# On the Geometry of Symmetry Breaking Inequalities

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**Abstract.** Breaking symmetries is a popular way of speeding up the branch-and-bound method for symmetric integer programs. We study fundamental domains, which are minimal and closed symmetry breaking polyhedra. Our long-term goal is to understand the relationship between the complexity of such polyhedra and their symmetry breaking capability.

Borrowing ideas from geometric group theory, we provide structural properties that relate the action of the group with the geometry of the facets of fundamental domains. Inspired by these insights, we provide a new generalized construction for fundamental domains, which we call generalized Dirichlet domain (GDD). Our construction is recursive and exploits the coset decomposition of the subgroups that fix given vectors in  $\mathbb{R}^n$ . We use this construction to analyze a recently introduced set of symmetry breaking inequalities by Salvagnin [27] and Liberti and Ostrowski [17], called Schreier-Sims inequalities. In particular, this shows that every permutation group admits a fundamental domain with less than nfacets. We also show that this bound is tight.

Finally, we prove that the Schreier-Sims inequalities can contain an exponential number of isomorphic binary vectors for a given permutation group G, which provides evidence of the lack of symmetry breaking effectiveness of this fundamental domain. Conversely, a suitably constructed GDD for this G has linearly many inequalities and contains unique representatives for isomorphic binary vectors.

Keywords: Symmetry breaking inequalities  $\cdot$  Fundamental domains  $\cdot$  Polyhedral theory  $\cdot$  Orthogonal groups.

## 1 Introduction

Symmetries are mappings from one object into itself that preserve its structure. Their study has proven fruitful across a myriad of fields, including integer programming, where symmetries are commonly present. For instance, almost 30% of mixed-integer linear programs (MILP) in the model library used by the solver CPLEX are considerably affected by symmetry [1]. Moreover, symmetry exploitation techniques are of importance in various situations. In particular, they help to avoid traversing symmetric branches of the tree considered by a branch-and-bound algorithm.

Roughly speaking, the symmetry group G of an optimization problem is the set of functions in  $\mathbb{R}^n$  that leave the feasible region and the objective function invariant (see Section 2 for a precise definition). The symmetry group G, or any of its subgroups, partitions  $\mathbb{R}^n$  into G-orbits, which are sets of isomorphic solutions. A natural technique for handling symmetries is to add a static set of symmetry breaking inequalities. That is, we add extra inequalities that remove isomorphic solutions while leaving at least one representative per G-orbit. This well established approach has been studied extensively, both in general settings and different applications; see e.g. [10,11,12,14,15,16,17,21,27,30]. In most of these works, the symmetry breaking inequalities select the lexicographically maximal vector in each G-orbit of binary vectors. However, this constitutes a major drawback when dealing with general permutation groups: selecting the lexicographically maximal vector in a G-orbit is an NP-hard problem [4]. Hence, the separation problem of the corresponding symmetry breaking inequalities is also NP-hard. On the other hand, there is nothing preventing us to select orbit representatives with a different criterion. In this article, we are interested in understanding fundamental domains of a given finite group G, which are minimal, closed and convex symmetry breaking sets for G. Ideally, a closed symmetry breaking set F contains a unique representative per G-orbit. However, such a set does not necessarily exist for every group. Instead, a fundamental domain F only contains a unique representative for G-orbits that intersect F in its interior, while it can contain one or more representatives of a G-orbit intersecting its boundary. Despite this, F is a minimal closed symmetry breaking set, as any proper closed subset of F leaves some G-orbit unrepresented. On the other hand, a given symmetry group can admit inherently different fundamental domains. While all fundamental domains for finite orthogonal groups, including permutation groups (the main focus when considering mixed integer linear programs), are polyhedral cones, their polyhedral structure and complexity might differ greatly.

Our long term and ambitious goal is to understand the tension (and potential trade-offs) between the symmetry breaking effectiveness and the complexity of fundamental domains. The complexity can be measured in several ways: from the sizes of the coefficients in its matrix description, the number of facets, or even its extension complexity. On the other hand, the symmetry breaking effectiveness is related to the number of representatives that each orbit contains. Hence, the boundary of a fundamental domain, which can contain overrepresented *G*-orbits, becomes problematic, in particular if our points of interest (e.g., binary points in a binary integer program) can lie within it.

More precisely, we contribute to the following essential questions: (i) Which groups admit fundamental domains in  $\mathbb{R}^n$  with poly(n) facets? (ii) What is the structure of these facets? (iii) Which algorithmic methods can we use to construct different fundamental domains? (iv) Which fundamental domains contain unique representatives for every orbit?

Related Work. The concept of fundamental domain traces back to the 19th century, as it corresponds to fundamental parallelepipeds for the symmetry group of a lattice. Fundamental domains are studied in several areas, for example crystallography, the theory of quadratic forms, and elliptic functions, among many others. In particular Dirichlet [9] gives a construction which implies the existence of a fundamental domain in a general context, including all groups of isometries in  $\mathbb{R}^n$ , later known as *Dirichlet domain*. For a historical overview see Ratcliffe [24] and the references therein.

Several techniques have been studied to handle symmetries in integer programming. Kaibel and Pfetsch [15] introduce the concept of *orbitopes* as the convex-hull of 0-1 matrices that are lexicographically maximal under column permutations, and give a complete description of the facets for the cyclic group and the symmetric group. Friedman [11] considers general permutation groups. Based on the Dirichlet Domain, he introduces the idea of a universal ordering vector, which yields a fundamental domain with unique representatives of binary points. On the other hand, this fundamental domain has an exponential number of facets, its defining inequalities can contain exponentially large coefficients in n, and the separation problem is NP-hard for general permutation groups [4,20]. Liberti [16] and later Dias and Liberti [8] also consider general permutation groups G and derive a class of symmetry breaking constraints by studying the orbits of G acting on  $[n] = \{1, \ldots, n\}$ . Liberti and Ostrowski [17], and independently Salvagnin [27], extend this construction and introduce a set of symmetry breaking inequalities based on a chain of pointwise coordinate stabilizers. We will refer to this set as the Schreier-Sims inequalities, as they are strongly related to the Schreier-Sims table from computational group theory [29]. Hojny and Pfetsch [14] study symretopes, defined as the convex hulls of lexicographically maximal vectors in binary orbits. They obtain a linear time algorithm for separating the convex hull of polytopes derived by a single lexicographic order enforcing inequality and show how to exploit this construction computationally.

For integer programming techniques, dynamic methods have been used to deal with symmetries within the Branch-and-Bound tree. Some methods are *Orbital Fixing* [19], *Isomorphism Pruning* [18] and *Orbital Branching* [22]. A more geometric approach for solving symmetric integer programs relies on the theory of *core points* [5,13]. For more details on these techniques and related topics see Margot [20], Pfetsch and Rehn [23], and Schürmann [28].

Our Contribution. In this article we focus on finite orthogonal groups in  $\mathbb{R}^n$ , that is, groups of linear isometries. We start by presenting basic structural results of the theory of fundamental domains for a given

orthogonal group G. A basic observation is that each facet is related to a group element g. We also show the following new property of the facets: for an interesting class of fundamental domains, which we call *subgroup* consistent, the vector defining a facet must be orthogonal to the fixed subspace of g. This implies that each inequality is of the form  $\alpha^t x \ge \alpha^t(gx)$  for some vector  $\alpha \in \mathbb{R}^n$  and some element  $g \in G$ . In other words, the inequalities of any subgroup consistent fundamental domain have the same structure as inequalities of Dirichlet domains.

Inspired by these new insights, we state our main contribution: a generalized construction of fundamental domains for any finite orthogonal group, including permutation groups. Our method is based on choosing a vector  $\alpha$  and finding the coset decomposition using the stabilizer subgroup  $G_{\alpha} = \{g \in G : g\alpha = \alpha\}$ . Next, we add inequalities to our symmetry breaking set, one for each member in the coset decomposition. For a well-chosen  $\alpha$ , the number of cosets can be bounded by a polynomial, yielding a polynomial number of inequalities. By proceeding recursively on the subgroup  $G_{\alpha}$ , we generate a fundamental domain after at most n iterations. We say that a fundamental domain obtained via this method is a *generalized Dirichlet domain* (GDD), as it generalizes the classical construction by Dirichlet [9]. To the best of our knowledge, this construction generalizes all convex fundamental domains found in the literature. For the special case of permutation groups, our algorithm can be implemented in polynomial time if the vector  $\alpha$  is well chosen.

A natural way of breaking symmetries is to choose the lexicographically maximal element for every Gorbit in  $\mathbb{R}^n$  (not only binary vectors, as in the construction by Friedman [11]). However, it is not hard to see that the obtained set is not necessarily closed. On the other hand, the set is convex. We show that the closure of this set coincides with the Schreier-Sims inequalities studied by Salvagnin [27] and Liberti and Ostrowski [17]. Moreover, we show that this set is a GDD, which implies that it is a fundamental domain. Finally, we give a stronger bound on the number of facets for this fundamental domain, implying that all permutation groups admit a fundamental domain with at most n-1 inequalities. We also notice that any fundamental domain for  $S_n$ , the full symmetric group of degree n, has n-1 facets, which shows that our bound is best possible.

Salvagnin [27] recognizes that the symmetry breaking efficiency of the Schreier-Sims inequalities might be limited: the orbit of a binary vector can be overrepresented in the set. We give a specific example of a permutation group in which an orbit of binary vectors can have up to  $2^{\Omega(n)}$  many representatives. Using the flexibility given by our GDD construction, we exhibit a fundamental domain for the same group with a unique representative for each binary orbit, while having O(n) facets. This illustrates that exploiting the structure of the given group can yield a relevant improvement in the way symmetries are broken. Moreover, we show that the only groups that admit a fundamental domain with a unique representative for *every* orbit are reflection groups. Finally, we propose a new way of measuring the effectiveness of fundamental domains, which we hope will pave the road for future work in deriving fundamental domains that exploit the structure of the groups involved.

## 2 Notation and Preliminaries

Throughout the whole paper, G denotes a group, and  $H \leq G$  means that H is a subgroup of G. The element id  $\in G$  denotes the identity. For a subset S of G,  $\langle S \rangle$  is the smallest group containing S. The set  $O_n(\mathbb{R})$  corresponds to the orthogonal group in  $\mathbb{R}^n$ , that is, the group of all  $n \times n$  orthogonal matrices (equivalently, linear isometries). Hence, it holds that if  $g \in O_n(\mathbb{R})$  then the inverse  $g^{-1}$  equals the transpose  $g^t$ . All groups considered in what follows are finite subgroups of  $O_n(\mathbb{R})$ . Also,  $G_{(S)}$  denotes the pointwise stabilizer of the set  $S \subseteq \mathbb{R}^n$ , and the set fix(g) denotes the invariant subspace of  $g \in G$ , that is,

$$G_{(S)} := \{ g \in G : x = gx \; \forall x \in S \} \text{ and } \operatorname{fix}(g) := \{ x \in \mathbb{R}^n : gx = x \}.$$

If  $S := \{x\}$ , we write  $G_x := G_{(S)}$ . For  $H \leq G$ , a transversal for H in G is a set of representatives from the left cosets of H in G, the set of left cosets being  $\{gH : g \in G\}$ . Given a set of elements  $S \subseteq G$ , we denote by  $S^{-1} := \{g^{-1} : g \in S\}$ . For  $x \in \mathbb{R}^n$ , the G-orbit of x is the set  $\operatorname{Orb}_G(x) := \{gx : g \in G\}$ . We denote by [n] the set  $\{1, \ldots, n\}$  for all  $n \in \mathbb{N}$  and  $S_n$  denotes the symmetric group, that is the group of all permutations over [n]. For  $G \leq S_n$ , each element  $g \in G$  acts on  $\mathbb{R}^n$  by the mapping  $x \mapsto gx := (x_{g^{-1}(i)})_{i=1}^n$ . Equivalently, we

consider  $G \leq S_n$  as a group of isometries where each  $g \in G$  is interpreted as the corresponding permutation matrix.

For an exhaustive introduction to group theory, see for instance Rotman [26]. For an exposition on computational aspects of permutation groups, see Seress [29].

For a set S we denote by  $S^c$  its complement. For  $S \subseteq \mathbb{R}^n$ , we write int(S) for its interior,  $\overline{S}$  for its closure, and  $\partial S$  for its boundary.

An optimization problem  $\min\{f(x) : x \in X\}$  is *G*-invariant if for all feasible x and  $g \in G$ ,

1. f(x) = f(gx), and

2. gx is feasible.

Given a G-invariant optimization problem, we can use the group G to restrict the search of solutions to a subset of  $\mathbb{R}^n$ , namely a fundamental domain.

**Definition 1.** A subset F of  $\mathbb{R}^n$  is a fundamental domain for  $G \leq O_n(\mathbb{R})$  if

- 1. the set F is closed and convex<sup>4</sup>,
- 2. the members of  $\{int(gF) : g \in G\}$  are pairwise disjoint,
- 3.  $\mathbb{R}^n = \bigcup_{g \in G} gF$ .

Notice that for any  $x \in \mathbb{R}^n$ , its *G*-orbit,  $\operatorname{Orb}_G(x)$ , satisfies that  $|\operatorname{Orb}_G(x) \cap F| \ge 1$ . Also,  $|\operatorname{Orb}_G(x) \cap F| = 1$ if  $x \in \operatorname{int}(F)$ . It is not hard to see that all fundamental domains for a finite subgroup of  $O_n(\mathbb{R})$  are fulldimensional sets. Moreover, if  $F' \subsetneq F$ , then there is some  $\operatorname{Orb}_G(x)$  such that  $\operatorname{Orb}_G(x) \cap F' = \emptyset$ , and hence some orbit is not represented in F.

**Definition 2.** A subset R of  $\mathbb{R}^n$  is a fundamental set for a group  $G \leq O_n(\mathbb{R})$  if it contains exactly one representative of each G-orbit in  $\mathbb{R}^n$ .

## 3 The Geometric Structure of Fundamental Domains

In this section we review some basic geometric properties of fundamental domains and derive new properties. Propositions 1 and 3 are well known; their proof can be found in [24, Ch. 6]. Proposition 2 extends a similar result for the particular case of *exact* fundamental domains [24, Ch. 6]. Theorem 1 and Corollary 1 are our main contributions of this section. To provide a self-contained presentation of the topic, we provide alternative proofs of some of the previously known results.

The following proposition, together with the existence of a vector  $\alpha$  whose stabilizer is trivial [24, Thm. 6.6.10.], guarantees the existence of a fundamental domain for any  $G \leq O_n(\mathbb{R})$ . We will refer to the construction  $F_{\alpha}$  in the proposition as a *Dirichlet domain*.

**Proposition 1.** Let  $G \leq O_n(\mathbb{R})$  be finite and non-trivial, and let  $\alpha \in \mathbb{R}^n$  whose stabilizer  $G_\alpha$  equals {id}. Then the following set is a fundamental domain for G,

$$F_{\alpha} = \{ x \in \mathbb{R}^n : \alpha^t x \ge \alpha^t g x, \quad \forall g \in G \}.$$

Proof. Let  $\alpha \in \mathbb{R}^n$  be a point such that  $G_\alpha = \langle id \rangle$ . Consider the linear functional  $y \mapsto \alpha^t y$ , for all  $y \in \mathbb{R}^n$ . Note that  $z \in F_\alpha$  if and only if z maximizes this linear functional over its finite G-orbit, i.e.  $z \in \operatorname{argmax}\{\alpha^t y : y \in \operatorname{Orb}_G(z)\}$ .

First note that  $F_{\alpha}$  is closed and convex by construction. Now, let  $x \in \mathbb{R}^n$ , and suppose that  $z \in \arg\max\{\alpha^t y : y \in \operatorname{Orb}_G(x)\}$ , and hence  $z \in F_{\alpha}$ . Then there exists a  $g \in G$  such that z = gx, i.e.  $x = g^{-1}z$ . Hence  $x \in g^{-1}F_{\alpha}$ . Now, note that

$$\begin{aligned} &\inf(F_{\alpha}) = \{ x \in \mathbb{R}^n \ : \ \alpha^t x > \alpha^t g x, \ \forall g \in G \setminus \{ \mathrm{id} \} \} \\ &= \{ x \in \mathbb{R}^n \ : \ G_x = \{ \mathrm{id} \} \text{ and for all } y \in \mathrm{Orb}_G(x) \setminus \{ x \}, \ \alpha^t x > \alpha^t y \}. \end{aligned}$$

<sup>&</sup>lt;sup>4</sup> Notice that in part of the literature, e.g. [24], convexity is not part of the definition.

Since every  $g \in G$  is a linear homeomorphism, we have that  $\operatorname{int}(gF_{\alpha}) = g\operatorname{int}(F_{\alpha})$ . Thus, if  $x \in \operatorname{int}(F_{\alpha})$ and  $x \in g\operatorname{int}(F_{\alpha})$ , for some  $g \in G$  non-trivial, there exists  $y \in \operatorname{int}(F_{\alpha})$ , such that x = gy. But this is a contradiction since the maximum is unique and  $G_x$  is trivial. In consequence,  $F_{\alpha}$  is a fundamental domain for G.

A specific kind of Dirichlet domains are k-fundamental domains. For any integer  $k \ge 2$ , we define  $\overline{k} := (k^{n-1}, k^{n-2}, \ldots, 1)$  as the k-universal ordering vector. The set  $F_{\overline{k}}$  is the k-fundamental domain for the symmetry group G. Friedman [11] observes that  $F_{\overline{2}}$  contains a unique representative per G-orbit of binary points in  $\mathbb{R}^n$ . This fact easily generalizes for points  $x \in \{0, \ldots, k-1\}^n$  with the k-ordering vector (see [20]).

Given a fundamental domain F and  $g \in G \setminus \{id\}$ , let  $H_g$  be any closed half-space that separates F and gF, that is,  $F \subseteq H_g$  and  $gF \subseteq \overline{H_g^c}$ . The existence of this half-space follows from the convex separation theorem. We say that a collection  $\{H_g\}_{g\in G}$  represents F if for every  $g \in G$ , the set  $H_g$  is a closed half-space that separates F and gF. Notice that representations are non unique.

Let us denote by  $H_g^{=} := \partial(H_g)$  the hyperplane defining  $H_g$ . Notice that  $H_g^{=}$  contains 0 as  $0 \in F \cap gF$ , since g is a linear isometry. We let  $\gamma_g \neq 0$  be some defining vector for  $H_g$ , i.e.,  $H_g = \{x \in \mathbb{R}^n : \gamma_g^t x \ge 0\}$ , and thus  $H_g^{=} = \{x \in \mathbb{R}^n : \gamma_g^t x = 0\}$ .

**Proposition 2.** Let  $G \leq O_n(\mathbb{R})$  be finite, let F be a fundamental domain and  $\{H_g\}_{g\in G}$  a collection that represents F. Then  $F = \bigcap_{g\in G} H_g$ . In particular, F is a polyhedral cone. Moreover, if A is the set of all  $g \in G$  such that  $\dim(F \cap gF) = n - 1$ , then A generates G.

*Proof.* Let  $H := \bigcap_{g \in G} H_g$ . Let us first show that F = H. Clearly  $F \subseteq H$  as  $F \subseteq H_g$  for every  $g \in G$ . For the other inclusion, suppose by contradiction that  $H \setminus F \neq \emptyset$ . Given that H is convex,  $\operatorname{int}(H) \neq \emptyset$  (as  $F \subseteq H$  is full-dimensional), and  $F^c$  is open, we have that  $\operatorname{int}(H \setminus F) \neq \emptyset$ . Hence, let  $x \in \operatorname{int}(H \setminus F)$ . As F is a fundamental domain for G, there exists a  $g \in G$  such that  $gx \in F$ . This implies that  $x \in g^{-1}F \subseteq \overline{H_{g^{-1}}}$ . By definition, we also have that  $x \in H \subseteq H_{g^{-1}}$ , thus  $x \in H_{g^{-1}}^{=}$ . But this contradicts the fact that x belongs to the interior of  $H_{q^{-1}}$ , because x belongs to the interior of  $H \setminus F$ .

Let us now show that A generates G. For a fixed  $g \in G$ , let us prove that  $g \in \langle A \rangle$ . First, take  $x \in int(F)$ and  $y \in int(gF)$ . Now, take  $\epsilon > 0$  so that  $B_{\epsilon}(x) \subseteq int(F)$ , and choose  $x_0 \in B_{\epsilon}(x)$  uniformly at random. For  $a, b \in \mathbb{R}^n$ , let [a, b] denote the interval  $\{\lambda a + (1 - \lambda)b : \lambda \in [0, 1]\}$ . The interval  $[x_0, y]$  is partitioned in several segments by the tessellation  $\{hF\}_{h \in G}$ . More precisely, notice that

$$[x_0, y] = \bigcup_{h \in G} ([x_0, y] \cap hF).$$
(1)

As hF is closed and convex, the set  $[x_0, y] \cap hF$  is a (possible empty) closed interval. Let  $\lambda_0 := 0$  and  $g_0 := id$ . Define  $\lambda_1$  as the maximum value such that  $x_1 := \lambda_1 x_0 + (1 - \lambda_1) y \in F$ . Hence,  $[x_0, x_1] \subseteq F$ . By (1), there must exist an element  $g_1 \neq id$  such that  $x_1 \in g_1 F$ . More generally, given  $\lambda_i \in (0, 1), g_i \neq g$ , and  $x_i \in g_i F$ , let  $\lambda_{i+1}$  be the maximum number such that  $x_{i+1} := \lambda_{i+1} x_0 + (1 - \lambda_{i+1}) y \in g_i F$ . As before, there must exists  $g_{i+1} \in G \setminus \{g_0, g_1, \ldots, g_i\}$  such that  $x_{i+1} \in g_{i+1}F$ . The construction finishes as G is finite, when we reach that  $x_m \in gF$  for some m. Defining  $x_{m+1} = y$  and  $g_m = g$  we obtain that

$$[x_0, y] = \bigcup_{i=1}^{m+1} [x_{i-1}, x_i],$$

where  $[x_{i-1}, x_i] \subseteq g_{i-1}F$  for all  $i \in \{1, ..., m+1\}$ .

By construction,  $x_i \in g_{i-1}F \cap g_iF$  for all  $i \in \{1, \ldots, m\}$ . Moreover, we have the following claim.

Claim 1: It holds almost surely (a.s.) that for all  $i \in \{1, ..., m\}$  the set  $g_{i-1}F \cap g_iF$  has dimension n-1. Let us show the claim. If the claim is not true, there must exists i such that  $\mathbb{P}(\dim(g_{i-1}F \cap g_iF) = n-1)$  with non-zero probability. For  $h, h' \in G$ , let E(i, h, h') be the event that  $g_{i-1} = h$  and  $g_i = h'$ . We will show that if  $\dim(hF \cap h'F) \leq n-2$  then the probability of E(i, h, h') is 0. This suffices to show the claim as G is finite. In the event E(i, h, h'),  $x_i$  belongs to  $R = hF \cap h'F$ , where  $\dim(R) \leq n-2$ . Notice now that

$$B'(R) := \{ z \in B_{\epsilon}(x) : [z, y] \cap R \neq \emptyset \}$$
$$= \left\{ z \in B_{\epsilon}(x) : z = \frac{1}{t}r + \frac{t-1}{t}y, r \in R, t \in (0, 1) \right\} \subseteq \operatorname{affine}(R \cup \{y\}),$$

where affine (S) denotes the affine span of S. Hence,  $\dim(B'(R)) \leq \dim(\operatorname{affine}(R \cup \{y\})) \leq n-1$ . This implies that the probability of E(i, h, h') is 0, and hence the claim follows.

By Claim 1 we know that for all  $i \in \{1, ..., m\}$  the set  $F \cap g_{i-1}^{-1}g_iF$  has dimension n-1 almost surely. Hence, we conclude the following.

**Claim 2:** For all  $i \in \{1, ..., m\}$  it holds that  $g_{i-1}^{-1}g_i \in A$  almost surely.

We now conclude the theorem from this claim. Let us pick a sequence  $g_0, \ldots, g_m$  that satisfies Claim 2, which exists as the claimed event has non-zero probability. Clearly,  $g_0 = id \in \langle A \rangle$ . Moreover,  $g_i = g_{i-1}h$  for some  $h \in A$ . Hence, if  $g_{i-1} \in \langle A \rangle$ , we have that  $g_i \in \langle A \rangle$  for all *i*. Inductively, we obtain that  $g = g_m \in \langle A \rangle$ .

We now introduce a new type of fundamental domain and characterize the structure of its facets.

**Definition 3.** A fundamental domain F is said to be subgroup consistent for the collection  $\{H_g\}_{g\in G}$  representing F if for every subgroup  $G' \leq G$  the set  $F' = \bigcap_{g\in G'} H_g$  is a fundamental domain for G'. We say that F is subgroup consistent if F is subgroup consistent for some collection  $\{H_g\}_{g\in G}$ .

It is not hard to see that Dirichlet domains are subgroup consistent. Moreover, subgroup consistent fundamental domains are amenable to be constructed iteratively, either by starting the construction of a fundamental domain for a subgroup and extending it to larger subgroups (bottom-up), or adding inequalities for G and recurse to smaller subgroups (top-down, as our technique in Section 4).

With the help of the following lemmas, we show a close relationship between supporting hyperplanes of a subgroup consistent fundamental domain F: all facet-defining inequalities of F are of the form  $\alpha^t x \ge \alpha^t g x$  for some  $\alpha$  and  $g \in G$ . In this case we say that the inequality is of *Dirichlet type*.

**Lemma 1.** Let  $g \in G$ . Then  $(\operatorname{fix}(g) \cap F) \setminus H_q^{=} = \emptyset$ .

*Proof.* Let  $x \in \text{fix}(g)$ . If  $x \in F \setminus H_g^=$ , then  $\gamma_g^t x > 0$ . Moreover,  $\gamma_g^t(gx) \leq 0$  since  $gx \in gF$ . But this is a contradiction as gx = x.

**Lemma 2.** If G is Abelian, then for every  $g \in G$ , the set fix(g) is G-invariant, i.e., h fix(g) = fix(g) for all  $h \in G$ .

Proof. Let  $g, h \in G$ . We show that  $h \operatorname{fix}(g) = \operatorname{fix}(g)$ . Indeed, if  $y \in h \operatorname{fix}(g)$ , i.e., y = hx for some  $x \in \operatorname{fix}(g)$ , then gy = g(hx) = h(gx) = hx = y. Therefore,  $y \in \operatorname{fix}(g)$ , and thus  $h \operatorname{fix}(g) \subseteq \operatorname{fix}(g)$ . The inclusion  $\operatorname{fix}(g) \subseteq h \operatorname{fix}(g)$  follows by applying the previous argument to  $h^{-1}$ , implying that  $h^{-1} \operatorname{fix}(g) \subseteq \operatorname{fix}(g)$ .  $\Box$ 

**Lemma 3.** Given a finite group  $G \leq O_n(\mathbb{R})$ , let  $F \subseteq \mathbb{R}^n$  be a subgroup consistent fundamental domain for the collection  $\{H_g\}_{g\in G}$ , where  $H_g = \{x \in \mathbb{R}^n : \gamma_g^t x \geq 0\}$ . Then  $\gamma_g$  belongs to the orthogonal complement of the fixed space of g, i.e.,

$$\gamma_g \in \operatorname{fix}(g)^{\perp} := \{ x \in \mathbb{R}^n : gx = x \}^{\perp}.$$

*Proof.* We start by showing the lemma for the case that G is Abelian. By Lemma 2 we have that fix(g) is G-invariant for every  $g \in G$ , and hence h fix(g) = fix(g) for any  $h \in G$ . Therefore,

$$\operatorname{fix}(g) = \operatorname{fix}(g) \cap \left(\bigcup_{h \in G} hF\right) = \bigcup_{h \in G} (\operatorname{fix}(g) \cap hF) = \bigcup_{h \in G} h(\operatorname{fix}(g) \cap F)$$

Let span(S) denote the linear span of a set S. Notice that  $\dim(\text{span}(\text{fix}(g) \cap F)) = \dim(\text{fix}(g))$ , otherwise, fix(g) would be contained in the union of finitely many subspaces of strictly smaller dimension, which is clearly a contradiction. Since  $F \cap \text{fix}(g) \subseteq \text{fix}(g)$ , we conclude that  $\text{span}(F \cap \text{fix}(g)) = \text{fix}(g)$ . As by Lemma 1 we have that  $F \cap \text{fix}(g) \subseteq H_g^=$ , this implies that  $\text{fix}(g) = \text{span}(F \cap \text{fix}(g)) \subseteq H_g^=$ . Since by definition  $\gamma_g$  is orthogonal to every vector in  $H_g^=$ , we conclude that  $\gamma_g \in \text{fix}(g)^{\perp}$ . The lemma follows if G is Abelian.

For the general case, assume that F is subgroup consistent for collection  $\{H_h\}_{h\in G}$ . Therefore, the Abelian subgroup  $G' = \langle g \rangle$  has  $F' = \bigcap_{h\in G'} H_h$  as a fundamental domain. Then our argument for the Abelian case implies that  $\gamma_q \in \text{fix}(g)^{\perp}$ .

The following is the main contribution of this section.

**Theorem 1.** Given a finite group  $G \leq O_n(\mathbb{R})$ , let  $F \subseteq \mathbb{R}^n$  be a subgroup consistent fundamental domain for a collection  $\{H_g\}_{g\in G}$ , where  $H_g = \{x : \gamma_g^t x \geq 0\}$ . Then, for every  $g \in G$  there exists  $\alpha_g \in \mathbb{R}^n$  such that  $\gamma_g = (\mathrm{id} - g)\alpha_g$ . In particular, any facet-defining inequality for F is of the form  $\alpha_g^t x \geq \alpha_g^t g^{-1}x$  for some  $g \in G$ , and hence it is of Dirichlet type.

*Proof.* Recall that any automorphism f of  $\mathbb{R}^n$  satisfies  $\operatorname{Im}(f)^{\perp} = \ker(f^t)$ . Since  $\operatorname{fix}(g) = \ker(\operatorname{id} - g)$ , and recalling that  $g^{-1} = g^t$  (interpreting g as a matrix), by Lemma 3 we have that

$$\gamma_g \in \operatorname{fix}(g)^{\perp} = \operatorname{fix}(g^{-1})^{\perp} = \operatorname{ker}(\operatorname{id} - g^t)^{\perp} = \operatorname{Im}(\operatorname{id} - g).$$

Hence, there exists  $\alpha_g \in \mathbb{R}^n$  such that  $\gamma_g = (\mathrm{id} - g)\alpha_g$ .

**Remark.** It is worth noticing that this theorem does not imply that every subgroup consistent fundamental domain is a Dirichlet fundamental domain. The difference relays in the fact that in Dirichlet domains  $\alpha = \alpha_g$  for all  $g \in G$ , while in subgroup consistent fundamental domains one can have different vectors  $\alpha_g$  for different group elements g. For concrete examples see Section 4.

We say that a fundamental domain F is *exact* if for every facet S of F there exists a group element  $g \in G$  such that  $S = F \cap gF$ . In this case we say that g defines a facet of F. Notice that it also holds that  $S = F \cap H_g^=$ . Exact fundamental domains are well structured and have been studied in the literature [24]. It is worth noticing that Dirichlet domains are exact.

For exact fundamental domains, facets come in pairs, i.e., if g defines a facet of F, then  $g^{-1}$  also does. The proof of the following proposition can be found in Ratcliffe [24, Thm. 6.7.5.].

**Proposition 3.** Let  $F \subseteq \mathbb{R}^n$  be an exact fundamental domain for  $G \leq O_n(\mathbb{R})$  finite. If S is a facet of F, then there is a unique non-trivial element  $g \in G$  such that  $S = F \cap gF$ , moreover  $g^{-1}S$  is a facet of F.

Proposition 3 and Theorem 1 together imply the following corollary which gives a stronger connection between the facets  $F \cap gF$  and  $F \cap g^{-1}F$ . Informally, the corollary says that we can take  $\alpha_g = \alpha_{g^{-1}}$  in Theorem 1.

**Corollary 1.** Let  $F \subseteq \mathbb{R}^n$  be an exact and subgroup consistent fundamental domain for  $G \leq O_n(\mathbb{R})$  finite. Suppose that  $H_g = \{x : \gamma_g^t x \geq 0\}$  defines the facet  $F \cap gF = F \cap H_g^=$  and  $H_{g^{-1}} = \{x : \gamma_{g^{-1}}^t x \geq 0\}$  defines the facet  $F \cap g^{-1}F = F \cap H_{g^{-1}}^=$ . Then there exists a vector  $\alpha_g$  such that

$$H_g = \{x : \alpha_q^t x \ge \alpha_q^t (g^{-1}x)\} \text{ and } H_{g^{-1}} = \{x : \alpha_q^t x \ge \alpha_q^t (gx)\}.$$

Proof. By Theorem 1,  $\gamma_g = (\mathrm{id} - g)\alpha_g$  for some  $\alpha_g$  and hence  $H_g = \{x : \alpha_g^t x \ge \alpha_g^t(g^{-1}x)\}$ . Now, for any  $x \in F \cap g^{-1}F$ , we have  $gx \in gF \cap F = F \cap H_g^=$ , and hence  $\gamma_g^t(gx) = (g^{-1}\gamma_g)^t x = 0$ . Thus,  $g^{-1}\gamma_g$  is orthogonal to  $F \cap g^{-1}F$ . As  $\dim(F \cap g^{-1}F) = n - 1$ , we obtain that  $H_{g^{-1}}^= \{x : (g^{-1}\gamma_g)^t x = 0\}$ . Now, notice that  $H_{g^{-1}} = \{x : (g^{-1}\gamma_g)^t x \le 0\}$ . Indeed, if  $H_{g^{-1}} = \{x : (g^{-1}\gamma_g)^t x \ge 0\}$  we have that for any  $x \in \operatorname{int}(g^{-1}F) \neq \emptyset$  it holds that  $(g^{-1}\gamma_g)^t x < 0$ , and hence  $gx \in \operatorname{int}(F)$  satisfies  $\gamma_g^t(gx) < 0$ , which contradicts the construction of  $H_g$ . We conclude that  $H_{g^{-1}} = \{x : (g^{-1}\gamma_g)^t x \le 0\}$ . The results follows by recalling that  $\gamma_g = (\operatorname{id} -g)\alpha_g$ , which implies that  $H_{g^{-1}} = \{x : \alpha_g^t x \ge \alpha_g^t(gx)\}$ .

## 4 Generalized Dirichlet Domains

In this section we present our main contribution: an algorithm which constructs a fundamental domain for an arbitrary finite orthogonal group. We use the insights gained from the geometric properties of subgroup consistent and exact fundamental domains to guide our search for new constructions. In particular we create subgroup consistent fundamental domains based on a sequence of nested stabilizers of the *G*-action on  $\mathbb{R}^n$ . This construction generalizes Dirichlet domains, and hence *k*-fundamental domains, as well as the *Schreier-Sims fundamental domain*, presented in Section 4.2. Both types of fundamental domains can be easily constructed using our algorithm. Moreover, in Section 5 we exploit the flexibility of our construction to define a new fundamental domain with better properties for a specific group.

Theorem 1 and Corollary 1 suggest that we should consider vectors  $\alpha_g$  for some  $g \in G$  and consider inequalities of the form  $\alpha_g^t x \ge \alpha_g^t g x$  and  $\alpha_g^t x \ge \alpha_g^t g^{-1} x$ , although it seems hard to decide whether we should pick different vectors  $\alpha_g$  for each pair  $g, g^{-1}$ , and if so, how to choose them. For instance, if we fix a vector  $\alpha = \alpha_g$  for all  $g \in G$ , we would obtain a Dirichlet domain. However, if  $\alpha$ 's stabilizer is non trivial, then all inequalities  $\alpha_g^t x \ge \alpha_g^t g^{-1} x$  in a coset of  $G_\alpha$  are equivalent. This hints that we should choose a vector  $\alpha$ , apply a coset decomposition using a stabilizer subgroup, and add the Dirichlet inequalities related to all members of the decomposition.

Furthermore, since all the elements of the group that fix  $\alpha$  constitute a subgroup, if a fundamental domain F for this subgroup were available, *residual symmetries* could be taken care of with F, while *non-residual symmetries* could be exploited via  $\alpha^t x \geq \alpha^t(gx)$  for  $g \notin G_{\alpha}$ . Our next result points in this direction and lays the ground for our generalized Dirichlet domain algorithm.

**Theorem 2.** Let  $\alpha \in \mathbb{R}^n$  be an arbitrary vector and consider the polyhedral cone

$$F_{\alpha} = \{ x \in \mathbb{R}^n : \alpha^t x \ge \alpha^t g x, \quad \forall g \in G \}.$$

Suppose that F is a fundamental domain for the subgroup  $G_{\alpha}$ , i.e., the pointwise stabilizer of  $\alpha$ . Then  $F \cap F_{\alpha}$  is a fundamental domain for G.

Moreover, for any transversal T for  $G_{\alpha}$  in G, the polyhedral cone  $F_{\alpha}$  can be described as

$$F_{\alpha} = \{ x \in \mathbb{R}^n : \alpha^t x \ge \alpha^t g x, \quad \forall g \in T \cup T^{-1} \},\$$

where  $T^{-1} := \{g^{-1} : g \in T\}.$ 

Proof. First, notice that  $F \cap F_{\alpha}$  is closed and convex. Now, we show that every  $x \in \mathbb{R}^n$  has a representative in  $F \cap F_{\alpha}$ . In other words, we show that there exists some  $g \in G$  such that  $gx \in F \cap F_{\alpha}$ . Let us consider two cases: (i)  $x \in F_{\alpha}$  and (ii)  $x \notin F_{\alpha}$ . In case (i), since F is a fundamental domain for  $G_{\alpha}$ , there exists  $g \in G_{\alpha}$ such that  $gx \in F$ . As  $\alpha = g^{-1}\alpha$  we have that

$$\alpha^t g x = (g^t \alpha)^t x = (g^{-1} \alpha)^t x = \alpha^t x.$$

Therefore,  $gx \in F \cap F_{\alpha}$ . Now, consider case (ii), i.e., there exists  $g' \in G$  such that  $\alpha^t g' x > \alpha^t x$ . Let  $h \in \operatorname{argmax}\{\alpha^t gx : g \in G\}$ . Clearly  $hx \in F_{\alpha}$ , and hence we are done if  $hx \in F$ . If  $hx \notin F$  there exists  $\tilde{g} \in G_{\alpha}$  such that  $\tilde{g}(hx) \in F$ . We conclude that  $\tilde{g}(hx) \in F \cap F_{\alpha}$  by the same argument as in case (i).

Now we prove that for any  $g \in G \setminus \{id\}$  we have that  $int(F \cap F_{\alpha})$  and  $int(g(F \cap F_{\alpha}))$  are disjoint. Let  $x \in int(F \cap F_{\alpha})$ . It suffices to show that  $gx \notin F \cap F_{\alpha}$ . Indeed, since  $x \in int(F) \cap int(F_{\alpha})$ , then  $gx \notin F \cap F_{\alpha}$  for all  $g \in G_{\alpha} \setminus \{id\}$  as F is a fundamental domain for  $G_{\alpha}$ . Moreover, since x belongs to the interior of  $F_{\alpha}$ , it holds that  $\alpha^{t}x > \alpha^{t}gx$  for all  $g \in G \setminus G_{\alpha}$ . Therefore,  $gx \notin F \cap F_{\alpha}$ . We conclude that  $F \cap F_{\alpha}$  is a fundamental domain for G.

Let us show that it suffices to consider the Dirichlet type inequalities associated to a transversal and its inverses  $T \cup T^{-1}$  to describe  $F_{\alpha}$ . Let  $T \subseteq G$  be a transversal for  $G_{\alpha}$  and let  $g \in G$ . If  $g \in G_{\alpha}$ , then clearly  $\alpha^t = \alpha^t g$  and hence the inequality  $\alpha^t x = \alpha^t g x$  is trivial. Consider  $g \notin G_{\alpha}$ , and thus  $g^{-1} \notin G_{\alpha}$ . Then there exists  $r \in T$  such that  $g^{-1} \in rG_{\alpha}$ , i.e.,  $g^{-1}\alpha = r\alpha$ . Therefore,

$$\alpha^t(gx) = (g^{-1}\alpha)^t x = (r\alpha)^t x = \alpha^t(r^{-1}x),$$

from which we can conclude that  $\alpha^t x \ge \alpha^t(gx)$  and  $\alpha^t x \ge \alpha^t(r^{-1}x)$  are equivalent.

An iterative application of Theorem 2 yields Algorithm 1. We say that a fundamental domain constructed by this algorithm is a *generalized Dirichlet domain* (GDD). See Examples 1 and 2 below for concrete examples of this construction.

**Algorithm 1** Construction of a generalized Dirichlet domain (GDD) **Input**: A set of generators  $S_G$  of a finite orthogonal group G**Output**: A fundamental domain F for G1: Set  $F := \mathbb{R}^n$ ,  $G_0 := G$ , and i := 12: while  $G_{i-1} \neq {\text{id}}$  do 3: Choose  $\alpha_i \in \mathbb{R}^n$  such that  $g\alpha_i \neq \alpha_i$  for some  $g \in G_{i-1}$ 4: Compute  $G_i := \{g \in G_{i-1} : g\alpha_i = \alpha_i\}$ Choose a transversal  $T_i$  for  $G_i$  in  $G_{i-1}$  and add the inverses  $R_i := T_i \cup T_i^{-1}$ 5:Set  $F_i := \{ x \in \mathbb{R}^n : \alpha_i^t x \ge \alpha_i^t h x \quad \forall h \in R_i \}$ 6:  $F := F \cap F_i$  and i := i + 17: 8: end while 9: return F

**Theorem 3.** Algorithm 1 terminates in at most n iterations and outputs a fundamental domain F.

Proof. We follow an inductive bottom-up argument. First we prove the base case. Given the output of Algorithm 1 let m be the smallest integer such that  $G_m = \langle id \rangle$ . Notice that  $m \leq n$  since the set  $\{\alpha_i\}_{i=1}^m$  must be linearly independent, otherwise some  $\alpha_i$  would belong to the linear span of  $\{\alpha_j\}_{j < i}$  implying that  $\alpha_i$  is fixed by  $G_{i-1}$ , which is a contradiction. Therefore the algorithm terminates in at most n iterations. Then, the transversal  $T_m$  for  $G_m$  in  $G_{m-1}$  computed in Line 5 corresponds to  $G_{m-1}$ , i.e.  $G_{m-1}$  is trivially decomposed by  $G_m$ . Hence,  $F_m = F_{\alpha_m}$  is a Dirichlet domain for  $G_{m-1}$ . Therefore,  $F_{m-1} \cap F_m$  is a fundamental domain for  $G_{m-2}$  by Theorem 2. Consequently, F is a fundamental domain for G since  $\bigcap_{i=2}^m F_i$  is a fundamental domain for  $G_1$ , by iteratively applying Theorem 2.

It is worth noticing that if we take  $\alpha_1$  such that  $G_1$  is trivial, then the algorithm finishes after one iteration. Indeed, the obtained fundamental domain is the Dirichlet domain  $F_{\alpha_1}$ . This justifies the name generalized Dirichlet domain.

We already know that Algorithm 1 terminates after at most n iterations. For the rest of the analysis of the running time, we focus on permutation groups. Lines 4 and 5 are the most challenging with respect to the algorithm's computational complexity. The result of the computation in line 4 is a setwise stabilizer of the coordinates of  $\alpha$ . Computing a set of generators for this subgroup can be performed in quasi-polynomial time with the breakthrough result by Babai [2,3] for String Isomorphism. In general, however,  $R_1$  might be of exponential size. Indeed, the number of cosets of  $G_1$  in G equals the size of the orbit  $|\operatorname{Orb}_G(\alpha_1)|$ , by the Orbit-Stabilizer Theorem. If we choose  $\alpha_1$  with pairwise different coordinates, then  $|\operatorname{Orb}_G(\alpha_1)| = |G|$ . This is exactly the case for the Dirichlet domain.

On the other hand, by choosing the  $\alpha_i$  vectors carefully we can avoid the described problem. In particular, suppose that  $\alpha = (\alpha^{(1)}, \ldots, \alpha^{(k)}, 0, \ldots, 0)$  such that  $\alpha^{(i)} \neq \alpha^{(j)}$  for  $i \neq j$  in [k], and  $\alpha^{(i)} \neq 0$  for  $i \in [k]$ . Hence, a set of generators for the stabilizer  $G_{\alpha}$  can be computed in polynomial time. Indeed, it corresponds to the pointwise stabilizers of coordinates 1 to k [29, Section 5.1.1]. Moreover, the number of cosets is  $O(n^k)$ , as again the number of cosets equals the cardinality of the orbit of  $\alpha$ . In other words, we have just proven the following proposition.

**Proposition 4.** Let  $G \leq S_n$  a permutation group and let  $k \in [n]$  be a constant. Suppose that each  $\alpha_i$  in Algorithm 1 satisfies

$$\alpha_i = (\alpha_i^{(1)}, \dots, \alpha_i^{(k)}, 0, \dots, 0),$$

 $\alpha_i^{(\ell)} \neq \alpha_i^{(m)}$  for  $\ell \neq m$  in [k], and  $\alpha_i^{(\ell)} \neq 0$  for  $i \in [k]$ . Then the associated GDD for G can be computed in time  $O(n^{O(k)})$ .

#### 4.1 Geometric Properties of Generalized Dirichlet Domains

In this section we study two important geometric properties of fundamental domains: subgroup consistency and exactness. To this end, first we show how can a *canonical* representation for generalized Dirichlet domains be defined via a partition of G into *layers*. Then, we use this representation for GDDs to show that they are subgroup consistent. Moreover, we show that they are not necessarily exact.

**Subgroup consistency.** Let  $F = \bigcap_{i=1}^{m} F_i$  be the output of Algorithm 1, where  $m \in [n]$  denotes the smallest index such that  $G_m = \langle id \rangle$ , and

$$F_i = \{ x \in \mathbb{R}^n : \alpha_i^t x \ge \alpha_i^t h x \quad \forall h \in R_i \}$$

where  $R_i = T_i \cup T_i^{-1}$ , with  $T_i$  a transversal for  $G_i$  in  $G_{i-1}$  and  $G_0 := G$ . We will define a partition of G and a representation of F using the nested coset decompositions produced by Algorithm 1. Notice that in the *i*-th iteration of our GDD algorithm a coset decomposition is computed using the subgroup  $G_i$ . In other words,  $G_{i-1}$  is partitioned into cosets as

$$G_{i-1} = \bigcup_{g \in T_i} gG_i$$

Now, fix  $i \in [m]$ . We say that  $g \in G \setminus \{id\}$  belongs to the *i*-th layer  $L_i$  of G induced by  $\{\alpha_i\}_{i=1}^m$  if  $g \in G_{i-1} \setminus G_i$ . Since  $G_{j-1} \geq G_j$  for all  $j \in [m]$ , g belongs to  $L_i$  if and only if i smallest index such that  $g \in G_i$ . Therefore, letting  $id \in L_m$ , we have that  $\{L_i\}_{i=1}^m$  is a partition of G as every g belongs to a unique  $L_j$ .

Now we are ready to define a *GDD representation* of *F*. First, note that  $T_i \setminus \{id\} \subseteq L_i$  since by definition  $T_i \subseteq G_{i-1}$  and  $T_i \setminus \{id\} \cap G_i = \emptyset$ . The latter implies that  $T_i^{-1} \setminus \{id\} \subseteq L_i$ , hence  $R_i \setminus \{id\} \subseteq L_i$ . Now, let  $g \in G \setminus \{id\}$ . Then  $g \in L_j$  for some  $j \in [m]$ . Since  $g \notin G_j$ , then so does  $g^{-1}$ , and it belongs to some coset  $rG_j$ , where  $r \in T_j$ . Since  $g^{-1}\alpha_j = r\alpha_j$ , then

$$\alpha_j^t g x = (g^{-1}\alpha_j)^t x = (r\alpha_j)^t x = \alpha_j^t r^{-1} x.$$

Since  $r^{-1}$  induces the same Dirichlet type inequality as g we say that g is associated to  $r^{-1}$ . Therefore, any  $g \in G$  can be associated to some  $h \in R_j$  in some layer  $L_j$  of G, i.e., we can define

$$H_q := \{ x \in \mathbb{R}^n : \alpha_j^t x \ge \alpha_j^t h x \},$$

and say that  $\{H_q\}_{q \in G}$  is a GDD representation of F induced by  $\{\alpha_i\}_{i=1}^m$ .

Proposition 5. Generalized Dirichlet domains are subgroup consistent.

*Proof.* Let  $\{H_g\}_{g\in G}$  be the *GDD representation* of *F* induced  $\{\alpha_i\}_{i=1}^m$  obtained via Algorithm 1. Let *G'* be any subgroup of *G*. We show that  $F' := \bigcap_{g\in G'} H_g$  is a fundamental domain for *G'*.

Clearly F' is closed and convex. Let us prove that for all  $x \in \mathbb{R}^n$ , there exists some  $g \in G'$  such that  $gx \in F'$ . Suppose that  $x \notin F'$  and let  $i_1 \in [m]$  denote the first layer such that  $\alpha_{i_1}^t x < \alpha_{i_1}^t gx$  for some  $g \in L_{i_1} \cap G'$ . Let  $h_{i_1} \in \operatorname{argmax} \{\alpha_{i_1}^t gx : g \in L_{i_1} \cap G'\}$ . Notice that  $\alpha_j^t x = \alpha_j^t h_{i_1} x$  for all  $j < i_1$  since  $h_{i_1} \in G_j$  for  $j < i_1$ , and then

$$h_{i_1} x \in \bigcap_{\substack{i \in [i_1]:\\g \in L_i \cap G'}} H_g.$$

If  $\tilde{x} := h_{i_1}x \notin F'$ , we can replicate the argument on the first layer  $i_2 > i_1$  such that  $\tilde{x} \notin H_{\tilde{g}}$  where  $\tilde{g} \in L_{i_2} \cap G'$ . Inductively we obtain an element  $h := h_{i_\ell} h_{i_{\ell-1}} \cdots h_{i_1} \in G'$  such that  $hx \in F'$ .

Now, we prove that  $\operatorname{int}(F') \cap g \operatorname{int}(F') = \emptyset$  for any non-trivial  $g \in G'$ . It suffices to show that if  $x \in \operatorname{int}(F')$  then  $gx \notin F'$ . Indeed, since  $x \in \operatorname{int}(F')$ , we have that

$$\begin{aligned} \alpha_i^t x &> \alpha_i^t r x \quad \text{for all } i \in [m] \text{ and } r \in L_i \cap G' \\ \iff \alpha_i^t x &> \alpha_i^t h x \quad \text{for all } i \in [m] \text{ and } h \in R_i \text{ associated to some } r \in G'. \end{aligned}$$

Suppose g belongs to layer  $L_j$  and it is associated to some  $h \in H_j$ . Therefore,  $\alpha_j^t g x = \alpha_j^t h$  and

$$\alpha_j^t gx < \alpha_j^t x = \alpha_j^t g^{-1}(gx)$$

where  $g^{-1} \in L_j \cap G'$ , i.e.,  $gx \notin F'$ .

**Exactness.** Recall that a fundamental domain is exact if every facet S of F is of the form  $S = F \cap gF$  for some  $g \in G$ . Dirichlet domains are exact [24, Theorem 6.7.4] though generalized Dirichlet domains may not be exact. This means that for some iteration i of Algorithm 1 there exists some  $h \in R_i$  such that  $F \cap H_h^=$  is a facet of F and it satisfies:

relint
$$(F \cap H_h^{=}) \cap hF \neq \emptyset$$
 and relint $(F \cap H_h^{=}) \cap gF \neq \emptyset$ 

for some  $g \neq h$ . The following examples show non-exact GDDs. The first one is an example for a permutation group in  $\mathbb{R}^4$ . The second one is a more geometrical example in  $\mathbb{R}^3$ .

*Example 1.* Let  $g := (1 \ 2 \ 3 \ 4)$  and consider  $G := \langle g \rangle$ . We construct a GDD for G with  $\alpha_1 := (1, 0, 1, 0)$  and  $\alpha_2 := (1, 0, 0, 0)$ .

Indeed, if we first choose  $\alpha_1$ , its stabilizer is  $G_{\alpha_1} = \{id, g^2\}$ , and a  $G_{\alpha_1}$ -transversal is  $H_1 = \{id, g\}$ . Hence,

$$F_1 = \{ x \in \mathbb{R}^4 : x_1 + x_3 \ge x_2 + x_4 \}.$$

Next, the only subgroup of  $G_{\alpha_1}$  that stabilizes  $\alpha_2$  is  $\langle id \rangle$ , hence

$$F_2 = \{ x \in \mathbb{R}^4 : x_1 \ge x_3 \}.$$

The resulting GDD for G is

$$F := F_1 \cap F_2 = \{ x \in \mathbb{R}^4 : x_1 + x_3 \ge x_2 + x_4, \ x_1 \ge x_3 \}.$$

Now, we exhibit two points that certify the non-exactness of F. Consider x = (2, 2, 1, 1) and  $\tilde{x} = (2, 1, 1, 2)$ . Clearly both points belong to the facet  $F \cap H_g^=$ , and since none of them satisfy  $x_1 = x_3$  they belong to the relative interior of  $F \cap H_g^=$ . Moreover, as  $g^{-1}x = (2, 1, 1, 2) \in F \iff x \in gF$  and  $g\tilde{x} = (2, 2, 1, 1) \in F \iff \tilde{x} \in g^{-1}F$ , then the relative interior of a facet of F intersects gF and  $g^{-1}F$ . Therefore F is not exact.  $\Delta$ 

Example 2. Let us consider the three-dimensional space  $\mathbb{R}^3$ , and let g be the isometry that consists of a rotation by 90 degrees around the  $x_3$ -axis, followed by a reflection with respect to the plane span $(e_1, e_2)$ . The matrix associated to g is

$$\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

The group  $G = \langle g \rangle = \{ \mathrm{id}, g, g^2, g^3 \}$  comprises four different elements. By taking  $\alpha_1 = (0, 0, 1)$ , and  $\alpha_2 = (0, 1, 0)$  when running Algorithm 1, where  $G_{\alpha_1} = \{ \mathrm{id}, g^2 \}$ , we obtain the following GDD

$$F = \left\{ x \in \mathbb{R}^3 : x_2 \ge 0, x_3 \ge 0 \right\}.$$

Then, we have

$$gF = \{x \in \mathbb{R}^3 : x_1 \le 0, x_3 \le 0\},\$$
  

$$g^2F = \{x \in \mathbb{R}^3 : x_2 \le 0, x_3 \ge 0\},\$$
  

$$g^3F = \{x \in \mathbb{R}^3 : x_1 \ge 0, x_3 \le 0\}.$$

It is easy to see that this tessellation is not exact, see Figure 1.

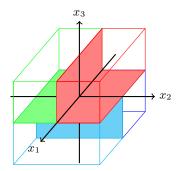


Fig. 1. The situation of Example 2, restricted to a cube. F is the red domain, gF the blue one,  $g^2F$  the green one, and  $g^3F$  the cyan one.

#### 4.2 The Lex-Max Fundamental Domain

In this section, we study a natural idea for breaking symmetries: in any orbit, choose the vector that is lexicographically maximal. We relate this idea to our generalized Dirichlet domain construction.

Let  $\succ$  denote a lexicographic order on  $\mathbb{R}^n$ , that is for any pair  $x, y \in \mathbb{R}^n$  we say that  $y \succ x$  if there exists  $j \in [n]$  such that  $y_j > x_j$  and  $y_i = x_i$  for all i < j. Therefore  $\succeq$  defines a total order on  $\mathbb{R}^n$ , where,  $y \succeq x$  if and only if  $y \succ x$  or y = x. Given a group  $G \leq S_n$  acting on  $\mathbb{R}^n$ , we define

$$\operatorname{Lex}_G := \{ x \in \mathbb{R}^n : x \succeq gx, \forall g \in G \}.$$

In what follows we show an alternative characterization of the set of lexicographically maximal points using k-fundamental domains. Recall that a k-fundamental domains is a Dirichlet domain  $F_{\overline{k}}$  where  $\overline{k} = (k^{n-1}, k^{n-2}, \ldots, k, 1)$  for some integer  $k \geq 2$ .

**Lemma 4.** Let  $n \in \mathbb{N}$  and  $x, y \in \mathbb{R}^n$ . If  $x \succ y$ , then there exists  $N \in \mathbb{N}$  such that for every integer k > N it holds that  $\overline{k}^t x > \overline{k}^t y$ .

Proof. Suppose  $x \succ y$ . This implies that  $x_1 > y_1$  or there exists  $i \in [n] \setminus \{1\}$  such that  $x_i > y_i$  and  $x_j = y_j$  for all  $j \in [i-1]$ . Let  $c := x_i - y_i > 0$  such that i is the smallest  $i \in [n]$  for which  $x_i - y_i > 0$ , and let  $m := \max\{|y_j - x_j| : j \in [n]\}$ . Note that if i = n our claim is trivially true since for any  $k \in \mathbb{N}$  we have that  $\overline{k}^t x - \overline{k}^t y = x_n - y_n > 0$ . If i = n - 1 we have  $\overline{k}^t x - \overline{k}^t y = kc + (x_n - y_n)$ , hence there exists  $N \in \mathbb{N}$  such that  $kc + (x_n - y_n) > 0$  for all  $k \ge N$ . Now, suppose  $i \in [n-2]$ . Then, for  $k \in \mathbb{N}$ ,

$$\overline{k}^{t}x - \overline{k}^{t}y = k^{n-i}c - k^{n-i-1}(y_{i+1} - x_{i+1}) \dots - k(y_{n-1} - x_{n-1}) - (y_n - x_n)$$
$$\geq k^{n-i}c - m\sum_{j=0}^{n-i-1} k^j = k^{n-i}c - m\left(\frac{k^{n-i} - 1}{k-1}\right).$$

Now, note that  $\lim_{k\to\infty} \left[k^{n-i}c - m\left(\frac{k^{n-i}-1}{k-1}\right)\right] = +\infty$ , because the sign of the leading coefficient of this rational function is positive and the degree of the numerator is greater than that of the denominator. Hence, there exists N such that  $k^{n-i}c - m\left(\frac{k^{n-i}-1}{k-1}\right) > 0$  for all k > N.

With the help of the previous lemma, we provide an alternative characterization of  $\text{Lex}_G$ . Recall that a fundamental set is a set that contains exactly one representative for each G-orbit.

**Lemma 5.** Let  $G \leq S_n$ . Then  $Lex_G$  is a convex fundamental set and

$$Lex_G = \bigcup_{i=1}^{\infty} \bigcap_{k=i}^{\infty} F_{\overline{k}} = \liminf_{k \to \infty} F_{\overline{k}}.$$

Proof. Let  $x \in \bigcup_{i=1}^{\infty} \bigcap_{k=i}^{\infty} F_{\overline{k}}$ , i.e. there exists  $N \in \mathbb{N}$  such that  $x \in F_{\overline{k}}$  for every integer  $k \ge N$ , and suppose on the contrary that  $x \notin \text{Lex}_G$ . This implies that there exists a non-trivial  $g \in G$  such that  $gx \succ x$ . By Lemma 4 there exists  $N' \in \mathbb{N}$ , such that for every integer  $k \ge N'$ , we have that  $\overline{k}^t gx > \overline{k}^t x$ . But this is absurd because  $x \in F_{\overline{k}}$  for  $k \ge \max\{N, N'\}$ . The other inclusion is analogously derived from Lemma 4.

absurd because  $x \in F_{\overline{k}}$  for  $k \ge \max\{N, N'\}$ . The other inclusion is analogously derived from Lemma 4. Furthermore, observe that  $\left(\bigcap_{k=i}^{\infty} F_{\overline{k}}\right)_{i=1}^{\infty}$  is a non-decreasing nested sequence of convex sets, which implies that Lex<sub>G</sub> is also convex. Finally, since the pair  $(\mathbb{R}^n, \succeq)$  is a total order, then Lex<sub>G</sub> must be a fundamental set for  $G \le S_n$ .

We now show that  $\overline{\text{Lex}_G}$ , the (topological) closure of  $\text{Lex}_G$ , is a fundamental domain for any  $G \leq S_n$ .

**Theorem 4.** For any  $G \leq S_n$ , the closure of  $Lex_G$  is a fundamental domain.

*Proof.* Let  $G \leq S_n$ . We want to show that the non-empty closed set  $\overline{\text{Lex}}_G \subseteq \mathbb{R}^n$  satisfies:

(i)  $\bigcup_{g \in G} g \overline{\operatorname{Lex}}_G = \mathbb{R}^n$ ,

(ii)  $g \operatorname{int}(\operatorname{Lex}_G) \cap \operatorname{int}(\operatorname{Lex}_G) = \emptyset, \forall g \in G \setminus \{\operatorname{id}\}.$ 

Notice that (i) follows directly as  $\bigcup_{q \in G} g \operatorname{Lex}_G = \mathbb{R}^n$  since  $\operatorname{Lex}_G$  is a fundamental set.

For (ii), note that  $\operatorname{int}(\operatorname{Lex}_G) = \operatorname{int}(\operatorname{Lex}_G)$  because  $\operatorname{Lex}_G$  is a convex set by Lemma 5. So it suffices to prove  $g \operatorname{int}(\operatorname{Lex}_G) \cap \operatorname{int}(\operatorname{Lex}_G) = \emptyset$  for every non-trivial  $g \in G$ . Suppose on the contrary that there exists a non-trivial  $g \in G$  such that  $x \in g(\operatorname{int}(\operatorname{Lex}_G)) \cap \operatorname{int}(\operatorname{Lex}_G)$ . Hence, x and  $g^{-1}x$  belong to  $\operatorname{int}(\operatorname{Lex}_G) \subseteq \operatorname{Lex}_G$ . This is clearly absurd as  $\preceq$  is a total order.

A Characterization of  $\overline{\text{Lex}}_G$  using the Schreier-Sims Table In what follows, we provide a characterization of  $\overline{\text{Lex}}_G$ , which in particular allows to compute its facets efficiently. Indeed, we show that its description coincides with the Schreier-Sims inequalities for  $G \leq S_n$  [27] (where computational results can be found).

The Schreier-Sims table is a representation of a permutation group  $G \leq S_n$ . The construction is as follows. Consider the chain of nested pointwise stabilizers defined as:  $G^0 := G$  and  $G^i := \{g \in G^{i-1} : g(i) = i\}$  for each  $i \in [n]$ . Note that the chain is not necessarily strictly decreasing (properly), and we always have that  $G^{n-1} = \{id\}$ . For a given  $i \in [n]$  and  $j \in \operatorname{Orb}_{G^{i-1}}(i)$ , let  $h_{i,j}$  be any permutation in  $G^{i-1}$  which maps i to j. Hence,  $U_i := \{h_{i,j} : j \in \operatorname{Orb}_{G^{i-1}}(i)\}$  is a transversal for the cosets of  $G^i$  in  $G^{i-1}$ .

We arrange the permutations in the sets  $U_i$ , for  $i \in [n]$ , in an  $n \times n$  table T where  $T_{i,j} = h_{i,j}$  if  $j \in \operatorname{Orb}_{G^{i-1}}(i)$  and  $T_{i,j} = \emptyset$  otherwise.

The most interesting property of this construction is that each  $g \in G$  can be uniquely written as  $g = g_1g_2 \cdots g_n$  with  $g_i \in U_i$ , for  $i \in [n]$ . Therefore, the permutations in the table form a set of generators of G which is called a *strong generating set* (SGS) for G [29].

The Schreier-Sims polyhedron, denoted by  $SS_G$ , is the polyhedron given by the inequalities  $x_i \ge x_j$  for all  $T_{i,j} \ne \emptyset$ . Theorem 5 states that  $\overline{Lex}_G = SS_G$ . A crucial observation to prove this is that for any vector  $x \in \mathbb{R}^n$ , x is in the closure of  $Lex_G$  if and only if x can be perturbed into the interior of  $\overline{Lex}_G$ , where the perturbed vector is lexicographically maximal in its orbit.

The following lemma characterizes the boundary of  $\overline{\text{Lex}}_G$  in terms of a special perturbation which we call "tie-breaker" perturbation, because it breaks all possible ties between the vector's entries. We will use this lemma to prove that the facets of  $\overline{\text{Lex}}_G$  are in fact Schreier-Sims inequalities.

**Lemma 6.** Let  $G \leq S_n$ ,  $x \in \mathbb{R}^n$ , and  $0 < \epsilon < M$ , where

$$M := \begin{cases} 1 & \text{if } x_i = x_j, \quad \forall i, j \in [n], \\ \min\{|x_i - x_j| > 0 : i, j \in [n]\} \text{ otherwise.} \end{cases}$$
(2)

We define the  $\epsilon$ -tie-breaker perturbation for x as

$$x_i^{\epsilon} := x_i - \frac{i\epsilon}{n^2} \quad for \ i \in [n].$$

Then x is in  $\overline{Lex_G}$  if and only if for any  $0 < \epsilon < M$ ,  $x^{\epsilon}$  belongs to  $Lex_G$ .

*Proof.* Let  $x \in \mathbb{R}^n$  and M be defined as above and suppose that  $x^{\epsilon} \in \text{Lex}_G$  for all  $0 < \epsilon < M$ . Since  $\lim_{\alpha} x^{\epsilon} = x$  then  $x \in \overline{\text{Lex}_G}$ .

For the converse, suppose  $x \in \mathbb{R}^n$  and let  $0 < \epsilon < M$ , with M defined as in (2). Notice that in  $x^{\varepsilon}$  ties in x are broken without changing the relative order of its coordinates, that is, if  $x_i < x_j$  then  $x_i^{\varepsilon} < x_j^{\varepsilon}$ . Also,  $x_i^{\varepsilon} \neq x_j^{\varepsilon}$  for  $i \neq j$ . Suppose that  $x^{\varepsilon}$  is not in Lex<sub>G</sub>. We want to show that x does not belong to Lex<sub>G</sub>. If  $x^{\varepsilon} \notin \text{Lex}_G$ , there exists a non-trivial  $g \in G$  such that  $gx^{\varepsilon} \succ x^{\varepsilon}$ . Let us characterize this g. Let  $i \in [n]$  denote the (largest) length of the prefix that g fixes in  $x^{\varepsilon}$ , i.e.,  $(gx^{\varepsilon})_j = x_j^{\varepsilon}$  for  $j \leq i$  and  $(gx^{\varepsilon})_{i+1} \neq x_{i+1}^{\varepsilon}$ . Hence, as the coordinates of  $x^{\varepsilon}$  are pairwise different, g belongs to the subgroup of G that fixes indices  $1, \ldots, i$  pointwise, i.e.  $g \in G_{([i])}$ . Then because g improves  $x^{\varepsilon}$  lexicographically and g fixes every  $j \leq i$ , the improvement should occur from entry i + 1 onwards. Hence, as  $gx^{\varepsilon} \succ x^{\varepsilon}$ , it must hold that  $(gx^{\varepsilon})_{i+1} = x_{g^{-1}(i+1)}^{\varepsilon} > x_{i+1}^{\varepsilon}$  and  $g^{-1}(i+1) > i+1$ .

By construction of our  $\epsilon$  perturbation, it must also hold that  $x_{g^{-1}(i+1)} > x_{i+1}$ . Indeed, it cannot hold that  $x_{g^{-1}(i+1)} = x_{i+1}$ , since the perturbation is increasing in the vector's indices and  $g^{-1}(i+1) > i+1$ . Neither it can happen that  $x_{g^{-1}(i+1)} < x_{i+1}$  since this implies that  $x_{g^{-1}(i+1)}^{\epsilon} < x_{i+1}^{\epsilon}$ . In consequence, it holds that  $gx \succ x$  and hence  $x \notin \text{Lex}_G$ . Moreover, the ball  $B_{M/2}(x) \subseteq \text{Lex}_G^{\epsilon}$ , as g fixes the indices  $1, \ldots, i$  pointwise and exchanges  $x_{i+1}$  for a strictly greater entry  $x_{g^{-1}(i+1)}$  in x, where  $g^{-1}(i+1) > i+1$ .

Now we are ready to show a characterization of  $\overline{\text{Lex}}_G$  by an explicit set of inequalities.

**Theorem 5.** Let  $G \leq S_n$ . Then  $\overline{Lex}_G = SS_G$ .

Proof. Suppose on the contrary that  $x \notin SS_G$  but  $x \in \overline{Lex}_G$ , i.e.,  $x^{\epsilon} \in Lex_G$  for all  $0 < \epsilon < M$  by Lemma 6. As  $x \notin SS_G$ , there exists a minimal  $i \in [n]$  and  $j \in Orb_{G_{i-1}}(i)$ , such that  $x_i < x_j$  where i < j, and thus  $x_i^{\epsilon} < x_j^{\epsilon}$ . Then, there exists  $g \in G_{i-1}$  such that  $gx^{\epsilon} \succ x^{\epsilon}$  which is a contradiction.

For the converse, suppose  $x \in SS_G$ . If for each index-orbit  $Orb \subseteq [n]$ , all the components of x indexed by Orb are different, then  $x \in Lex_G$  since for any pair (i, j) such that  $i \in [n]$ ,  $j \in Orb_{G_{i-1}}(i)$ , and i < j, the corresponding Schreier-Sims inequality is strict, i.e.  $x_i > x_j$ . If not, for every coordinate-tie within an orbit apply the tie-breaker perturbation. Therefore, the perturbed vector belongs to  $Lex_G$ , i.e.,  $x \in Lex_G$  by Lemma 6.

The next result exhibits the generality of our GDD method for constructing fundamental domains. It shows that by choosing  $\alpha_i$  as the canonical basis vectors in our GDD construction the algorithm outputs  $SS_G$ . We note that this also gives an alternative proof to Theorem 4.

## **Proposition 6.** For any group $G \leq S_n$ the set $SS_G$ is a GDD.

*Proof.* We show that  $SS_G$  can be obtained from Algorithm 1 by choosing  $\alpha_i$  equal to the canonical vectors. We begin the procedure with  $\alpha_1 := e_1$ , then  $G_1$ , in Line 4 of Algorithm 1, corresponds to the pointwise stabilizer of the index  $1 \in [n]$ . Hence, if in iteration  $i \in [n]$  we choose  $\alpha_i := e_i$ , then the subgroup  $G_i$  which stabilizes  $\alpha_1, \ldots, \alpha_i$  is equal to  $G_{([i-1])}$ . After at most n iterations we have that  $F = SS_G$ .

As the Schreier-Sims table has  $O(n^2)$  many entries, the number of facets of the Schreier-Sims fundamental domain is at most  $O(n^2)$ . In what follows we show a tighter bound of O(n). To this end, we notice that several of the added inequalities are redundant.

**Theorem 6.** Let us consider a group  $G \leq S_n$  and let f denote the number of G-orbits in [n]. Then  $SS_G$  is a polyhedron with at most n - f facets.

*Proof.* Let D = ([n], E) be a directed graph defined as follows. For each  $i \in [n]$  we have that  $(i, j) \in E$  for each  $j \in \operatorname{Orb}_{G^{i-1}}(i)$ . By construction, D is a topological sort, and hence it is a directed acyclic graph (DAG).

Claim: Let  $j \in [n]$ . If  $(i, j), (k, j) \in E$  then either  $(i, k) \in E$  or  $(k, i) \in E$ .

Indeed, without loss of generality, let us assume that i < k. As  $(i, j) \in E$  then  $j \in \operatorname{Orb}_{G^{i-1}}(i)$ . Similarly, it holds that  $j \in \operatorname{Orb}_{G^{k-1}}(k) \subseteq \operatorname{Orb}_{G^{i-1}}(k)$ . Therefore, by transivity,  $k \in \operatorname{Orb}_{G^{i-1}}(i)$ , and hence  $(i, k) \in E$ . This shows the claim.

Let  $\tilde{D} = ([n], \tilde{E})$  be the *minimum equivalent graph* of D, that is, a subgraph with a minimum number of edges that preserves the reachability of D. Hence, there exists a (u, v)-dipath in D if and only if there exist a (u, v)-dipath in  $\tilde{D}$ . Notice that

$$SS_G = \{x : x_i \ge x_j \text{ for all } (i,j) \in E\}.$$

We define

$$SS_G = \{x : x_i \ge x_j \text{ for all } (i,j) \in \tilde{E}\}$$

then  $SS_G = \widetilde{SS}_G$ . Clearly we have that  $SS_G \subseteq \widetilde{SS}_G$ . On the other hand, if  $x_i \ge x_j$  is an inequality of  $SS_G$ , then there exists an (i, j)-dipath in  $\widetilde{SS}_G$  and hence  $x_i \ge x_{i_1} \ge x_{i_2} \ge \ldots x_{i_k} \ge x_j$  is a valid set of inequalities for  $\widetilde{SS}_G$ , for certain nodes  $i_1, \ldots, i_k$ . We conclude that  $SS_G = \widetilde{SS}_G$ .

No we argue that  $\tilde{D}$  is a collection of at least f out-trees. Indeed, lets assume by contradiction that for  $j \in [n]$  there exists two distinct nodes i, k such that  $(i, j), (k, j) \in \tilde{E}$ . By our previous claim, k is reachable from i in D (or analogously i is reachable from k), and hence the same is true in  $\tilde{D}$ . This is a contradiction as the edge (i, j) could be removed from  $\tilde{D}$  preserving the reachability. As  $\tilde{D}$  is a DAG, then  $\tilde{D}$  must be a collection of node-disjoint out-trees. Finally, note that the smallest element in each orbit of G in [n] has in-degree 0 in D, and hence also in  $\tilde{D}$ . Therefore  $\tilde{D}$  has at least f different trees, which implies that  $\tilde{D}$  has at most n - f edges.

This means that every permutation group admits a fundamental domain with at most n-1 facets. We complement this theorem by the following observation.

## **Proposition 7.** Any fundamental domain for $S_n$ has n-1 facets.

Proof. Since  $S_n$  is generated by the transpositions  $(i \ j)$  for all  $i \neq j \in [n]$  which correspond to reflections with reflection axis  $x_i = x_j$ , we conclude that  $S_n$  is a reflection group. Moreover, since fundamental domains for reflection groups are unique (up to actions of the group), see Coxeter [6, pp. 79 – 81], any fundamental domain for  $S_n$  is equivalent to the Schreier-Sims fundamental domain for  $S_n$ . This symmetry breaking set has n-1 facets and can be described by the inequalities  $x_i \geq x_{i+1}$  for every  $i \in [n-1]$ .

## 5 Overrepresentation of Orbit Representatives

A desirable property of symmetry breaking polyhedra is that they select a unique representative per G-orbit. In general, the definition of fundamental domains only guarantees this for vectors in their interior. Recall that a subset R of  $\mathbb{R}^n$  which contains exactly one point from each G-orbit is called a *fundamental set*. The following result shows that closed convex fundamental sets are only attained by reflection groups. In other words, the only groups that admit fundamental domain containing unique representatives for every orbit are reflection groups.

**Theorem 7.** Let  $G \leq O_n(\mathbb{R})$  finite. Then G admits a fundamental domain F with  $|F \cap O| = 1$  for every G-orbit  $O \subseteq \mathbb{R}^n$  if and only if G is a reflection group.

*Proof.* Suppose G admits a closed convex fundamental set  $F \subseteq \mathbb{R}^n$ , i.e. F is a fundamental domain and for every  $x \in \mathbb{R}^n$  we have that

$$\operatorname{Orb}_G(x) \cap F = \{gx\},\$$

for some  $q \in G$ . By Proposition 2 we know that F is a polyhedral cone and we can write it as

$$F = \bigcap_{g \in A} H_g$$

where A is a generating set for G. We want to show that A is a set of reflections.

Let g be a non-trivial element of A and consider its associated half-space  $H_g$ . We know that  $H_g^=$  is a supporting hyperplane for F, and  $F \cap gF$  has dimension n-1. Suppose x is an arbitrary vector in  $F \cap gF$ . Then  $g^{-1}x \in F$ , and hence gx = x because F contains a unique representative of x. Now consider the span of  $F \cap gF$  and let  $\hat{g}$  denote the restriction of the orthogonal transformation g to this linear subspace. As  $\hat{g}$ fixes every point in the relative interior of  $F \cap gF$ , which is n-1 dimensional, we have that  $\hat{g}$  acts trivially in span $(F \cap gF) = H_g^=$ . Since g is a non-trivial isometry, every vector  $y \in (H_g^=)^{\perp}$  must satisfy that gy = -y. We conclude that g is a reflection with respect to the hyperplane  $H_g^=$ . For the converse implication, see Coxeter [6, pp. 79 – 81] and notice that his construction gives an exact fundamental domain as its facets are defined by reflections.

As a corollary we can characterize when the fundamental set  $\text{Lex}_G$  is closed. Alternatively, this characterizes when  $SS_G$  contains a unique representative for *every* orbit. Equivalently, this characterizes the groups for which the fundamental set  $\text{Lex}_G$  is closed. Our proof utilizes the next lemma which provides an orthogonal decomposition of  $\text{Lex}_G$  when G is a direct product.

**Lemma 7.** Consider  $G \leq S_n$ . Assume that  $O_1, O_2$  is a partition of [n], and  $G_i \leq S_{O_i}$  for  $i \in \{1, 2\}$ . If  $G = G_1 \times G_2$ , then  $Lex_G = Lex_{G_1} \times Lex_{G_2}$ .

*Proof.* For  $x \in \mathbb{R}^n$  and  $S \subseteq [n]$ , let us denote by  $x_S$  the vector x restricted to the coordinates in S. Let us also denote  $x_{O_i} \succ_i y_{O_i}$  if  $x_{O_i}$  is lexicographically larger than  $y_{O_i}$  (without altering the order of elements in  $O_i$ ). Also, for  $(g_1, g_2) \in G_1 \times G_2$ , we denote by  $x \to (g_1, g_2)x$  the action where  $g_1$  permutes the coordinates in  $O_1$  and  $g_2$  permutes the coordinates in  $O_2$ .

We must show that the following are equivalent:

- (i)  $x \succeq gx$  for all  $g \in G_1 \times G_2$ .
- (ii)  $x_{O_i} \succeq_i g_i x_{O_i}$  for  $i \in \{1, 2\}$  for every  $(g_1, g_2) \in G_1 \times G_2$ .

Clearly, (ii) is equivalent to  $x \succeq (g_1, id)x$  and  $x \succeq (id, g_2)x$  for every  $(g_1, g_2) \in G_1 \times G_2$ . This last condition is necessary for (i). To see that is also sufficient, assume that  $x \prec (g_1, g_2)x$  for some  $(g_1, g_2) \in G_1 \times G_2$ . Let ibe the first coordinate where  $x_i < ((g_1, g_2)x)_i$ . Let us assume that  $i \in O_1$  (the case  $i \in O_2$  is analogous), and hence  $x_j = (g_1x_{O_1})_j$  for all j < i such that  $j \in O_1$ . This implies that  $x_{O_1} \prec_1 g_1x_{O_1}$ . The lemma follows.  $\Box$ 

**Corollary 2.** Let  $G \leq S_n$ . Suppose that G partitions [n] into a collection of orbits  $O_1, \ldots, O_m \subseteq [n]$ ,  $m \in [n]$ . Then Lex<sub>G</sub> is closed if and only if

$$G = S_{|O_1|} \times \dots \times S_{|O_m|}.$$

*Proof.* Suppose that  $G \leq S_n$  is transitive. Given that the only transitive reflection group of  $S_n$  is  $S_n$  itself, Theorem 7 implies that if G is a proper transitive group of  $S_n$  then G does not admit a closed convex fundamental set. Hence Lex<sub>G</sub> cannot be closed since Lex<sub>G</sub> is a convex fundamental set for any  $G \leq S_n$ .

Suppose G is not transitive on [n]. Then the if part is straightforward by Lemma 7 and Theorem 7. For the converse, without loss of generality assume that G is a subgroup of  $S_{|O_1|} \times \cdots \times S_{|O_m|}$  and that the orbits are reordered (relabeled) as  $\{1, \ldots, n_1\}$ ,  $\{n_1 + 1, \ldots, n_2\}$ ,  $\ldots$ ,  $\{n_{m-1} + 1, \ldots, n\}$ , where  $|O_1| = n_1$ ,  $|O_2| = n_2 - n_1, \ldots, |O_{m-1}| = n_{m-1} - n_{m-2}, |O_m| = n - n_{m-1}$ . We perform this reordering without changing the order of the variables in the lexicographic order, so that  $\text{Lex}_G$  is maintained.

Now, suppose that  $\operatorname{Lex}_G$  is closed, i.e. G is a group generated by reflections, and that  $G \leq S_{|O_1|} \times \cdots \times S_{|O_m|}$ . Note that if  $g \in G$  is a reflection, then it must be a transposition  $(i \ j)$  for some  $i, j \in [n]$ . Indeed, consider the decomposition of g into disjoint cycles  $\{c_1, \ldots, c_L\}$ , i.e.  $g = c_1 \cdots c_L$ , and note that the invariant subspace of any cycle  $c_l$  is given by the equalities  $x_i = x_j$  for all i, j moved by  $c_l$ . Since the invariant subspace of g is n-1, then g must be equal to a single transposition  $(i \ j)$ . Therefore, G is generated by transpositions, and since it acts transitively on each G-orbit  $O_k$ , then the action of G restricted to  $O_k$  is isomorphic to  $S_{|O_k|}$ . Moreover, the direct product follows after noting that every g is a product of cycles of order 2, hence  $S_{|O_k|} \subseteq G$  for every  $k \in [m]$ .

In integer programming problems, we are concerned about the number of representatives of binary orbits in a fundamental domain. The Schreier-Sims domain can be weak in this regard, as shown in the following example.

*Example 3.* Let  $n \in \mathbb{N}$  be divisible by 3, and consider the direct product

$$G := C^1 \times C^2 \times \dots \times C^{n/3},$$

where  $C^i$  for  $i \in [n/3]$  is the cyclic group on the triplet

$$(3(i-1)+1, 3(i-1)+2, 3(i-1)+3).$$

Consider the binary vector x := (1, 1, 0, 1, 1, 0, ..., 1, 1, 0). For each vector in the *G*-orbit of *x*, there are three possible values for each triplet:

$$1, 1, 0$$
 or  $0, 1, 1$  or  $1, 0, 1$ .

Therefore, the orbit of x has cardinality  $3^{n/3}$ . The fundamental domain SS<sub>G</sub> for G can be described as follows

$$SS_G = \{x \in \mathbb{R}^n : x_{3(i-1)+1} \ge x_{3(i-1)+2} \text{ and } x_{3(i-1)+1} \ge x_{3(i-1)+3}, \forall i \in [n/3]\}$$

It is clear that each vector in  $SS_G \cap Orb_G(x)$  admits two options for its index triplets: 1, 1, 0 and 1, 0, 1. As a result  $|SS_G \cap Orb_G(x)| = 2^{n/3}$ .

We propose a definition for a theoretical classification of symmetry breaking systems inspired by our findings, and we consider two attributes to rank symmetry breaking systems: the complexity of their separation, and their symmetry breaking power, i.e. their effectiveness to cut isomorphic points. These two properties seem to be a longstanding trade-off in mathematical programming with respect to symmetry breaking systems [20,14], and this trade-off has also been recognized in *constraint satisfaction problems* [25]. In the latter, it is challenging to identify a symmetry breaking system which is both *effective*, in the sense that it rules out a large portion of the search space, and *compact*, which means that the symmetry breaking inequalities can be checked in a reasonable amount of time [31,7].

Let X be a G-invariant subset of  $\mathbb{R}^n$  (e.g.  $X = \{0,1\}^n$ ). Let  $\mathcal{O}(G,X)$  be the set of all G-orbits in X. Motivated by our previous discussion, we define, for a fixed G, the worst-case effectiveness of F on X as

$$\Lambda_{G,X}(F) := \max_{O \in \mathcal{O}(G,X)} |F \cap O|.$$

Now, we use our GDD algorithm to obtain a suitable fundamental domain in Example 3 with  $\Lambda_{G,\{0,1\}^n}(F) = 1$  while  $\Lambda_{G,\{0,1\}^n}(SS_G) = 2^{\Omega(n)}$ .

*Example 3 (continued).* We construct a GDD F with  $\Lambda_{G,\{0,1\}^n}(F) = 1$ . First, note that G has n/3 orbits in [n] given by:

$$\Delta_i := \{3(i-1)+1, 3(i-1)+2, 3(i-1)+3\}$$

for  $i \in [n/3]$ . Therefore the following vectors, and their associated stabilizers, construct a generalized Dirichlet domain

10 1

$$\alpha_{1} = (4, 2, 1, 0, 0, 0, 0, \dots, 0), \quad G_{\alpha_{1}} = (C_{3})^{n/3-1}$$
$$\alpha_{2} = (0, 0, 0, 4, 2, 1, 0, \dots, 0), \quad G_{\alpha_{2}} = (C_{3})^{n/3-2}$$
$$\vdots$$
$$\alpha_{n/3} = (0, 0, 0, 0, \dots, 0, 4, 2, 1), \quad G_{\alpha_{n/3}} = \langle \text{id} \rangle.$$

such that  $\operatorname{Orb}_G(x) \cap F = \{x\}$  for any  $x \in \{0,1\}^n$ . The number of cosets in each iteration is 3. Omitting the trivial coset, the number of inequalities that defines our GDD is  $2 \cdot (n/3)$ .

## 6 Future Work

Our work leaves several major questions.

**Q1:** Does our GDD construction exhaust all possible fundamental domains for a group of isometries, or are there other fundamental domains that are not GDDs?

Any light on this question can help creating new fundamental domains with potential practical relevance, or help us show impossibility results. This can also have consequences regarding our long term goal: understanding the tension (potentially trade-off) between the symmetry breaking effectiveness of a polyhedron and its complexity. A closely related question is whether we need the hypothesis of being subgroup consistent in Theorem 1. If the answer to Q1 is positive, we would immediately conclude that Theorem 1 holds without assuming that the fundamental domain is subgroup consistent.

**Q2:** Does every group of isometries admit a fundamental domain with a single representative of each binary orbit, and with a polynomial number of facets?

It is not hard to imagine other interesting variants of this question. For example, we could be interested either in the extension complexity or complexity of the separation problem, instead of the number of facets. At the moment, the only information we have is that blindly choosing lexicographically maximal binary vectors as representatives should not help, as finding them is NP-hard [4]. It is worth noticing that an answer to Q1 might help answering Q2, either positively or negatively. Alternatively, the relation between  $\Lambda_{G,X}(F)$  and the number of facets of a fundamental domain F is of interest, for example for  $X = \{0,1\}^n$ . On the other hand, we know that only reflection groups admit fundamental domains with  $\Lambda_{G,\mathbb{R}^n}(F) = 1$ . Characterizing, for example, the class of groups that allows for  $\Lambda_{G,\mathbb{R}^n}(F) = O(1)$  might also give us a better understanding on the limitations of symmetry breaking polyhedra.

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## References

- Achterberg, T., Wunderling, R.: Mixed Integer Programming: Analyzing 12 Years of Progress. In: M. Jünger, G. Reinelt (eds.) Facets of Combinatorial Optimization, pp. 449 – 481. Springer Berlin Heidelberg (2013)
- 2. Babai, L.: Graph Isomorphism in Quasipolynomial Time. arXiv preprint arXiv:1512.03547v2 (2016)
- 3. Babai, L.: Graph Isomorphism in Quasipolynomial Time. In: Proceedings of the Forty-eighth Annual ACM Symposium on Theory of Computing, pp. 684–697 (2016)
- Babai, L., Luks, E.M.: Canonical labeling of Graphs. In: Proceedings of the Fifteenth Annual ACM Symposium on Theory of Computing, pp. 171 – 183 (1983)
- Bödi, R., Herr, K., Joswig, M.: Algorithms for highly Symmetric Linear and Integer Programs. Mathematical Programming Series A 137, 65 – 90 (2013)
- 6. Coxeter, H.S.M.: Regular Polytopes. Methuen & Co. Ltd. (1948)
- Crawford, J.M., Ginsberg, M.L., Luks, E.M., Roy, A.: Symmetry-Breaking Predicates for Search Problems. In: Proceedings of the Fifth International Conference on Principles of Knowledge Representation and Reasoning, pp. 148 – 159. Morgan Kaufmann Publishers Inc. (1996)
- 8. Dias, G., Liberti, L.: Exploiting Symmetries in Mathematical Programming via Orbital Independence. Annals of Operations Research **298**, 149 182 (2021)
- 9. Dirichlet, G.L.: Über die Reduction der Positiven Quadratischen Formen mit drei unbestimmten ganzen Zahlen. Journal für die reine und angewandte Mathematik **1850**, 209 – 227 (1850)
- Faenza, Y., Kaibel, V.: Extended Formulations for Packing and Partitioning Orbitopes. Mathematics of Operations Research 34, 686 – 697 (2009)

- 11. Friedman, E.: Fundamental Domains for Integer Programs with Symmetries. In: Proceedings of Conference on Combinatorial Optimization and Applications, pp. 146 153 (2007)
- 12. Ghoniem, A., Sherali, H.D.: Defeating Symmetry in Combinatorial Optimization via Objective Perturbations and Hierarchical Constraints. IIE Transactions 43, 575 588 (2011)
- Herr, K., Rehn, T., Schürmann, A.: Exploiting Symmetry in Integer Convex Optimization using Core Points. Operations Research Letters 41, 298 – 304 (2013)
- Hojny, C., Pfetsch, M.: Polytopes associated with Symmetry handling. Mathematical Programming Series A 175, 197 – 240 (2018)
- 15. Kaibel, V., Pfetsch, M.: Packing and Partitioning Orbitopes. Mathematical Programming 114, 1 36 (2008)
- Liberti, L.: Reformulations in Mathematical Programming: Automatic Symmetry Detection and Exploitation. Mathematical Programming Series A 131, 273 – 304 (2012)
- 17. Liberti, L., Ostrowski, J.: Stabilizer-based Symmetry Breaking constraints for Mathematical Programs. Journal of Global Optimization **60**, 183 194 (2014)
- 18. Margot, F.: Pruning by Isomorphism in Branch-and-Cut. Mathematical Programming Series A 94, 71 90 (2002)
- Margot, F.: Exploiting Orbits in Symmetric Integer Linear Program. Mathematical Programming Series B 98, 3 - 21 (2003)
- Margot, F.: Symmetry in Integer Linear Programming. In: M. Jünger, T.M. Liebling, D. Naddef, G.L. Nemhauser, W.R. Pulleyblank, G. Reinelt, G. Rinaldi, L.A. Wolsey (eds.) 50 Years of Integer Programming 1958-2008, pp. 647 – 686. Springer Berlin Heidelberg (2010)
- 21. Ostrowski, J., Anjos, M.F., Vannelli, A.: Symmetry in Scheduling Problems (2010). Cahier du GERAD G-2010-69
- Ostrowski, J., Linderoth, J., Rossi, F., Smriglio, S.: Orbital Branching. Mathematical Programming Series A 126, 147 – 178 (2011)
- Pfetsch, M.E., Rehn, T.: A computational comparison of symmetry handling methods for mixed integer programs. Mathematical Programming Computation 11, 37 – 93 (2019)
- 24. Ratcliffe, J.G.: Foundation of Hyperbolic Manifolds, 3rd edn. Springer (2019)
- Rossi, F., Van Beek, P., Walsh, T. (eds.): Handbook of Constraint Programming, 1st edn. Foundations of artificial intelligence. Elsevier (2006)
- 26. Rotman, J.J.: An Introduction to the Theory of Groups, 4th edn. Springer (1995)
- Salvagnin, D.: Symmetry Breaking Inequalities from the Schreier-Sims table. In: International Conference on the Integration of Constraint Programming, Artificial Intelligence, and Operations Research, pp. 521 – 529 (2018)
- Schürmann, A.: Exploiting Symmetries in Polyhedral Computations. In: Discrete Geometry and Optimization, pp. 265 – 278. Springer International Publishing (2013)
- 29. Seress, A.: Permutation Group Algorithms. Cambridge University Press (2003)
- Sherali, H.D., Smith, J.C.: Improving Discrete Model Representations via Symmetry Considerations. Management Science 47, 1396 – 1407 (2001)
- Shlyakhter, I.: Generating effective Symmetry-breaking Predicates for Search problems. Discrete Applied Mathematics 155, 1539 1548 (2007)