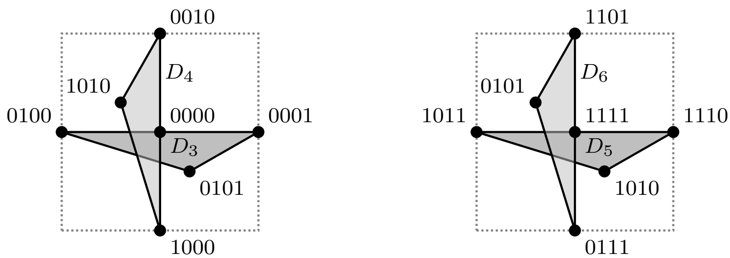

Figure 6: The disks D_3, D_4, D_5 and D_6.

Note that the sphere S and disks $D_1, D_2, \ldots D_6$ are pairwise face-disjoint and account for all squares of Q_4^2. Further the boundaries of the disks are pairwise edge-disjoint. We now have eight spheres in Q_5^2: $S \times \{0\}$, $S \times \{1\}$, $\partial(D_1 \times [0,1]), \cdots, \partial(D_6 \times [0,1])$. By construction they are face-disjoint. (See Figure 7.) Moreover the total number of squares used is $12 + 12 + 16 + 16 + 6 + 6 + 6 + 6 = 80$, so we have used all the squares in Q_5^2.

We have now decomposed the 2-skeleton of Q_5 into a pairwise face-disjoint union of spheres, two of which are rhombic dodecahedrons, two of which have the structure shown in Figure 7 (left), and four of which are the boundaries of a 3-cube, as in Figure 7 (right).

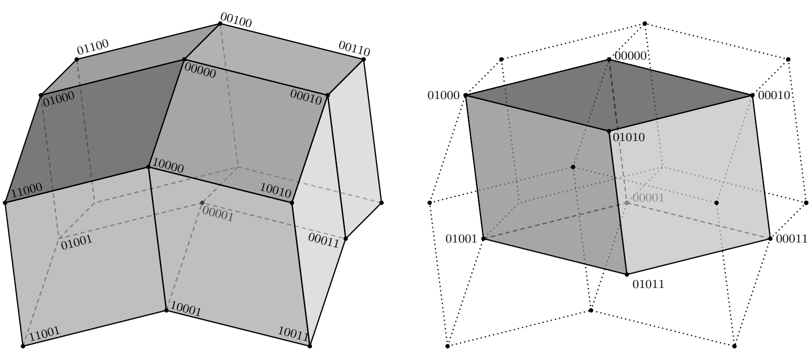

Figure 7: The spheres $\partial(D_1 \times I)$ (left) and $\partial(D_3 \times I)$ (right) intersect at the hexagon 00000–00010–00011–00001–01001–01000–00000. Our decomposition of of Q_5 uses two spheres of the type on the left, four of the type on the right, and two rhombic dodecahedra.

Having obtained a sphere decomposition of Q_5^2, we get a generalization. Consider the finite field $\mathbb{F}_5$ consisting of the integers modulo 5. The vector space $\mathbb{F}_5^n$ then consists of 5^n elements, or **points**, and each 1-dimensional subspace $V = \{\lambda \mathbf{v} \mid \lambda \in \mathbb{F}_5\}$ consists of five points. A **line** L is a translate $L = \{\mathbf{w} + \lambda \mathbf{v} \mid \lambda \in \mathbb{F}_5\}$ of a 1-dimensional subspace. We can realize $S(5, 5^n)$ by letting the blocks be the lines in $\mathbb{F}_5^n$. (Each line consists of 5 of the 5^n points in $\mathbb{F}_5^n$, and any two points in $\mathbb{F}_5^n$ lie on a unique line.) From each block we can extract 10 pairs of points, so the total number of blocks is $\frac{1}{10}\binom{5^n}{2} = \frac{5^{n-1}(5^n-1)}{4}$. Using the development from Section 1, it follows that the 2-skeleton of Q_{5^n} is the face-disjoint union of $\frac{5^{n-1}(5^n-1)}{4}2^{5^n-5}$ 5-cubes, each of which is decomposable into a pairwise face-disjoint union of spheres. We can thus decompose the 2-skeleton of Q_{5^n} into a pairwise face-disjoint union of spheres. Indeed, the total number of faces used in this decomposition is $80\frac{5^{n-1}(5^n-1)}{4}2^{5^n-5} = \frac{5^n(5^n-1)}{2}2^{5^n-2} = \binom{5^n}{2}2^{5^n-2}$, the number of faces of $Q^2_{5^n}$. □

Notice that $5^n \equiv 5 \pmod 6$ if and only if n is odd, so Theorem 2.1 yields a new class of hypercubes with sphere decompositions that is not covered by Theorem 1.1.

3 Discussion

Design theory applies to additional cases where $d \equiv 5 \pmod 6$ by using the technique of the previous section. Suppose one has a sphere decomposition of some Q_k^2 and there is a k-design on $[d]$. Then there is a sphere decomposition for Q_d^2. We illustrate this for $k = 5$.

In [5, Thm. 2], Hanani showed that a 5-design exists if and only if $d \equiv 1$ or $5 \pmod{20}$. So for $d = 41, 65,$ etc., any $S(5, d)$ and any sphere decomposition of Q_5^2 can be combined to construct a sphere decomposition of Q_d^2 for some $d \neq 5^n$.

We conjecture that sphere decompositions exist for Q_d^2 for all odd d, but that spherical factorizations exist if and only if $d \equiv 1$ or $3 \pmod 6$.

Note that cyclical configurations of points and lines were constructed by Grünbaum through a similar use of Steiner triple systems. See [3, pp. 253 and 325].

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Strongly regular graphs with parameters $(37, 18, 8, 9)$ having nontrivial automorphisms*

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Abstract

All strongly regular graphs having at most 36 vertices have been enumerated. Hence, the first open case is enumeration of the SRGs with parameters $(37, 18, 8, 9)$. In this paper we show that there are exactly forty SRGs with parameters $(37, 18, 8, 9)$ having nontrivial automorphisms. Comparing the constructed graphs with previously known SRGs with these parameters we conclude that six of the SRGs with parameters $(37, 18, 8, 9)$ constructed in this paper are new, and that up to isomorphism there are at least 6766 strongly regular graphs with parameters $(37, 18, 8, 9)$.

Keywords: Strongly regular graph, automorphism group, orbit matrix.

Math. Subj. Class. (2020): 05E30, 20D45

1 Introduction

One of the main problems in the theory of strongly regular graphs (SRGs) is constructing and classifying SRGs with given parameters. A frequently used method of constructing combinatorial structures is a construction with a prescribed automorphism group using orbit matrices. While orbit matrices of block designs have been used for such a construction of designs since 1980s, orbit matrices of strongly regular graphs have not been introduced until 2011 (see [2]). Using orbit matrices we construct all strongly regular graphs with parameters $(37, 18, 8, 9)$ having nontrivial automorphisms. In that way we have constructed forty SRGs with parameters $(37, 18, 8, 9)$, and six of them are new. Thereby we proved that there are exactly forty SRGs with parameters $(37, 18, 8, 9)$ having nontrivial automorphisms, and at least 6766 strongly regular graphs with these parameters.

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The paper is organized as follows: after a brief description of the terminology and some background results in Section 2, in Section 3 we describe the concept of orbit matrices. In Section 4 we apply the method of constructing SRGs using orbit matrices to construct all strongly regular graphs with parameters $(37, 18, 8, 9)$ having nontrivial automorphisms.

2 Background and terminology

We assume that the reader is familiar with basic notions from the theory of finite groups. For basic definitions and properties of strongly regular graphs we refer the reader to [3, 9, 14].

A graph is regular if all its vertices have the same valency. A simple regular graph $\Gamma = (\mathcal{V}, \mathcal{E})$ is strongly regular with parameters (v, k, λ, μ) if it has $|\mathcal{V}| = v$ vertices, valency k, and if any two adjacent vertices are together adjacent to λ vertices, while any two nonadjacent vertices are together adjacent to μ vertices. A strongly regular graph with parameters (v, k, λ, μ) is usually denoted by SRG(v, k, λ, μ). An automorphism of a strongly regular graph Γ is a permutation of vertices of Γ, such that every two vertices are adjacent if and only if their images are adjacent.

Let $\Gamma_1 = (\mathcal{V}, \mathcal{E}_1)$ and $\Gamma_2 = (\mathcal{V}, \mathcal{E}_2)$ be strongly regular graphs and $G \leq Aut(\Gamma_1) \cap Aut(\Gamma_2)$. An isomorphism $\alpha : \Gamma_1 \to \Gamma_2$ is called a G-isomorphism if there exists an automorphism $\tau : G \to G$ such that for each $x, y \in \mathcal{V}$ and each $g \in G$ the following holds:

$$(\tau g).(\alpha x) = \alpha y \Leftrightarrow g.x = y.$$

Strongly regular graphs having at most 36 vertices have been enumerated, so SRGs with parameters $(37, 18, 8, 9)$ are the first open case that still have to be classified (see [4]). It is known that there exists at least 6760 SRGs$(37, 18, 8, 9)$, which are obtained as the descendants of the 191 regular two-graphs on 38 vertices constructed in [11]. The adjacency matrices of these 6760 SRGs$(37, 18, 8, 9)$ can be found at [12]. In this paper we classify SRGs$(37, 18, 8, 9)$ having nontrivial automorphisms, showing that there are at least 6766 strongly regular graphs with parameters $(37, 18, 8, 9)$.

3 Orbit matrices of strongly regular graphs

Orbit matrices of block designs have been frequently used for construction of block designs, see e.g. [6, 7, 8, 10]. In this section we describe the concept of orbit matrices of SRGs, which is introduced in 2011 by Behbahani and Lam (see [2]).

Let Γ be a SRG(v, k, λ, μ) and A be its adjacency matrix. Suppose an automorphism group G of Γ partitions the set of vertices V into b orbits $O_1, \ldots, O_b$, with sizes $n_1, \ldots, n_b$, respectively. The orbits divide A into submatrices $[A_{ij}]$, where A_{ij} is the adjacency matrix of vertices in O_i versus those in O_j. We define matrices $C = [c_{ij}]$ and $R = [r_{ij}]$, $1 \leq i, j \leq b$, such that

$c_{ij} =$ column sum of A_{ij},
$r_{ij} =$ row sum of A_{ij}.

The matrix R is related to C by

$$r_{ij} n_i = c_{ij} n_j. \tag{3.1}$$

Since the adjacency matrix is symmetric, it follows that

$$R = C^T. \tag{3.2}$$

The matrix R is the row orbit matrix of the graph Γ with respect to G, and the matrix C is the column orbit matrix of the graph Γ with respect to G.

Let us assume that a group G acts as an automorphism group of a SRG(v, k, λ, μ). Behbahani and Lam showed that orbit matrices $R = [r_{ij}]$ and $R^T = C = [c_{ij}]$ satisfy the condition

$$\sum_{s=1}^{b} c_{is} r_{sj} n_s = \delta_{ij}(k-\mu)n_j + \mu n_i n_j + (\lambda-\mu)c_{ij}n_j.$$

Since $R = C^T$, it follows that

$$\sum_{s=1}^{b} \frac{n_s}{n_j} c_{is} c_{js} = \delta_{ij}(k-\mu) + \mu n_i + (\lambda-\mu)c_{ij} \tag{3.3}$$

and

$$\sum_{s=1}^{b} \frac{n_s}{n_j} r_{si} r_{sj} = \delta_{ij}(k-\mu) + \mu n_i + (\lambda-\mu)r_{ji}.$$

In order to enable a construction of SRGs with a presumed automorphism group G, each matrix with the properties of an orbit matrix will be called an orbit matrix for parameters (v, k, λ, μ) and a group G (see [1]). Therefore, we introduce the following definition of orbit matrices of strongly regular graphs (see [5]).

Definition 3.1. A $(b \times b)$-matrix $R = [r_{ij}]$ with entries satisfying conditions:

$$\sum_{j=1}^{b} r_{ij} = \sum_{i=1}^{b} \frac{n_i}{n_j} r_{ij} = k \tag{3.4}$$

$$\sum_{s=1}^{b} \frac{n_s}{n_j} r_{si} r_{sj} = \delta_{ij}(k-\mu) + \mu n_i + (\lambda-\mu)r_{ji} \tag{3.5}$$

where $0 \le r_{ij} \le n_j$, $0 \le r_{ii} \le n_i - 1$ and $\sum_{i=1}^{b} n_i = v$, is called a **row orbit matrix** for a strongly regular graph with parameters (v, k, λ, μ) and the orbit lengths distribution $(n_1, \ldots, n_b)$.

Definition 3.2. A $(b \times b)$-matrix $C = [c_{ij}]$ with entries satisfying conditions:

$$\sum_{i=1}^{b} c_{ij} = \sum_{j=1}^{b} \frac{n_j}{n_i} c_{ij} = k \tag{3.6}$$

$$\sum_{s=1}^{b} \frac{n_s}{n_j} c_{is} c_{js} = \delta_{ij}(k-\mu) + \mu n_i + (\lambda-\mu)c_{ij} \tag{3.7}$$

where $0 \le c_{ij} \le n_i$, $0 \le c_{ii} \le n_i - 1$ and $\sum_{i=1}^{b} n_i = v$, is called a **column orbit matrix** for a strongly regular graph with parameters (v, k, λ, μ) and the orbit lengths distribution $(n_1, \ldots, n_b)$.

Not every orbit matrix gives rise to strongly regular graphs while, on the other hand, a single orbit matrix may produce several nonisomorphic strongly regular graphs. For the elimination of orbit matrices that produce G-isomorphic strongly regular graphs we use the same method as for the elimination of orbit matrices of G-isomorphic designs (see for example [7]). We could use row or column orbit matrices, but since we construct matrices row by row, it is more convenient for us to use column orbit matrices.

3.1 Orbit lengths distribution

Suppose an automorphism group G of the graph Γ partitions the set of vertices V into b orbits $O_1, \dots, O_b$, with sizes $n_1, \dots, n_b$, respectively. It is well known that n_i divides $|G|$, for $i = 1, \dots, b$. Further,

$$\sum_{i=1}^{b} n_i = v.$$

In this paper we will be interested in groups that act in orbits having at most two lengths, since we will consider automorphism groups of prime order. If the group G acts with d_1 orbits of length 1 and d_h orbits of length h, we will denote this distribution with $(d_1 \times 1, d_h \times h)$. When determining the orbit lengths distributions we use the following result that can be found in [1].

Theorem 3.3. *Let $s < r < k$ be the eigenvalues of a SRG(v, k, λ, μ), then*

$$\phi \leq \frac{\max(\lambda, \mu)}{k - r} v,$$

where ϕ is the number of fixed points for a nontrivial automorphism.

In the case of SRGs with parameters $(37, 18, 8, 9)$ we obtain that $\phi \leq 20$, so to find all feasible orbit length distributions $(d_1 \times 1, d_h \times h)$ we need to solve the system

$$\begin{aligned} & d_1 + h \cdot d_h = 37 \\ & d_1 \leq 20. \end{aligned}$$

4 Classification of SRGs with parameters $(37, 18, 8, 9)$ having nontrivial automorphisms

It is known that there exists at least 6760 SRGs with parameters $(37, 18, 8, 9)$ (see [11]). Spence [12] listed adjacency matrices of all of them. In Table 1 we give information on orders of the full automorphism groups of these 6760 SRGs$(37, 18, 8, 9)$. The graph having the full automorphism group of order 666 is the Paley graph obtained from the field $GF(37)$, having the full automorphism group isomorphic to $Z_{37} : Z_{18}$ (see [14]).

In this section we give the classification of strongly regular graphs with parameters $(37, 18, 8, 9)$ having nontrivial automorphisms. We show that there are exactly 6 strongly regular graphs with parameters $(37, 18, 8, 9)$ having an automorphism group of order two,

Table 1: Orders of the full automorphism groups of the known SRGs$(37, 18, 8, 9)$

$\lvert\mathrm{Aut}(\Gamma_i)\rvert$	#SRGs
1	6726
2	3
3	24
9	4
18	2
666	1

all of them isomorphic to the graphs given at [12]. Further, we show that there are exactly 37 strongly regular graphs with parameters $(37, 18, 8, 9)$ having an automorphism group of order three, 6 of them nonisomorphic to any of the graphs listed at [12]. Finally we show that there is no SRG$(37, 18, 8, 9)$ having an automorphism group Z_p, where p is prime and $3 < p < 37$, and that there is exactly one SRG$(37, 18, 8, 9)$ having the automorphism of order 37 (the Paley graph with 37 vertices). Comparing the constructed SRGs with the SRGs given at [12], we establish that six of the strongly regular graphs having a nontrivial automorphism group of prime order constructed in this paper have not been previously known.

In order to construct orbit matrices of SRGs with parameters $(37, 18, 8, 9)$ that have automorphism of prime order p, we first find all permissible distibutions $(d_1 \times 1, d_p \times p)$. Then for each distribution we find all prototypes (see [1]). Using prototypes we construct orbit matrices row by row and we eliminate mutually G-isomorphic orbit matrices during this process. In the next step we construct adjacency matrices of SRGs$(37, 18, 8, 9)$.

Table 2: Number of orbit matrices and SRGs$(37, 18, 8, 9)$ for the automorphism group Z_2

distribution	#OM	#SRGs	distribution	#OM	#SRGs
$(1 \times 1, 18 \times 2)$	24	6	$(11 \times 1, 13 \times 2)$	0	0
$(3 \times 1, 17 \times 2)$	0	0	$(13 \times 1, 12 \times 2)$	0	0
$(5 \times 1, 16 \times 2)$	6	0	$(15 \times 1, 11 \times 2)$	0	0
$(7 \times 1, 15 \times 2)$	0	0	$(17 \times 1, 10 \times 2)$	0	0
$(9 \times 1, 14 \times 2)$	0	0	$(19 \times 1, 9 \times 2)$	0	0

4.1 SRGs with parameters $(37, 18, 8, 9)$ having an automorphism group of order two

Using the program Mathematica we get all the possible orbit lengths distribution that satisfy Theorem 3.3, and using our own programs written in GAP [13] we construct all orbit matrices for the given orbit lengths distributions. In Table 2 we present the number of mutually nonisomorphic orbit matrices for Z_2 for each orbit lengths distribution. In the next step we obtain the adjacency matrices of strongly regular graphs with parameters $(37, 18, 8, 9)$. Finally, we check isomorphisms of strongly regular graphs using GAP. Thereby we prove Theorem 4.1. The number of the constructed nonisomorphic SRGs with parameters $(37, 18, 8, 9)$ are presented in Table 2. Orders of the full automorphism groups of these SRGs, also determined by using GAP, are shown in Table 3.

Table 3: SRGs with parameters $(37, 18, 8, 9)$ that have automorphisms of order 2

$\lvert \mathrm{Aut}(\Gamma_i) \rvert$	#SRGs
2	3
18	2
666	1

Theorem 4.1. *Up to isomorphism there exists exactly* 6 *strongly regular graphs with parameters* $(37, 18, 8, 9)$ *having an automorphism group of order 2.*

4.2 SRGs with parameters $(37, 18, 8, 9)$ having an automorphism group of order three

Using the program Mathematica we get all the possible orbit lengths distribution that satisfy Theorem 3.3, and using our own programs written in GAP [13] we construct all orbit matrices for given orbit lengths distributions. In Table 4 we present the number of mutually nonisomorphic orbit matrices for Z_3 for each orbit lengths distribution. In the next step we obtain the adjacency matrices of strongly regular graphs with parameters $(37, 18, 8, 9)$. Finally, we check isomorphisms of strongly regular graphs using GAP. Thereby we prove Theorem 4.2. The number of the constructed nonisomorphic SRGs with parameters $(37, 18, 8, 9)$ are presented in Table 4. Orders of the full automorphism groups of these SRGs are presented in Table 5.

Table 4: Number of orbit matrices and SRGs$(37, 18, 8, 9)$ for the automorphism group Z_3

distribution	#OM	#SRGs	distribution	#OM	#SRGs
$(1 \times 1, 12 \times 3)$	18	37	$(13 \times 1, 8 \times 3)$	0	0
$(4 \times 1, 11 \times 3)$	0	0	$(16 \times 1, 7 \times 3)$	0	0
$(7 \times 1, 10 \times 3)$	0	0	$(19 \times 1, 6 \times 3)$	0	0
$(10 \times 1, 9 \times 3)$	0	0			

Theorem 4.2. *Up to isomorphism there exists exactly* 37 *strongly regular graphs with parameters* $(37, 18, 8, 9)$ *having an automorphism group of order 3.*

Table 5: SRGs with parameters $(37, 18, 8, 9)$ that have automorphisms of order 3

$\lvert \mathrm{Aut}(\Gamma_i) \rvert$	#SRGs
3	30
9	4
18	2
666	1

4.3 SRGs $(37, 18, 8, 9)$ for Z_p, where p is a prime and $3 < p \leq 37$

We show that there is no orbit matrix for Z_p, where p is a prime and $3 < p < 37$. The results are presented in Table 6. Hence, there is no SRG$(37, 18, 8, 9)$ having an automorphism group isomorphic to Z_p, where p is a prime and $3 < p < 37$. Furher, there is exactly one SRG$(37, 18, 8, 9)$ admitting an automorphism group isomorphic to Z_{37}, namely the Paley graph with 37 vertices having the full automorphism group isomorphic to $Z_{37} : Z_{18}$.

Table 6: Possible distributions for Z_p, p a prime and $3 < p < 37$

distribution	#OM	distribution	#OM
$(2 \times 1, 7 \times 5)$	0	$(15 \times 1, 2 \times 11)$	0
$(7 \times 1, 6 \times 5)$	0	$(11 \times 1, 2 \times 13)$	0
$(12 \times 1, 5 \times 5)$	0	$(3 \times 1, 2 \times 17)$	0
$(17 \times 1, 4 \times 5)$	0	$(20 \times 1, 1 \times 17)$	0
$(2 \times 1, 5 \times 7)$	0	$(18 \times 1, 1 \times 19)$	0
$(9 \times 1, 4 \times 7)$	0	$(14 \times 1, 1 \times 23)$	0
$(16 \times 1, 3 \times 7)$	0	$(8 \times 1, 1 \times 29)$	0
$(4 \times 1, 3 \times 11)$	0	$(6 \times 1, 1 \times 31)$	0

We summarize the presented information in Theorem 4.3.

Theorem 4.3. *Up to isomorphism there exists at least* 6766 *strongly regular graphs with parameters* $(37, 18, 8, 9)$. *These are exactly forty SRGs*$(37, 18, 8, 9)$ *having nontrivial automorphisms, and at least* 6726 *SRGs*$(37, 18, 8, 9)$ *having the full automorphism group of order one.*

The adjacency matrices of the six newly constructed SRGs can be found at the link:

`http://www.math.uniri.hr/~mmaksimovic/srg37.txt`.

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