Symmetries in polynomial optimization

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Abstract This chapter investigates how symmetries can be used to reduce the computational complexity in polynomial optimization problems. A focus will be specifically given on the Moment-SOS hierarchy in polynomial optimization, where results from representation theory and invariant theory of groups can be used. In addition, symmetry reduction techniques which are more generally applicable are also presented.

1 Introduction

Symmetry is a vast subject, significant in art and nature. Mathematics lies at its root, and it would be hard to find a better one on which to demonstrate the working of the mathematical intellect.

Hermann Weyl

Polynomial optimization is concerned with optimization problems expressed by polynomial functions. Problems of this kind can arise in many different contexts, including engineering, finance, and computer science. Although these problems may be formulated in a rather elementary way, they are in fact challenging and solving such problems is known to be algorithmically hard in general. It is therefore beneficial to explore the algebraic and geometric structures underlying a given problem to design

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more efficient algorithms, and a kind of structure which is omnipresent in algebra and geometry is symmetry. In the language of algebra, symmetry is the invariance of an object or a property by some action of a group. The goal of the present chapter is to present techniques which allow to reduce the complexity of an optimization problem with symmetry. Since it is impossible to give an exhaustive and detailed description of this vast domain, our goal here is to focus mainly on the Moment-SOS hierarchy in polynomial optimization and elaborate how the computation of such approximations can be simplified using results from representation theory and invariant theory of groups. In addition to these approaches we also mention some more general results, which allow to reduce the symmetry directly on the formulation of the polynomial optimization problem.

Overview

We begin first with a short presentation of the basic Moment-SOS hierarchy in global polynomial optimization and semidefinite programming in the following Section. We do not give a very extended exposition of this topic but limit Section 2 to defining the concepts which are essential for this chapter. Section 3, which is devoted to the representation theory of (finite) groups, lays out a first set of tools allowing for reduction of complexity. We begin in Subsection 3.1 with a survey of the central ideas of representation theory from the point of view of symmetry reduction, where the main focus is on Schur's Lemma and its consequences. Subsection 3.2 then gives a short collection of central combinatorial objects which are used to understand the representation theory of the symmetric group. Finally, Subsection 3.3 outlines how representation theory can be used to simplify semidefinite programs via blockdiagonalization of matrices which are commuting with the group action. Building on representation theory we then turn to invariant theory in Section 4 which allows to closer study the specific situation of sums of squares which are invariant by a group. We begin with a basic tutorial on invariant theory in Subsection 4.1. Since this theory is easier in the particular situation of finite reflection groups, we put a special emphasis on these groups. Following this introduction we show in Subsection 4.2 how the algebraic relationship between polynomials and invariant polynomials can be used to gain additional understanding of the structure of invariant sums of squares. These general results are then exemplified in Subsection 4.3 for the case of symmetric sums of squares. Finally, Section 5 highlights some additional techniques for symmetry reduction: firstly, we overview in Subsection 5.1 how rewriting the polynomial optimization problem in terms of invariants and combining it with the semialgebraic description of the orbit space of the group action can be used. In Subsection 5.2, we show that even in situations where Schur's Lemma from representation theory does not directly apply, one can already obtain good complexity reduction by structuring computations per orbit, and we illustrate this idea in the context of so-called SAGE certificates. We conclude, in Subsection 5.3 with some results guaranteeing the existence of structured optimizers in the context of polynomial optimization problems with symmetries.

2 Preliminaries on the Moment-SOS hierarchy in polynomial optimization and semidefinite programming

Given real polynomials $f, g_1, \dots, g_m \in \mathbb{R}[X_1, \dots, X_n]$, a polynomial optimization problem is an optimization task of the following kind

$$f^* = \inf \{ f(x) : g_1(x) \ge 0, \dots, g_m(x) \ge 0, x \in \mathbb{R}^n \}.$$
 (1)

As motivated above, the task of finding the optimal value of a such problems arises naturally in many applications. However, it is also known that this class of problems is algorithmically hard ([50]) and a given problem might be practically impossible to solve. One approach to overcome such challenges consists in relaxing the problem: instead of solving the original hard problem, one can relax the hard conditions and define a new problem, easier to solve, and whose solution might still be close to the solution of the original problem. This idea has produced striking new ways to approximate hard combinatorial problems, such as the Max-Cut problem [28]. One quite successful approach to relax polynomial optimization problems uses the connection of positive polynomials to moments and sums of squares of polynomials. We shortly outline this approach in the beginning since a big focus of this chapter deals with using symmetries in this setup. The overview we give here is short and a reader who is not familiar with the concepts is also advised to consult [45, 43] and in particular the original works by Lasserre [42] and Parrilo [53]. For simplifications we explain the main ideas only in the case of global optimization, i.e., when the additional polynomial constraints are trivial. In this case the problem we are interested to solve is to find

$$f^* = \inf \left\{ f(x) : x \in \mathbb{R}^n \right\}. \tag{2}$$

This problem is in general a non-convex optimization problem and it can be beneficial to slightly change perspective in order to obtain the following equivalent formulations which are in fact convex optimization problems. Firstly, one can associate to a point $x \in \mathbb{R}^n$ the Dirac measure δ_x which leads to the following reformulation of the problem:

$$f^* = \inf \left\{ \int f(x) d\mu(x) : \int 1 d\mu(x) = 1 \right\},\tag{3}$$

where the infimum is considered over all probability measures μ supported in \mathbb{R}^n . Since the Dirac measures δ_x of every point are feasible solutions this reformulation clearly yields the same solution. Secondly, one can also reformulate in the following way:

$$f^* = \sup \left\{ \lambda : f(x) - \lambda \ge 0 \ \forall x \in \mathbb{R}^n \right\}. \tag{4}$$

It follows from results of Haviland [31] that both of the above presented reformulations are dual to each other. Even though the second formulation is equivalent from the algorithmic perspective, it points to the core of the algorithmic hardness of the polynomial optimization problem: it is algorithmically hard to test if a given polynomial $f \in \mathbb{R}[X_1, \dots, X_n]$ is non-negative, i.e., if $f(x) \ge 0$ for all $x \in \mathbb{R}^n$. Therefore an approach to obtain approximations for f^* which are easier to calculate consists in replacing this condition with one that is easier to check, but still ensures non-negativity. We say that a polynomial $f \in \mathbb{R}[X_1, \dots, X_n]$ is a *sum of squares (SOS)* if it can be written as $f = p_1^2 + \dots + p_l^2$ for some polynomials $p_1, \dots, p_l \in \mathbb{R}[X_1, \dots, X_n]$. Clearly every such polynomial is also non-negative and we can consider the problem

$$f^{SOS} = \sup \{ \lambda : f(x) - \lambda \text{ is a SOS} \}.$$
 (5)

Clearly we have $f^{SOS} \leq f^*$, and as not every non-negative polynomial is a sum of squares, as was shown by Hilbert [34], this inequality will not be sharp in general. On the other hand, having a concrete decomposition into sums of squares provides an *algebraic certificate* of non-negativity. So one obtains an algebraically verifiable proof for the solution of the bound. This strengthening of the optimization problem gives, on the dual side, a relaxation of the moment formulation. The main feature which makes this approach also interesting for practical purposes comes from the fact that one can find a SOS-decomposition with the help of semidefinite programming. This was used by Lasserre [42] to define a hierarchy for polynomial optimization based on the sums of squares strengthening (5) and the corresponding relaxation of (3). In the context of polynomial optimization on compact sets semi algebraic sets this yields (some additional assumptions) yields a converging sequence of approximations each of which can be obtained by a semidefinite program (see [45, 43] for more details on these hierarchies).

Semidefinite programming

Semidefinite programming (SDP) is an optimization paradigm which was developed in the 1970s as a generalization of linear programming. The main setup is to maximize/minimize a linear function over a convex set which is defined by the requirement that a certain matrix is positive semidefinite. We denote by $\operatorname{Sym}_n(\mathbb{R})$ the set of all real symmetric $n \times n$ matrices. Then a matrix $A \in \operatorname{Sym}_n(\mathbb{R})$ is called *positive semidefinite* if $x^T A x \geq 0$ for all $x \in \mathbb{R}^n$. In this case, we write $A \geq 0$. Furthermore for $A, B \in \operatorname{Sym}_n(\mathbb{R})$ we consider their scalar product

$$\langle A, B \rangle = \text{Tr}(A \cdot B).$$

The set of all symmetric matrices $A \in \operatorname{Sym}_n(\mathbb{R})$ which are positive semidefinite defines a convex cone inside $\operatorname{Sym}_n(\mathbb{R})$. With these notations we can define what an SDP is.

Definition 1 Let $C, A_1, \ldots, A_m \in \operatorname{Sym}_n(\mathbb{R})$ be symmetric matrices and let $b \in \mathbb{R}^m$ Then a semidefinite program is an optimization problem of the form

$$y^* := \inf \langle X, C \rangle$$

 $s.t. \quad \langle X, A_i \rangle = b_i, \quad 1 \le i \le m,$
 $X \ge 0, \text{ where } X \in \operatorname{Sym}_n(\mathbb{R}).$

The feasible set

$$\mathcal{L} := \{ X \in \operatorname{Sym}_n(\mathbb{R}) : \langle A_i, X \rangle = b_i, 1 \le i \le m, X \ge 0 \}$$

is a convex set.

The main feature which spiked the interest in this class of optimization problem is that they are on the one hand practically solvable (see [52, 56] for more details) but on the other hand can be used to design good approximation of otherwise algorithmically hard optimization problems (see for example [78] for a detailed overview).

The Lovász number of a graph

One example in which SDPs have proven to be especially powerful is in combinatorial optimization. In fact the seminal paper [46] in which Lovász introduced the parameter ϑ defined below as the solution to a semidefinite program was one of the first instances where the formulation of SDPs arose. The combinatorial problem for which these notions were designed is related to the following parameters of a graph.

Definition 2 Let $\Gamma = (V, E)$ be a finite graph.

- 1. A set $S \subset V$ is called *independent*, if no two elements in S are connected by an edge. Let $\alpha(\Gamma)$ denote the cardinality of the *largest independent set* in Γ .
- 2. For $k \in \mathbb{N}$ a k-coloring of the vertices of Γ is a distribution of k colors to the vertices of Γ such that two neighbouring vertices obtain different colors. The number $\chi(\Gamma)$ denotes the smallest k such that there is a k-coloring of the vertices in Γ .

Let $V = v_1, ..., v_n$ and $S \subset V$ be any independent vertex set. We consider the characteristic function $\mathbf{1}_S$ of S. Using this function, we can construct the following $n \times n$ matrix M:

$$M_{i,j} = \frac{1}{|S|} \mathbf{1}_S(v_i) \mathbf{1}_S(v_j).$$

It is clear that $M \in \operatorname{Sym}_n(\mathbb{R})$. Furthermore, clearly $M \geq 0$. Additionally, since $\mathbf{1}_S$ is the characteristic function of S and S consists only of vertices that do not share an edge, the following three properties of the matrix M hold:

- 1. $M_{i,j} = 0$ if $\{v_i, v_j\} \in E$,
- 2. $\sum_{v_i \in V} M_{i,j} = 1$,
- 3. $\sum_{\{v_i,v_j\}\in V\times V} M_{i,j} = |S|$.

With these properties of M in mind, one defines the ϑ -number of a graph Γ .

Definition 3 Let $\Gamma = (V, E)$ be a graph with vertex set $V = \{v_1, v_2, \dots, v_n\}$. Then the ϑ -number of Γ is defined as the solution to the following SDP:

$$\vartheta(\Gamma) = \sup \left\{ \sum_{i,j} B_{i,j} : B \in \operatorname{Sym}_n(\mathbb{R}), \ B \ge 0 \right.$$

$$\sum_i B_{i,i} = 1,$$

$$B_{i,j} = 0 \quad \forall (i,j) \in E \right\}$$

$$(6)$$

Note that the above mentioned graph invariants are known to be hard to compute (see [25, 40]). On the other hand, the ϑ -number is defined as the optimal solution of a semidefinite program and thus easier to calculate. In fact, Lovász could show the following remarkable relationship.

Theorem 1 (Sandwich theorem) With the notions defined above we have:

$$\alpha(\Gamma) \le \vartheta(\Gamma) \le \chi(\overline{\Gamma})$$

Furthermore, for the class of perfect graphs the ϑ -number actually provides a sharp bound. Thus, in these cases, and as $\alpha(\Gamma)$ is an integer, semidefinite programming yields polynomial time algorithms for computing these graph parameters.

Following Lovász's work, various different SDP approximations of hard problems have been proposed, for instance in coding theory and sphere packing (see [27, 44, 4, 18, 17]).

Connecting SDPs with sums of squares

In the context of polynomial optimization the relation to semidefinite approximations comes through the following observation originally due to Powers and Wörmann [54] that one can obtain a sums of squares decomposition of a given polynomial f via the so-called Gram Matrix method, which transfers this question into a semi-definite program. This connection is established in the following way: Let $p \in \mathbb{R}[X_1, \ldots, X_n]$ be a polynomial of even degree 2d. With a slight abuse of notation we denote by Y^d a vector containing all $\binom{n+d}{d}$ monomials in the variables X_1, \ldots, X_n of degree at most d. Thus, every polynomial s = s(X) of degree d is uniquely determined by its coefficients relative to Y. Now assume that p decomposes into a form

$$p = \sum_{i} (s_{i}(X))^{2}$$
 with polynomials s_{i} of degree at most d .

Then with the above notation we can rewrite this as

$$p = (Y^d)^T \left(\sum_j s_j s_j^T \right) Y^d,$$

where now each s_j denotes the coefficient vector of the polynomials $s_j(X)$. In this case the matrix $Q := \sum_j s_j s_j^T$ is positive semi-definite. Since by the so called Cholesky decomposition every positive semidefinite matrix $A \in \operatorname{Sym}_n(\mathbb{R})$ can be written in the form $A = \sum_j a_j a_j^T$ for some $a_j \in \mathbb{R}^n$ we see that the above line of argument is indeed an equivalence and so the existence of a sum of squares decomposition of p follows by providing a feasible solution to a semi-definite program, i.e we have

Proposition 1 A polynomial $p \in \mathbb{R}[X]$ of degree 2d is a sum of squares, if and only if there is a positive semi-definite matrix Q with

$$p = Y^T Q Y.$$

With this observation the formulation (5) can be directly transferred into the framework of semidefinite programming. This first approximation can already yield good bounds for the global optimum f^* and in particular in the constraint case, it can be developed further to a hierarchy of SDP-approximations: for a given optimization problem in the form (2) which satisfies relatively general conditions on the feasible set K one can construct a hierarchy of growing SDP-approximations whose optimal solutions converge towards the optimal solution of the initial problem. This approach gives a relatively general method to approximate and in some cases solve the initial problem.

Even though the Moment-SOS formulation described above yields a computational viable way to approximate the optimal solution the dimension of the matrices in the resulting SDPs can grow fast with the problem size. This is why this approach is limited to small or medium size problems unless some specific characteristics are taken into account. The focus of this chapter is on presenting ways to overcome this bottleneck in the case when additional symmetry is present in the problem.

3 Using Representation theory in SDPs for sums-of-squares

Representation theory is a branch of mathematics that studies symmetries and their relation to algebraic structures. More concretely, it studies the ways in which groups can be represented as linear transformations of vector spaces by representing the elements of the groups as invertible matrices. In this way it becomes possible to examine the structure of the group using the tools of linear algebra, making easier the study of structural algebraic properties of the group. Representation theory has also proven to be a powerful tool to simplify computations, in the situation where a group action is assumed on a vector space of matrices. In this situation we can use representation theory to describe the set of matrices stabilized by the action in a simplified way, reducing the sizes of the matrices as well as the dimension of the matrix spaces. In turn, this allows to study other algebraic properties, such as positive semidefiniteness of the invariant matrices in a more efficient way. This computational aspect of representation theory gives rise to practical applications in many fields, including physics, chemistry, computer science, and engineering. For example, it can be used to study the behavior of particles in quantum mechanics and the properties of molecules in chemistry and many more (see for example [39, 73, 77, 30, 11]). In this section, we outline the basic ideas of representation theory and its use in particular in semidefinite programming, where representation theory has successfully served as a key for many fascinating applications (see [3, 74] for other tutorials on the topic). Our main focus here lies in the reduction of semi-definite optimization problems and sums of squares representations of invariant polynomials. We start by providing a basic introduction to representation theory. A comprehensive and approachable introduction to this topic can be found in Serre's book [65]. Further readings on the subject can be found in [68, 70, 24, 38].

3.1 Basic representation theory

We begin by introducing the central definitions of representation theory.

Definition 4 Let G be a group.

- 1. A representation of G is a pair (V, ρ) , where V is a vector space over a field \mathbb{K} and $\rho: G \to \operatorname{GL}(V)$ is a group homomorphism from G to the group of invertible linear transformations of V. The degree of the representation is the dimension of the vector space V.
- 2. Two representations (V, ρ) and (V', ρ') of the same group G are considered equivalent, or isomorphic, if there exists an isomorphism $\phi: V \to V'$ such that $\rho'(g) = \phi \rho(g) \phi^{-1}$ for all $g \in G$.
- 3. Given a representation (V, ρ) , we can associate to it its character $\chi_V : G \to \mathbb{K}$, which is defined as

$$\chi_V(g) = \text{Tr}(\rho(g)).$$

Remark 1 A character of a group is a class function: it is constant on the conjugacy classes of *G*.

If V is a finite-dimensional vector space, we can identify the image of G under ρ as a matrix subgroup M(G) of the invertible $n \times n$ matrices with coefficients in \mathbb{K} by choosing a basis for V. We will denote the matrix corresponding to $g \in G$ as M(g) and refer to the family $\{M(g) \mid g \in G\}$ as a matrix representation of G.

Examples of representations

To give a selection of examples, we consider the group \mathfrak{S}_n of permutations of a set $S = \{1, 2, ..., n\}$. The group \mathfrak{S}_n has several representations:

- 1. The trivial representation $V = \mathbb{C}$ with g(v) = v for all $g \in \mathfrak{S}_n$ and $v \in \mathbb{C}$. This trivial representation can analogously be defined for all groups.
- 2. The *natural representation* of \mathfrak{S}_n on \mathbb{C}^n . In this representation, \mathfrak{S}_n acts linearly on the *n*-dimensional space

$$V = \mathbb{C}^n = \bigoplus_{i=1}^n \mathbb{C}e_i.$$

For $g \in \mathfrak{S}_n$, we define $g \cdot e_i = e_{g(i)}$ and extend this to a linear map on V. With respect to the basis e_1, \ldots, e_n we obtain thus a matrix representation given by *permutation matrices* which are defined as $M(g) = (x_{ij}) \in \mathbb{C}^{n \times n}$ with entries

$$x_{ij} = \delta_{g(i),j} = \begin{cases} 1, & \text{if } g(i) = j \\ 0, & \text{else.} \end{cases}$$

3. A representation of \mathfrak{S}_n on the polynomial ring $\mathbb{C}[X_1,\ldots,X_n]$. In this representation, we define

$$g \cdot X_i = X_{g(i)}$$
 for $g \in \mathfrak{S}_n$ and $i \in 1, \ldots, n$,

and extend it to a morphism of \mathbb{C} -algebras $\mathbb{C}[X_1, \dots, X_n] \longrightarrow \mathbb{C}[X_1, \dots, X_n]$. In this case we write f^g for the image of a polynomial f under the action of σ . This notation analogously applies to more general groups.

4. The regular representation, where (\mathfrak{S}_n, \circ) acts on the vector space

$$\mathbb{C}\mathfrak{S}_n = \bigoplus_{s \in \mathfrak{S}_n} \mathbb{C}e_s$$

with formal symbols e_s ($s \in \mathfrak{S}_n$) via $g(e_s) = e_{g \circ s}$. Also, this regular representation can analogously be defined for other finite groups.

The notion of G-module

Another way to define representations is to consider the linear action of a group G on a vector space V which gives V the structure of a G-module. A G-module is an abelian group M on which the action of G respects the abelian group structure on M. In the case when M is a vector space V, this just means that the group action is compatible with the operations on V. Given a vector space V that is a G-module, we can define a map $\phi: G \to \operatorname{GL}(V)$ that sends an element $g \in G$ to the linear map $v \mapsto gv$ on V. This map ϕ is then a representation of G. Thus in the context of linear spaces, the notions of G-modules and representations of G are equivalent, and it can be more convenient to use the language of G-modules. In this case, we call a linear map

$$\phi: V \to W$$

between two G-modules a G-homomorphism if

$$\phi(g(v)) = g(\phi(v))$$
 for all $g \in G$ and $v \in V$.

The set of all G-homomorphisms between V and W is denoted by $\operatorname{Hom}_G(V,W)$. Two G-modules are considered *isomorphic* (or equivalent) as G-modules if there exists a G-isomorphism from V to W.

Given a representation V, the set of all G-homomorphisms from V to itself is called the *endomorphism algebra* of V. It is denoted by $\operatorname{End}(V)$. If we have a matrix

representation M(G) of a group G, the endomorphism algebra corresponds to the *commutant algebra* Com((M(G))). This is the set of all matrices commuting with the group action, i.e.,

$$Com(M(G)) := \{ T \in \mathbb{C}^{n \times n} \text{ such that } TM(g) = M(g)T \text{ for all } g \in G \}.$$

When studying the action of a group G on a vector space V, it is important to consider subspaces that are closed under the action. Such a subspace is called a *subrepresentation* or G-submodule of V. If a representation V has a proper submodule, it is called *reducible*. If the only submodules of V are V and the zero subspace, the representation is called *irreducible*.

Decomposition of the natural representation of \mathfrak{S}_n

Consider the natural representation of \mathfrak{S}_n on the *n*-dimensional vector space \mathbb{C}^n . This representation is not irreducible. It has in fact two non-trivial subrepresentations, namely

$$W_1 = \mathbb{C} \cdot (e_1 + e_2 + \ldots + e_n)$$
 and $W_2 = W_1^{\perp}$

the orthogonal complement of W_1 for the usual inner product. Clearly, W_1 is irreducible since it is one-dimensional. Furthermore, also W_2 is in fact irreducible.

In the previous example, the vector space V is an orthogonal sum of irreducible representations. This is generally the case when the order of the group is not divisible by the characteristic of the ground field. In this case, a G-invariant inner product can be defined starting from any inner product $\langle \cdot, \cdot \rangle$ via

$$\langle x, y \rangle_G = \frac{1}{|G|} \sum_{g \in G} \langle g(x), g(y) \rangle.$$

The existence of such a G-invariant scalar product is in fact the key to the following Theorem.

Theorem 2 (Maschke's Theorem) Let G be a finite group and consider a representation (V, ϕ) defined over a field with a characteristic which is prime to |G|. Then, for every subrepresentation W we have that the orthogonal complement of W with respect to $\langle \cdot, \cdot \rangle_G$ is also a subrepresentation.

Remarks on Maschke's Theorem

As a consequence of Maschke's Theorem, every reducible representation V can be decomposed as an orthogonal sum of irreducible representations. Note that such a decomposition is not necessarily unique. Indeed, if we consider a group G which acts trivially on a n-dimensional vector space, every one-dimensional subspace is an irreducible subrepresentation. Furthermore, the assumption that the group is finite

is not necessary and a G-invariant inner product also exists in the case of compact groups. So, a version of Maschke's theorem also holds, for example, for compact groups, like O(n).

A very central statement in representation theory, which is, in particular, the key to the symmetry reductions in the further sections, is the following statement which goes back to Schur.

Theorem 3 (Schur's Lemma) Let V and W be two irreducible G-modules of a group G. Every G-endomorphism from V to W is either zero or invertible. Furthermore, $\operatorname{End}(V)$ is a skew field over \mathbb{K} . In particular, if the ground field \mathbb{K} is algebraically closed, every G invariant endomorphism between V and V is a scalar multiple of the identity.

Corollary 1 Let V be a complex irreducible G-module and $\langle \cdot, \cdot \rangle_G$ be an invariant Hermitian form on V. Then $\langle \cdot, \cdot \rangle_G$ is unique up to a real scalar multiple.

One can define an inner product on the set of complex valued functions on a finite group G by

$$\langle \phi, \psi \rangle = \frac{1}{|G|} \sum_{g \in G} \phi(g) \overline{\psi(g)}.$$

Using Schur's Lemma, one can show the following important property of irreducible characters.

Theorem 4 Let G be a finite group and \mathbb{K} be algebraically closed. Then, for every pair of characters (χ_i, χ_j) corresponding to a pair of non-isomorphic irreducible representations we have

$$\langle \chi_i, \chi_i \rangle = 0.$$

Moreover, the set of irreducible characters $\{\chi_i, i \in I\}$ form an orthonormal basis for the \mathbb{K} -vector space of class functions of G.

Recall that a *class function* on G is a function $G \to \mathbb{K}$ which is constant on the different conjugacy classes of G. Therefore, the following is a direct consequence.

Corollary 2 Assume that G is finite. Then there exists a finite number of non-equivalent irreducible representations of G. If \mathbb{K} is algebraically closed, this number is equal to the number of conjugacy classes of G.

Motivated by the notion of irreducible representations is the following notion of the *isotypic decomposition* of a representation. Here, isotypic means that we aim to decompose a representation V as a direct sum of subrepresentations, where each summand is the direct sum of equivalent irreducible subrepresentations. Specifically, for a finite group G, suppose that $I = \{W_1, W_2, \ldots, W_k\}$ are all the isomorphism classes of irreducible representations of G. Then the isotypic decomposition of V is a decomposition

$$V = \bigoplus_{i=1}^k \bigoplus_{j=1}^{m_i} V_{ij},$$

where each V_{ij} is a subrepresentation of V that is equivalent to the irreducible representation W_i . In other words, for each i, there exist G-isomorphisms

$$\phi_{i,j}: W_i \to V_{ij}$$
, for all $1 \le j \le m_i$

The subspace

$$V_i = \bigoplus_{i=1}^{m_i} V_{ij}$$

is called the isotypic component associated of type W_i . Since there is a bijection between the set of characters and the set of isomorphism classes of representations, we can also index the isotypic components of a representation by the corresponding irreducible character. We then denote by V^{χ} the isotypic component of V associated to the irreducible representation of character χ . The resulting isotypic decomposition of V

$$V = \bigoplus_{i=1}^{k} V_i = \bigoplus_{\chi} V^{\chi}$$

is unique up to the ordering of the direct sum.

Computing an isotypic decomposition

Using the characters of the irreducible representations, it is possible to calculate the isotypic decomposition as images of the projections

$$\pi_i: V \longrightarrow V
x \longmapsto \frac{\dim W_i}{|G|} \sum_{g \in G} \overline{\chi_i(g)} g \cdot x \tag{7}$$

where χ_i is the character associated to the irreducible representation W_i .

Combining the isotypic decomposition with Schur's Lemma, we obtain the following for representations defined over \mathbb{C} .

Corollary 3 Let $V := m_1 W_1 \oplus m_2 W_2 \oplus \ldots \oplus m_k W_k$ be a complete decomposition of a representation V over \mathbb{C} such that $\dim W_i = d_i$. Then we have:

- 1. dim $V = m_1 d_1 + \dots m_k d_k$, 2. End $V \simeq \bigoplus_{i=1}^k \mathbb{C}^{m_i \times m_i}$.
- 3. Let χ be the character of V and χ_i the character of W_i then we have $\langle \chi, \chi_i \rangle = m_i$.
- 4. There is a basis of V such that
 - a. The matrices of the corresponding matrix group M(G) are of the form

$$M(g) = \bigoplus_{l=1}^k \bigoplus_{j=1}^{m_l} M^{(l)}(g),$$

where $M^{(l)}(G)$ is a matrix representation of G corresponding to W_l . b. The corresponding commutant algebra is of the form

$$\operatorname{Com} M(G) \simeq \bigoplus_{l=1}^{k} (N_l \otimes I_{d_l}),$$

where $N_l \in \mathbb{C}^{m_l \times m_l}$ and I_{d_l} denotes the identity in $\mathbb{C}^{d_l \times d_l}$.

A basis for V as in the corollary above is called *symmetry adapted* basis. Given a matrix representation X of a representation V of a group G, Corollary 3 amounts to construct a basis of V such that the corresponding matrix representation has a particularly simple form. Specifically, we can decompose V into a direct sum of subrepresentations $V_{I,\beta}$ that are isomorphic to an irreducible representation W_I of G, and the matrices of the representation will be block diagonal with blocks corresponding to these subrepresentations.

How to construct a symmetry adapted basis

To construct such a basis, we consider a matrix representation Y^l corresponding to an irreducible representation W_l of dimension d_l and define the map

$$\pi_{\alpha,\beta}: V \to V$$
 for each $\alpha, \beta = 1, \ldots, d_l$,

as

$$\pi_{\alpha,\beta} = \frac{m_l}{|G|} \sum_{g \in G} Y_{\beta,\alpha}^l(g^{-1}) M(g).$$

Here, m_l is the number of copies of W_l that appear in the decomposition of V. It can be shown (see [65, Section 2.6]) that the map $\pi_{1,1}$ is a projection from V onto a subspace $V_{l,1}$ isomorphic to W_l , and $\pi_{1,\beta}$ maps $V_{l,1}$ onto $V_{l,\beta}$, which is another subrepresentation of V isomorphic to W_l . Thus we arrive at the announced decomposition and can use the maps to construct a symmetry-adapted basis.

A representation that admits a very beautiful isotypic decomposition is the regular representation of a finite group G. Recall that this is defined on the vector space

$$V^{reg} = \bigoplus_{g \in G} \mathbb{C}e_g,$$

via $\rho(g)(e_h) = e_{g \cdot h}$ for every $g, h \in G$.

Theorem 5 Let G be a finite group and (V, ρ) isomorphic to the regular representation of G. Then,

$$V \simeq \bigoplus_{W \in I} (\dim W) W,$$

and in particular, we have

$$|G| = \dim V = \sum_{W \in \mathcal{I}} (\dim W)^2.$$

Cyclic permutation matrices and the associated commutant

Consider the cyclic group C_4 and let g be a generating element of this group, i.e., $C_4 = \{g^0, g^1, g^2, g^3\}$. The regular representation of this group is of dimension 4. It can be defined as a matrix representation via the *cyclic permutation matrices* given via

$$g \mapsto M^{reg}(g) = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{pmatrix}.$$

Furthermore, C_4 has 4 pairwisely non-isomorphic irreducible representations, each of which is one-dimensional and we get these representations via

$$\rho_j: G \longrightarrow \mathbb{C}$$
$$g \longmapsto e^{\frac{2\pi i}{4}j}$$

for $0 \le i \le 3$. With the projection defined above in (7) we obtain that the symmetry adapted basis

$$B := \{(1, 1, 1, 1), (1, i, -1, -i), (1, -1, 1, -1), (1, -i, -1, i)\}.$$

With respect to this basis, the representation V^{reg} is given via the diagonal matrix

$$g \mapsto \tilde{X}^{reg}(g) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \mathbf{i} & 0 & 0 \\ 0 & 0 - 1 & 0 \\ 0 & 0 & 0 & -\mathbf{i} \end{pmatrix}$$

Now, consider a circulant matrix, i.e., a matrix of the from

$$T := \begin{pmatrix} \alpha & \beta & \gamma & \delta \\ \beta & \gamma & \delta & \alpha \\ \gamma & \delta & \alpha & \beta \\ \delta & \alpha & \beta & \gamma \end{pmatrix}.$$

Clearly, this matrix commutes with the matrix representation X^{reg} and doing the change of basis to the symmetry adapted basis we obtain

$$\tilde{T} = \begin{pmatrix} \alpha + \beta + \gamma + \delta & 0 & 0 & 0 \\ 0 & \alpha + i\beta - \gamma - i\delta & 0 & 0 \\ 0 & 0 & \alpha - \beta + \gamma - \delta & 0 \\ 0 & 0 & 0 & \alpha - i\beta - \gamma + i\delta \end{pmatrix}$$

More generally, for the cyclic group C_n we see that this regular representation will contain n irreducible representations $\rho_0, \ldots, \rho_{n-1}$, all of which are 1-dimensional and given by

$$\rho_i: g \mapsto e^{\frac{2\pi i}{n}j},$$

and corresponding symmetric adapted bases is also known as the Fourier-basis.

Complex irreducible versus real irreducible

The statements in Corollary 3 rely on the ground field to be algebraically closed. Therefore, a little bit of caution is necessary when working, for example, over the real numbers. Since this will be important for optimization we briefly highlight this situation. For a real irreducible representation (V, ρ) , there are two possible situations that lead to three different types (see [65, Section 13.2]):

- 1. If the complexification $V \otimes \mathbb{C}$ is also irreducible (type I), then representation can be directly transferred from $V \otimes \mathbb{C}$ to V and we can directly apply Corollary 3.
- 2. If the complexification $V \otimes \mathbb{C}$ is reducible, then it will decompose into two complex-conjugate irreducible G-submodules V_1 and V_2 . These submodules may be non-isomorphic (type II) or isomorphic (type III).

If the complexification $V \otimes \mathbb{C}$ of a real G-module V has the isotypic decomposition

$$V \otimes \mathbb{C} = V_1 \oplus \cdots \oplus V_{2l} \oplus V_{2l+1} \oplus \cdots \oplus V_h$$

where each pair (V_{2j-1}, V_{2j}) is complex conjugate $(1 \le j \le l)$ and V_{2l+1}, \ldots, V_h are real, we can keep track of this decomposition in the real representation, in the following way: consider a pair of complex conjugated G-modules (V_{2j-1}, V_{2j}) with $d = \dim V_{2j-1}$. Then a basis \mathcal{B}_{2j-1} of V_{2j-1} and the conjugated basis $\mathcal{B}_{2j} = \overline{\mathcal{B}_{2j-1}}$ of V_{2j} can be used to obtain a real basis of $V_{2j-1} \oplus V_{2j}$ by considering

$$\left\{b_1 + b'_1, \dots, b_d + b'_d, \frac{1}{i}(b_1 - b'_1), \dots, \frac{1}{i}(b_d - b'_d)\right\}$$

where $b_i \in \mathcal{B}_{2j-1}$ and $b_i' \in \mathcal{B}_{2j-1}$. Therefore, with a slight abuse of notation, we can translate the isotypic decomposition of $V \otimes \mathbb{C}$ above to a decomposition into real irreducible G representations via

$$V = (V_1 + V_2) \oplus \frac{1}{i} \Big(V_1 - V_2 \Big) \oplus \cdots \oplus (V_{2l-1} + V_{2l}) \oplus \frac{1}{i} \Big(V_{2l-1} - V_{2l} \Big) \oplus V_{2l+1} \oplus \cdots \oplus V_h.$$

Note that in the case of a real irreducible representation W, also the structure of the corresponding endomorphism algebras differs from the complex case, depending on which of the three cases we are in. Indeed, in the case of non-algebraically closed fields, the second statement in Schur's Lemma 3 only yields that $\operatorname{End}(W)$ is isomorphic to a skew field. There are exactly three skew fields over $\mathbb R$, namely $\mathbb R$ itself, $\mathbb C$, and the Quaternions $\mathbb H$, and these three cases exactly correspond to the types discussed above. Therefore, in the case of a real irreducible representation, we get that the endomorphism algebra is isomorphic to $\mathbb R$ if it is of (type I), it is isomorphic to $\mathbb C$ if we are of (type II) and it is isomorphic to $\mathbb H$ in the case of (type III).

Real symmetry adapted basis for circulant matrices

We consider again the cyclic group C_4 acting linearly on \mathbb{R}^4 by cyclically permuting coordinates. This representation is isomorphic to the regular representation, and we know a complex symmetry-adapted basis. If we denote by $b^{(1)}, \ldots, b^{(4)}$ the basis elements of the symmetry-adapted basis given above, then the 4 real vectors

$$\mathcal{B} := \left\{ b^{(1)}, b^{(3)}, b^{(2)} + b^{(4)}, \frac{1}{i} (b^{(2)} - b^{(4)}) \right\}$$

yield a decomposition into real irreducible representations. The matrix T considered in the example above is then of the form

$$T_{\mathcal{B}} = \begin{pmatrix} \alpha + \beta + \gamma + \delta & 0 & 0 & 0 \\ 0 & \alpha - \beta + \gamma - \delta & 0 & 0 \\ 0 & 0 & \delta - \beta - \alpha + \gamma \\ 0 & 0 & \alpha - \gamma & \delta - \beta \end{pmatrix}.$$

We thus see that the two non-real irreducible representations of C_4 give one real irreducible representation. We are in (type II) as these two complex irreducible representations are not isomorphic and therefore the corresponding endomorphism algebra decomposes into the blocks as above. Note that in the case of a *symmetric circulant matrix* we would have obtained the same diagonal form as in the complex case.

3.2 Representation theory of \mathfrak{S}_n

The representation theory of the symmetric group, which is of particular importance due to its historical significance and connections to combinatorics, is outlined here for future reference. It is known that the conjugacy classes of the symmetric group \mathfrak{S}_n correspond one-to-one with partitions of n, which are non-decreasing sequences of positive integers that sum to n. A Young diagram, corresponding to a partition $\lambda = (\lambda_1, \dots, \lambda_k) \vdash n$, is a collection of cells arranged in left-aligned rows, with λ_1 cells in the top row, λ_2 cells in the row below, and so on.

Example of a Young diagram

Consider the partition $(4,3,1) \vdash 8$. To this partition we associate the following Young diagram:



A *Young tableau* of shape λ is obtained by filling the cells of the Young diagram of λ with the integers 1 to n. Two tableaux are considered equivalent if their corresponding rows contain the same integers. Given a tableau T, its row-equivalent class $\{T\}$ can be visualized by removing the vertical lines separating the boxes in each row. Such a row equivalence class is also called a tabloid. We call the formal \mathbb{K} -vector space \mathcal{M}^{λ} which is spanned by all λ -tabloids the *partition module* associated to λ .

Example of equivalent Young tableaux

Continuing with the above example and the partition (4,3,1) + 8 we have, for example, the following two equivalent tableaux

$$T_1 = \frac{1573}{624}$$
 and $T_2 = \frac{7531}{246}$.

We can represent the row equivalence class to which these two tableaux belong by

$$\{T_1\} = \{T_2\} = \frac{\boxed{3 \ 1 \ 7 \ 5}}{\boxed{4 \ 6 \ 2}}.$$

Combinatorics reveals further that the associated permutation module $\mathcal{M}^{(4,3,1)}$ is spanned by the $\frac{8!}{4!\cdot 3!} = 280$ different tabloids.

Given a tableau T, we denote its columns by C_1, \dots, C_c and consider the column stabilizer subgroup $CStab_T \subset \mathfrak{S}_n$ defined by

$$CStab_T = \mathfrak{S}_{C_1} \times \mathfrak{S}_{C_2} \times \cdots \times \mathfrak{S}_{C_c}.$$

This setup of notations allows to define the following class of \mathfrak{S}_n representations, which turn out to give a complete list of irreducible representations in the case $\operatorname{char}(\mathbb{K}) = 0$.

Definition 5 Let $\lambda \vdash n$ be a partition. For a Young tableau T of shape λ we define

$$E_T := \sum_{\sigma \in \text{CStab}_T} \text{sgn}(\sigma) \{ \sigma T \}.$$

Then, the Specht module $W^{\lambda} \subseteq \mathcal{M}^{\lambda}$ associated to λ is the \mathbb{K} -vector space spanned by the E_T corresponding to all Young tableaux of shape λ .

A tableau is standard if every row and every column is filled in increasing order and it can be shown that the set of Young tabloids corresponding to standard Young tableaux is a minimal generating set of a Specht module. More importantly we have the following theorem:

Theorem 6 If $char(\mathbb{K}) = 0$ then the set $\{W^{\lambda}, \lambda \vdash n\}$ is the set of non-isomorphic irreducible representations of \mathfrak{S}_n .

The Specht modules of \mathfrak{S}_3

The Specht modules, and hence the irreducible representations of \mathfrak{S}_3 , are the following three.

$$W^{(3)} = \langle \frac{\overline{1} \ 2 \ 3}{\rangle},$$

$$W^{(2,1)} = \langle \frac{\overline{1} \ 2}{3} - \frac{\overline{3} \ 2}{1}, \frac{\overline{1} \ 3}{2} - \frac{\overline{2} \ 3}{1} \rangle,$$

$$W^{(1,1,1)} = \langle \frac{\overline{1}}{2} - \frac{\overline{2}}{1} - \frac{\overline{3}}{2} - \frac{\overline{1}}{3} + \frac{\overline{3}}{2} + \frac{\overline{3}}{1} \rangle.$$

We further give the associated characters. These are constant on the 3 conjugacy classes of \mathfrak{S}_3 , namely $C_1 = \{\text{Id}\}, C_2 = \{(12), (13), (23)\}$ and $C_3 = \{(123), (132)\}$.

$$\begin{array}{c|cccc} & C_1 & C_2 & C_3 \\ \hline \chi_{(3)} & 1 & 1 & 1 \\ \chi_{(2,1)} & 2 & 0 & -1 \\ \chi_{(1,1,1)} & 1 & -1 & 1 \\ \end{array}$$

This understanding of the irreducible representations allows us to examine the following example.

Diagonalization of a S₃-invariant Gram matrix

We consider the permutation action of the group \mathfrak{S}_3 on \mathbb{R}^3 and construct a Gram Matrix of the invariant scalar product. Since it is supposed to be \mathfrak{S}_3 -invariant, we find

$$\langle e_j, e_j \rangle_{\mathfrak{S}_3} = \alpha$$
 for $j = 1..3$, and $\langle e_i, e_j \rangle_{\mathfrak{S}_3} = \beta$ for $j \neq i$.

The associated Gram matrix is therefore of the form

$$\begin{pmatrix} \alpha & \beta & \beta \\ \beta & \alpha & \beta \\ \beta & \beta & \alpha \end{pmatrix}.$$

We further have seen that this representation decomposes into two irreducible ones, one of them being the trivial one, the other one being $W^{(2,1)}$. Thus, we find that, in this situation, the vectors $\{e_1 + e_2 + e_3, e_1 - e_2, e_1 - e_3\}$ form a symmetry adapted basis. Indeed, with respect to this basis, the Gram matrix is of the form

$$\begin{pmatrix} a+2 & 0 & 0 \\ 0 & a-b & 0 \\ 0 & 0 & a-b \end{pmatrix}.$$

3.3 Using representation theory to simplify semidefinite formulations

We have seen that Schur's Lemma allows for a block-diagonalization for matrices which commute with a given group action. Now assume that (\mathbb{R}^n, ρ) is an n-dimensional representation of a finite group G. As we can always choose an orthonormal basis for \mathbb{R}^n with respect to a G-invariant scalar product, we can assume without loss of generality that the corresponding matrices are unitary, i.e we have $M(g)M(g)^T = \operatorname{Id}$ for all $g \in G$. Now this representation naturally carries over to a representation on $\operatorname{Sym}_n(\mathbb{R})$ via

$$X^g := M(g)XM(g)^T$$
, for $X \in \text{Sym}_n(\mathbb{R})$ and $g \in G$.

A set $\mathcal{L} \subseteq \operatorname{Sym}_n(\mathbb{K})$ is called *invariant with respect to G* if for all $X \in \mathcal{L}$ we have $X^g \in \mathcal{L}$, for all $g \in G$. A linear functional $\langle C, X \rangle$ is *G-invariant*, if $\langle X^g, C \rangle = \langle X, C \rangle$ for all $g \in G$ and an SDP is *G-invariant* if both the cost function $\langle X, C \rangle$ as well as the feasible set \mathcal{L} are *G*-invariant.

Definition 6 For a given SDP we consider

$$y_G^* := \inf \langle X, C \rangle$$

s.t. $\langle X, A_i \rangle = b_i$, $1 \le i \le m$,
 $X = X^g$ for all $g \in G$,
 $X \ge 0$, where $X \in \text{Sym}_n(\mathbb{R})$.

Clearly, $y^* \leq y_G^*$. Even more, we have the following.

Theorem 7 If the original SDP is G-invariant then we have $y_G^* = y^*$.

Proof For every feasible X and $g \in G$ the matrix X^g is feasible. We have $\langle X, C \rangle = \langle X^g, C \rangle$ for every $g \in G$. Since the feasible region is convex we have

$$X_G := \frac{1}{|G|} \sum_{g \in G} X^g$$

is feasible with $\langle X, C \rangle = \langle X_G, C \rangle$ and $X_G^g = X_G$ for all $g \in G$. Thus $y_G^* = y^*$.

Notice that the additional condition we impose in the above formulation, namely that $X = X^g$ for all $g \in G$ clearly reduces the dimension of the space of possible solutions and therefore the number of free variables in the formulation. This first step of a *reduction to orbits* therefore reduces the intrinsic dimension of the problem. But in order to further simplify the formulation we also notice that Theorem 7 allows us to restrict to invariant matrices (i.e., the commutant of the associated matrix representation). By Schur's Lemma we know that we can find a basis that *block-diagonalises* the matrices in this space. Let

$$\operatorname{Sym}_{n}(\mathbb{R}) = H_{1,1} \perp H_{1,2} \perp H_{1,m_{i}} \perp H_{2,1} \perp \cdots \perp H_{k,m_{k}}$$

be an orthogonal decomposition into irreducibles, and pick an orthonormal basis $e_{l,1,u}$ for each $H_{l,1}$. Choose $\phi_{l,i}: H_{l,1} \to H_{l,i}$ to obtain orthogonal bases

$$e_{l,u,v} = \phi_{l,i}(e_{l,1,v})$$

for each $H_{l,u}$. This then gives us an *orthonormal symmetry adapted basis*. Now, for ever irreducible representation and every $(i, j) \in \{1, ..., n\}^2$ we can define *zonal matrices* $E_l(i, j)$ with coefficients

$$(E_l(i,j))_{u,v} := \sum_{h=1}^{d_l} e_{l,u,h}(i) \cdot \overline{e_{l,v,h}^k(j)}.$$

These characterise invariant $X \in \operatorname{Sym}_n(\mathbb{R})$ via $X_{i,j} = \sum_{l=1}^k \langle E_l(i,j), M_l \rangle$, for some $M_l \in \operatorname{Sym}_{m_l}(\mathbb{R})$, $1 \le l \le k$. Summing up we have provided:

Theorem 8 A G-invariant SDP is equivalent to the following reduced SDP:

$$\begin{split} \inf \langle C, X \rangle \\ s.t. \quad & \langle A_{i,j}, X \rangle = b_i \,, \quad 1 \leq j, \leq m \,, 1 \leq i \leq k \,, \\ & X_{i,j} = \sum_{l=1}^k \langle E_l(i,j), M_l \rangle \,, \\ & M_l \geq 0, \; where \; M_l \in \operatorname{Sym}_{m_l}(\mathbb{R}), 1 \leq l \leq k \,. \end{split}$$

Some remarks

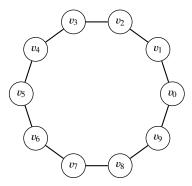
The main work that has to be done to obtain this nice form (i.e., the actual calculation of the zonal matrices) is far from trivial. However the possible reductions can make

a difference that enables one to actually compute a given SDP which otherwise might be too big to be handled by a SDP-solver. Furthermore, in the context of semidefinite programming the issue with real irreducible representations versus complex irreducible representations can be easily avoided by replacing symmetric matrices with hermitian matrices. This is why the definition of the zonal matrices was given with the complex conjugate, which is necessary only in the case of a complex symmetry adapted basis.

We want to highlight this potential reduction of complexity by studying the example of the ϑ -number introduced in Definition 3 for graphs with symmetry.

Symmetry reduction for the ϑ -number of a cyclic graph C_n

Consider a cyclic graph C_n shown in the picture below for n = 10.



The ϑ -number in this case is given by

$$\vartheta(C_n) = \sup \left\{ \sum_{i,j} B_{i,j} : B \in \operatorname{Sym}_n(\mathbb{R}), \ B \ge 0 \right.$$

$$\sum_{i=1}^n B_{i,i} = 1,$$

$$B_{i,j} = 0 \quad j \equiv i+1 \pmod{n} \right\}.$$
(8)

We see that this SDP is invariant under the natural action of the cyclic group $\mathbb{Z}/n\mathbb{Z}$. We get a symmetry adapted basis for the (complexification) of this representation through the Fourier basis, and a corresponding real decomposition. Then one obtains the following equivalent formulation for the SDP (8)

$$\vartheta(C_n) = \sup \left\{ n \cdot x_0 : (x_0, \dots, x_{\lfloor \frac{n}{2} \rfloor}) \in \mathbb{R}_{\geq 0} \right.$$

$$\sum_{\substack{j=0 \\ \lfloor \frac{n}{2} \rfloor \\ j=0}} x_j = 1,$$

$$\sum_{j=0}^{\lfloor \frac{n}{2} \rfloor} x_j \cdot \cos(\frac{2j\pi}{n}) = 0 \right\}$$
(9)

Through this formulation of the ϑ -number as a linear program, it is possible to calculate the ϑ -number directly. Indeed, we can deduce [46, Corollary 5]

$$\vartheta(C_k) = \begin{cases} \frac{n\cos(\pi/k)}{1+\cos(\pi/k)} & \text{for odd } k, \\ \frac{k}{2} & \text{for even } k. \end{cases}$$

Recall that our main objective is polynomial optimization. We now turn our attention to specific SDPs stemming from sums of squares approximations. Note that in this situation the action of a group G on \mathbb{R}^n also induces an action on the \mathbb{R} -vector space $\mathbb{R}[X]$, as we have seen before and a matrix representation M(G) for the space of polynomials of degree at most d. Thus, if $p^g = p$ for all $g \in G$ we can define

$$Q^G := \frac{1}{|G|} \sum_{g \in G} M(g)^T Q M(g),$$

and will have

$$p = (Y)^T Q^G Y$$

with the property that now Q^G commutes with the matrix representation M(G). Therefore the above methods for general SDPs can be used again to block-diagonalize the matrix Q^G and thus simplify the calculations. This was first explored in detail by Gatermann and Parillo [26] and several other authors [16, 62, 21]. We want to highlight this in the following example.

Symmetry reduction of the SOS decomposition of a symmetric quadratic

Consider the homogeneous polynomial

$$p = a \cdot \sum_{i=1}^{n} X_i^2 + b \cdot \sum_{i < j} X_i X_j.$$

We want to examine the conditions on a and b such that p is a sum of squares. Since p is homogeneous and of degree 2, a sum of squares decomposition will involve only squares of homogeneous polynomials of degree 1. In other words, by Proposition 1 we consider the vector $Y = (X_1, \ldots, X_n)$ comprised of all monomials of degree 1 and have that the polynomial p is a sum of squares if and only if we can find a positive semidefinite matrix Q of size $n \times n$ such that

$$p = Y^T Q Y$$
.

Now, by construction, p remains invariant by the permutation action of \mathfrak{S}_n on the monomials X_1, \ldots, X_n . This action is represented by the *permutation matrices*, and we can therefore assume that Q commutes with every permutation matrix. As we have seen above, this representation decomposes into two non-isomorphic irreducible

representations, one isomorphic to the trivial representation and the other one to the Specht module $W^{(n-1,1)}$. Therefore, in a symmetry adapted basis, we may assume that the matrix Q is of the from

$$Q = \begin{pmatrix} \alpha & 0 & 0 & \dots & 0 \\ 0 & \beta & 0 & \dots & 0 \\ \vdots & \ddots & & & \\ 0 & 0 & \dots & \beta \end{pmatrix}.$$

Doing the calculations we obtain that a sums of squares decomposition of p is of the form

$$p = \alpha (X_1 + X_2 + \ldots + X_n)^2 + \beta \sum_{i < j} (X_i - X_j)^2 = (\alpha + (n-1)\beta) \sum_{i = 1}^n X_i^2 + 2(\alpha - \beta) \sum_{i < j} X_i X_j,$$

with $\alpha, \beta \geq 0$.

In the above example we have seen that the sum of squares decomposition essentially consisted of two type of summands. Firstly the square of the invariant polynomial $X_1 + X_2, + \ldots + X_n$ and summands which are squares of elements in the \mathfrak{S}_n -orbit of $X_1 - X_2$. This observation can be made more precise with the following setup: if we want to decide for a given polynomial f of degree 2d which is invariant by a group G if it is a sum of squares we consider the vector space $\mathbb{R}[X]_{\leq d}$ of polynomials of degree at most d, which is finite dimensional. Then the linear action of a group G on \mathbb{R}^n also induces a linear action on $\mathbb{R}[X]_{\leq d}$ and we can consider the isotypic decomposition

$$\mathbb{R}[X]_{\leq d} = \bigoplus_{i \in I} V_i = \bigoplus_{i \in I} \bigoplus_{j=1}^{\eta_i} W_{i,j}$$
 (10)

where the W_i are again the non-isomorphic irreducible representations of G, and any $W_{i,j}$ is an irreducible representation isomorphic to W_i . For the discussion we now assume for simplicity that every irreducible component W_i of this decomposition is real irreducible. In this case we can construct a set of real polynomials

$$\{f_{11}, f_{12}, \dots, f_{l\eta_l}\} \subset \mathbb{R}[X]_{\leq d}$$

with the following two properties:

1. The polynomial f_{i1} cyclically generates W_{i1} i.e., for every fixed i the G-span

$$\langle f_{i1} \rangle_G = W_{i,1}.$$

2. The polynomial $f_{ij} \in W_{i,j}$ is the image of f_{i1} under the (up to scalar multiplication) unique G-isomorphism between $W_{i,1}$ to $W_{i,j}$. This in particular implies that f_{ij} generates cyclically $W_{i,j}$.

We denote by $(\langle f_{i1}, \ldots, f_{i\eta_i} \rangle_{\mathbb{R}}^2)$ a sum of squares of elements in the vector space spanned by the polynomials $f_{i1}, \ldots, f_{i\eta_i}$. With this notation, and integrating the described construction with the consequences of Schur's Lemma (Theorem 3), one arrives at the following which agrees with the observation from the example above (see also [13, 16, 26, 62, 19] for more details on the following statement).

Theorem 9 With the notation defined above any G-invariant polynomial p of degree 2d that is a sum of squares can be written in the from

$$p = \sum_{i \in I} \sum_{j=1}^{\eta_i} \sum_{g \in G} p_{ij}^g$$

where every $p_{ij} \in (\langle f_{i1}, \ldots, f_{in_i} \rangle_{\mathbb{D}}^2)$.

Proof Let p be a sum of squares. Then there is symmetric positive semidefinite bilinear from

$$B: \mathbb{R}[X]_{\leq d} \times \mathbb{R}[X]_{\leq d} \to \mathbb{R}$$

which is a Gram matrix for p, i.e. for every $x \in \mathbb{R}^n$ we can write

$$p(x) = B(Y^d, Y^d),$$

where Y^d stands for the vector of monomials up to degree d. Since p is G-invariant, by linearity, we may assume that B is a G-invariant bilinear form. We get from Corollary 3 that $B^{ij}(v,w) = 0$ for all $v \in V_i$ and $w \in V_j$, i.e., the isotypic components appearing in (10) are orthogonal with respect to B and hence it suffices to look at

$$B^{jj}: V_i \times V_i \to \mathbb{R}$$

individually. If $B^{jj} = 0$, there is nothing to prove. Otherwise, consider the decomposition

$$V_j := \bigoplus_{k=1}^{\eta_j} W_{j,k},$$

where with the notation above each $W_{j,k}$ is generated by the orbit of a polynomial $f_{j,k}$. We can freely identify V_j with its complexification $V_j^{\mathbb{C}}$ since by assumption all irreducible representations are irreducible over \mathbb{C} . Furthermore, since B is positive semidefinite and f_{j1} cylically generates W_{j1} , we may assume that $B(f_{j1}, f_{j1}) > 0$. We extend f_{j1} to a basis

$$f_{i1} = f_{i11}, f_{i12}, \cdots, f_{i1d}$$

of $W_{j,1}$, and denote by $f_{ji1}, f_{ji2}, \dots, f_{jid}$ the image of this basis under the unique G-isomorphism sending f_{j1} to f_{ji} . Consider the vector space U generated by

 $f_{j1}, \dots, f_{j\eta_j}$. Since the restriction $B|_{U\times U}$ is a positive semi-definite bilinear form, we obtain

$$\sum_{a=1}^{\eta_j} \sum_{b=1}^{\eta_j} B(f_{ja}, f_{jb}) f_{ja} f_{jb} = \sum_{t=1}^{z} g_t^2$$

for some $g_t \in \langle f_{j1}, \dots, f_{j\eta_j} \rangle_{\mathbb{R}}$. Now, clearly there exists a symmetric, G-invariant, bilinear form $C: V_j \times V_j \to \mathbb{R}$ for which we have

$$\mathcal{R}_G(\sum_{t=1}^z g_t^2) = C(Z, Z),$$

where

$$Z = (f_{j11}, \dots, f_{j1d}, f_{j21}, \dots, f_{jn_i1}, \dots, f_{jn_id}).$$

To conclude we need to see that the form C is essentially B^{jj} , i.e., that it is obtained from B^{jj} by multiplication with a positive scalar. This can be done by direct calculations using the fact that each f^g_{jab} for $g \in G$ can be expressed in the basis of $W_{j,a}$ defined above. It then follows that there exists a $\lambda_{jbb'}$, independent on a, a' such that

$$C(f_{jab}, f_{ja'b'}) = \lambda_{jbb'}C(f_{jab}, f_{ja'b'}).$$

Since B and C can be seen as elements of $\operatorname{Hom}_G(W_{j1}, W_{j1}^*)$, applying Schur's lemma one can prove that $\lambda_{jbb'}$ is actually independent of b, b', that is $C = \lambda B^{jj}$ for some constant $\lambda \in \mathbb{R}_+^*$.

In analogy to the zonal matrices defined before, we can also reformulate Theorem 9 in terms of matrix polynomials, i.e., matrices with polynomial entries. To do this we define a block-diagonal symmetric matrix B with j blocks $B^{(1)}, \ldots, B^{(j)}$ with the entries of each block given by:

$$B^{(j)} = \left(\sum_{g \in G} (f_{ju}^g \cdot f_{jv}^g)\right)_{u,v}.$$
 (11)

With these notations Theorem 9 can be stated in the following equivalent form.

Corollary 4 Let $g \in \mathbb{R}[X]_{\leq 2d}^G$. Then g is a sum of squares if and only if

$$g = \langle A_1 \cdot B^{(1)} \rangle + \ldots + \langle A_l \cdot B^{(l)} \rangle,$$

for some symmetric and positive semidefinite matrices $A_i \in \operatorname{Mat}_{\eta_i \times \eta_i}(\mathbb{R})$.

Remark 2 The restriction to type I real irreducible representations in the description above is mainly due to convenience of the presentation. Using the discussion in in Section 3 on real irreducible representations it is possible to generalize to type II and to adapt to type III representations.

These first examples give a hint on the power of symmetry reduction to simplify optimization problems affording some symmetries. This approach has been used

quite successfully in a wide range of applications and settings. In the next section, we focus on the case of sums of squares and explore how the additional algebraic structure of polynomials can be combined with the above approach to get a better understanding of invariant sums of squares.

4 Invariant theory

Polynomial functions that remain unchanged under the action of a symmetry transformation naturally appeared in the previous section. Such functions are called *polynomial invariants*, and they play a crucial role in *invariant theory*, a branch of algebra that studies symmetry in algebraic structures, such as groups, rings, and fields. The structural insights into the set of invariant polynomials can give important additional comprehension and different ways of simplifications for polynomial optimization, as we will outline in this section. In order to do this, we give first an overview of the basic concepts and important results in invariant theory which will prove useful in order to take advantage of symmetries in polynomial optimization problems. For details and further insights we refer the reader to [71, 20, 9, 67, 37].

4.1 Basics of invariant theory

We begin with examining the situation of a linear action of a group on the ring of polynomials more closely. As was introduced before, given a finite group G and a representation $\rho: G \longrightarrow \mathbb{K}^n$ we can define a linear action f^g on the polynomial functions on V, denoted $\mathbb{K}[V]$ via $f^g := f \circ \rho(g^{-1})$. Choosing a basis of V we can identify $\mathbb{K}[V]$ with $\mathbb{K}[X_1, \ldots, X_n]$ and consider the associated isotypic decomposition of the G module:

$$\mathbb{K}[X_1,\ldots,X_n] = \bigoplus_{i\in I} \mathbb{K}[X_1,\ldots,X_n]^{\chi_i},\tag{12}$$

where as before I is the set of isomorphism classes of irreducible representations and χ_i for $i \in I$ is a list of irreducible characters. In addition to being a \mathbb{K} -vector space with group action, $\mathbb{K}[X_1, \ldots, X_n]$ is in fact an algebra and this additional algebraic structure also allows for a finer analysis of the group action. If χ corresponds to the trivial character the polynomials in $\mathbb{K}[X_1, \ldots, X_n]^{\chi}$ will not be affected by the action of G. Polynomials with this property, i.e, elements

$$f \in \mathbb{K}[X_1, \dots, X_n]$$
 such that $f^g = f$ for all $g \in G$

are called *invariant polynomials*. Since the property of being invariant is not affected by addition or multiplication with other invariant polynomials the set of invariant

polynomials forms a sub-algebra denoted by $\mathbb{K}[X]^G$. The polynomials belonging to the other isotypic components are sometimes also called semi-invariants.

The Motzkin polynomial as an example for a symmetric polynomial

We consider the group \mathfrak{S}_2 acting linearly on \mathbb{C}^2 by permuting coordinates. Then, the Motzkin polynomial

$$M := X_1^4 X_2^2 + X_1^2 X_2^4 - 3X_1^2 X_2^2 + 1$$

is invariant with respect to this action. In the case of \mathfrak{S}_n invariant polynomials we also speak of symmetric polynomials.

A very useful tool to work with polynomials in invariant setting is the so-called Reynolds operator defined as follows.

Definition 7 For a finite group G the map

$$\mathcal{R}_G(f) := \frac{1}{|G|} \sum_{g \in G} f^g$$

is called the *Reynolds operator* of *G*.

The Reynolds operator of a finite group G has the following properties:

- 1. \mathcal{R}_G is a $\mathbb{K}[X]^G$ linear map.
- 2. For $f \in \mathbb{K}[X]$ we have $\mathcal{R}_G(f) \in \mathbb{K}[X]^G$. 3. \mathcal{R}_G is the identity map on $\mathbb{K}[X]^G$, i.e $\mathcal{R}_G(f) = f$ for all $f \in K[X]^G$.

Remark 3 Whereas we introduced the Reynolds operator for finite groups, it can be more generally defined for compact and reductive groups and most of the results we state for finite groups mostly can be adapted for this more general case. We refer the reader to [71, 20] for more details and algorithmic questions.

As seen above, $\mathbb{K}[X]^G$ is a subalgebra of $\mathbb{K}[X]$. In the second half of the 19th century, invariant theory was very much concerned with the following question: is this subalgebra generated by finitely many elements? The following Theorem, proven by Hilbert in 1890, initiated modern invariant theory.

Theorem 10 (Hilbert) Let G be a finite group. Then the invariant subalgebra $\mathbb{K}[X]^G$ is generated by finitely many homogeneous invariants, i.e., there is a finite set of invariant homogeneous polynomials π_1, \ldots, π_m such that every invariant polynomial $f \in \mathbb{K}[X]^G$ can be written as a polynomial in π_1, \ldots, π_m .

Remark 4 Hilbert himself asked in his 14th problem whether the above Theorem holds generally for all groups. Indeed, it holds for a large class of infinite groups. However, with a concrete counter example, Nagata [51] could prove in 1959 that not all invariant algebras are finitely generated.

In the case of the symmetric group \mathfrak{S}_n the following families of generators are well known and used in many different parts of algebra and combinatorics.

Definition 8 For $n \in \mathbb{N}$, consider the following two families of symmetric polynomials

- 1. For $0 \le k \le n$ let $p_k := \sum_{i=1}^k x_i^k$ denote the k-th power sum polynomial,
- 2. For $0 \le k \le n$ let $e_k := \sum_{1 \le i_1 < i_2 < \dots < i_k \le n} x_{i_1} x_{i_2} \cdots x_{i_k}$ denote the k-th elementary symmetric polynomial.

Theorem 11 The two families $\{p_1, \ldots, p_n\}$ and $\{e_1, \ldots, e_n\}$ both are algebraically independent generating sets for the algebra of \mathfrak{S}_n -invariant polynomials, namely

$$\mathbb{C}[X_1,\ldots,X_n]^{\mathfrak{S}_n}=\mathbb{C}[e_1,\ldots,e_n]=\mathbb{C}[p_1,\ldots,p_n].$$

The Motzkin polynomial expressed in elementary symmetric polynomials

Consider the action of \mathfrak{S}_2 on \mathbb{C}^2 . Then, every symmetric polynomial can be uniquely written as a polynomial in $e_1 := X_1 + X_2$, and $e_2 := X_1 X_2$, and the Motzkin polynomial M from the example above can be expressed as

$$M = e_1^2 e_2^2 - 2e_2^3 - 3e_2^2 + 1.$$

Remark 5 Since both the power sum polynomials and the elementary symmetric polynomials generate the ring of symmetric polynomials, each of two families of symmetric polynomials can be expressed by the other. The expression can be deduced from the so-called Newton identities (see e.g.[47]):

$$k(-1)^k e_k(x) + \sum_{i=1}^k (-1)^{i+k} p_i(x) e_{k-i}(x) = 0.$$
 (13)

In contrast to the above example of the symmetric polynomials, for general groups we might need more than n generators. We can, however, give a bound for the number of generators needed.

Theorem 12 (Noether's bound) Let G be a finite group acting linearly on \mathbb{K}^n . Then $\mathbb{K}[X]^G$ is generated as an algebra over \mathbb{K} by not more than $\binom{n+|G|}{n}$ many homogeneous invariants of degree not exceeding |G|.

So, in particular, it is not guaranteed that a set of algebraically independent generators exists. However, more generally, it can be shown that the invariant ring is Cohen-Macaulay and that a Hironaka decomposition exists, i.e., that we can find n algebraically independent polynomials $\theta_1, \ldots, \theta_n$ and polynomials η_1, \ldots, η_k such that

$$\mathbb{K}[X]^G = \bigoplus_{i=1}^k \eta_i \mathbb{K}[\theta_1, \dots, \theta_n].$$

The algebraic invariant polynomials $\theta_1, \ldots, \theta_n$ are called *primary invariants*, and the η_1, \ldots, η_k are called *secondary invariants*. With these families of polynomials, every invariant polynomial can be uniquely written in such a way that the secondary invariants appear only linearly.

Invariant polynomials for the alternating group

Consider the group \mathfrak{A}_3 which is the subgroup of \mathfrak{S}_3 of even permutations and define $\Delta = (X_1 - X_2)(X_1 - X_3)(X_2 - X_3)$ Then for every \mathfrak{A}_3 invariant polynomial f there exist two unique symmetric polynomials $g_0(p_1, p_2, p_3)$ and $g_1(p_1, p_2, p_3)$ such that

$$f(X_1, X_2, X_3) = g_0(p_1, p_2, p_3) + g_1(p_1, p_2, p_3) \cdot \Delta.$$

In other words, the p_1, p_2, p_3 (or any other generating set for the \mathfrak{S}_3 -invariant polynomials) can be used as primary invariants and Δ serves as the secondary invariant.

As we have seen now, the trivial component of the isotypic decomposition (10) enjoys the property of being a finitely generated \mathbb{K} -algebra. We now turn to the other isotypic components. Let χ be any character of G and $f \in \mathbb{K}[X]^G$ be an invariant polynomial. Then clearly the application

$$\begin{array}{ccc} \cdot f : \ \mathbb{K}[X]^{\chi} & \longrightarrow & \mathbb{K}[X]^{\chi} \\ q & \longmapsto & q \cdot f \end{array}$$

which corresponds to multiplication by f is a G-homomorphism. So $\mathbb{K}[X]^X$ has in turn the structure of a $\mathbb{K}[X]^G$ -module. We have in fact the following.

Theorem 13 Let χ be an irreducible character of a finite group G. Then $\mathbb{K}[X]^{\chi}$ is a is a finitely generated (even Cohen-Macaulay) $\mathbb{K}[X]^G$ -module and $\mathbb{K}[X]^{\chi}$ is generated by homogeneous elements of degree not exceeding |G|. In particular, also $\mathbb{K}[X]$ is a finitely generated $\mathbb{K}[X]^G$ (Cohen-Macaulay) module.

Decomposition of polynomials in two variables

We consider the case of polynomials in two variables $\mathbb{K}[X_1, X_2]$ and their relation to \mathfrak{S}_2 symmetric polynomials. Here we have that $\mathbb{K}[X_1, X_2]$ is generated as an $\mathbb{K}[X_1, X_2]^{\mathfrak{S}_2}$ -module by 1 and $X_1 - X_2$, i.e., every polynomial f can be written as

$$f = g_0 + g_1 \cdot (X_1 - X_2),$$

where $g_1, g_2 \in \mathbb{K}[X_1, X_2]^{\mathfrak{S}_2}$. Moreover, in this case the representation is in fact unique.

Definition 9 A *reflection* is a mapping from a Euclidean space to itself that is an isometry whose set of fixed points is a hyperplane. If V is an Euclidean vector space we can view a reflection as an element in O(V) that has exactly one eigenvalue different from 1, i.e., one other eigenvalue that is -1. If (V, ρ) is a representation of G, then $g \in G$ is a reflection if the mapping $v \mapsto \rho(g)v$ is a reflection and we say that G is a *reflection group* if it is generated by reflections.

It is very important to remember that the property of being a reflection group is not a property of the group itself, but it is crucially linked to the representation. This can be seen in the following example.

Two different representations of \mathfrak{S}_n

We consider the symmetric group \mathfrak{S}_n . This group is generated by the transpositions $\tau_i = (i, i+1)$ for $i \in \{1, \dots, n-1\}$.

- 1. Consider the defining representation of \mathfrak{S}_n given by permuting the coordinates in \mathbb{R}^n . In this representation, elements in O(V) corresponding to transpositions have the eigenvectors e_j for $j \neq i, i+1$ with eigenvalue 1, as well as $e_i + e_{i+1}$ with eigenvalue 1 and $e_i e_{i+1}$ with eigenvalue -1. Therefore these elements are reflections, which geometrically correspond to the reflection through the hyperplane of equation $x_i x_{i+1} = 0$ in V. With this representation \mathfrak{S}_n is acting as a reflection group.
- 2. Now, let n = 2 and consider the representation on

$$V = \mathbb{R} \cdot e_1 \oplus \mathbb{R} \cdot e_2 \oplus \mathbb{R} \cdot e_3 \text{ given by}$$

$$(1,2) \cdot e_1 = e_2, (1,2) \cdot e_2 = e_1 \text{ and } (1,2) \cdot e_3 = -e_3.$$

Then, the image of the transposition (1,2) has eigenvalues 1,-1,-1 and thus is not a reflection. Therefore, \mathfrak{S}_2 is not a reflection group if acting in this way.

The following theorem is due to Shephard, Todd, Chevalley and motivates the study of reflection groups.

Theorem 14 (Shephard, Todd, Chevalley) *Let G be a group with a finite dimensional representation V. Then the following properties are equivalent:*

- 1. G is a reflection group;
- 2. the corresponding invariant ring $\mathbb{K}[V]^G$ is a polynomial algebra;
- 3. the polynomial ring $\mathbb{K}[V]$ is a free $\mathbb{K}[V]^G$ module.

In the case of a finite reflection group G the collection π_1, \ldots, π_n which generate the invariant ring are called *basic invariants*. These basic invariants are not unique, but their sequence of degrees $d_i(G) := \deg \pi_i$ is unique. The following example highlights the equivalence of the statements in Theorem 14.

Invariants of a different \mathfrak{S}_2 action

We consider the group \mathfrak{S}_2 with the action on \mathbb{K}^3 above such that \mathfrak{S}_2 is not acting as a reflection group. Then,

$$\mathbb{K}[x_1, x_2, x_3]^G = \mathbb{K}[\tau_1, \tau_2, \tau_3, \tau_4]$$

with $\tau_1 = x_1 + x_2$, $\tau_2 = x_1x_2$, $\tau_3 = x_3^2$ and $\tau_4 = x_3(x_1 - x_2)$. Clearly, these three polynomials cannot be algebraically independent and indeed, there is an algebraic dependency between the τ_i 's, namely

$$\tau_1^2 \tau_3 - 4\tau_2 \tau_3 - \tau_4^2 = 0.$$

Similarly one can find that $\mathbb{K}[x_1, x_2, x_3]$ is not a free $\mathbb{K}[\tau_1, \tau_2, \tau_3, \tau_4]$ -module.

Definition 10 Let G be a finite reflection group. Then, the quotient \mathbb{K} -algebra of the polynomial ring modulo the ideal generated by the non-constant elements of the invariant ring is called the covariant algebra of G and denoted by $\mathbb{K}[X_1,\ldots,X_n]_G$. If π_1,\ldots,π_n are a minimal set of algebraically independent generators of the invariant ring, we have

$$\mathbb{K}[X_1,\ldots,X_n]_G := \mathbb{K}[X_1,\ldots,X_n]/(\pi_1,\ldots,\pi_n)_{\mathbb{K}[X_1,\ldots,X_n]}$$

The covariant algebra of G has the structure of a G-module and we find in fact the following.

Theorem 15 Let G be a real reflection group acting linearly on \mathbb{R}^n . Then the covariant algebra $\mathbb{R}[X_1, \dots, X_n]_G$ is as G-module isomorphic to the regular representation $\mathbb{R}[G]$ and

$$\mathbb{R}[X_1,\ldots,X_n] \cong \mathbb{R}[X_1,\ldots,X_n]^G \otimes_{\mathbb{R}} \mathbb{R}[X_1,\ldots,X_n]_G$$

as graded \mathbb{R} -algebras.

In fact, for general finite groups we have the following analog which follows from the Hironaka decomposition.

Theorem 16 Let G be a finite group with a linear action on a finite dimensional vector space V. Let $\theta_1, \ldots, \theta_n$ be the primary invariants and suppose that the rank of the $\mathbb{K}[\theta_1, \ldots, \theta_n]$ -module $\mathbb{K}[V]^G$ is m. Then $\mathbb{K}[V]/(\theta_1, \ldots, \theta_n)$ is isomorphic as G-module to m times the regular representation.

An algorithmic approach to efficiently compute the decomposition above can for example be found in [35].

Going via G- harmonic polynomials

Computing a basis of the covariant algebra may be complicated and involve calculation of a Groebner basis. We shortly mention that also the set of G-harmonic polynomials defined below can be efficiently used.

Definition 11 For a polynomial $f = \sum_{\alpha} c_{\alpha} X_1, \dots, X_n^{\alpha} \in \mathbb{R}[X_1, \dots, X_n]$ we denote by $f(\partial)$ the linear operator

$$f(\partial): \mathbb{R}[X_1, \dots, X_n] \longrightarrow \mathbb{R}[X_1, \dots, X_n]$$
$$g \longmapsto \sum_{\alpha} c_{\alpha} \frac{\partial^{|\alpha|}}{\partial X_1^{\alpha_1} \dots \partial X_n^{\alpha_n}} g,$$

i.e., $f(\partial)$ is the formal sum of scaled partial derivatives considered as a linear map.

Example for $f(\partial)$

Let
$$f = X_1^2 + X_1 X_2 \in \mathbb{R}[X_1, X_2, X_3]$$
, then $f(\partial) = \frac{\partial^2}{\partial X_1 \partial X_1} + \frac{\partial^2}{\partial X_1 \partial X_2}$ and

$$f(\partial)\left(X_1^2 + X_2^2 + X_3^2 + X_1X_2X_3\right) = 1 + X_3.$$

Definition 12 Let G be a reflection group with invariant ring $\mathbb{R}[\pi_1, \dots, \pi_n]$. Then the R-vector space of harmonic polynomials is defined as

$$\mathcal{H}_G := \left(\mathbb{R}[X_1,\ldots,X_n]^G\right)^{\perp},$$

with respect to the scalar product on $\mathbb{R}[X_1,\ldots,X_n]$ given by

$$\langle \cdot, \cdot \rangle : \mathbb{R}[X_1, \dots, X_n] \times \mathbb{R}[X_1, \dots, X_n] \longrightarrow \mathbb{R}[X_1, \dots, X_n]$$

$$(f, g) \longmapsto \operatorname{eval}_{(0, \dots, 0)} (f(\partial)g(X_1, \dots, X_n)).$$

Now the following statement shows that G-harmonic polynomials have some remarkable similarities with the covariant algebra as presented in Theorem 15. We refer the reader also to [10] for details on the following Theorem.

Theorem 17 Let G be a real reflection group and $\Delta := \prod L_i$, be the product of the linear polynomials defining the reflection hyperplanes.

- 1. The vector space of G-harmonic polynomials \mathcal{H}_G is generated by all partial derivatives of Δ , i.e., $\mathcal{H}_G = \langle \frac{\partial^{\alpha}}{\partial x^{\alpha}} \Delta : \alpha \in \mathbb{N}_0^n \rangle_{\mathbb{R}}$. 2. Furthermore, \mathcal{H}_G is as G-representation isomorphic to the regular representation
- of G and $\mathbb{R}[X_1,\ldots,X_n]=\mathbb{R}[\pi_1,\ldots,\pi_n]\otimes_{\mathbb{R}}\mathcal{H}_G$.

Let G be a finite reflection group and ψ_1, \dots, ψ_n be generators of the invariant ring. Consider the map

$$\Psi: \mathbb{R}^n \longrightarrow \mathbb{R}^n$$

$$X_1, \dots, X_n \longmapsto (\psi_1(X_1, \dots, X_n), \dots, \psi_n(X_1, \dots, X_n)).$$

Then, thanks to a statement of Steinberg in [69], we have

$$\Delta = c \cdot Jac \Psi$$

where $c \in \mathbb{R} \setminus \{0\}$ and $Jac \Psi$ denotes the Jacobian matrix of Ψ . The choice of fundamental invariants ψ_1, \ldots, ψ_n does not matter.

Jacobian of \mathfrak{S}_n

For \mathfrak{S}_n the symmetric group acting on \mathbb{R}^n via coordinate permutation and

$$\psi_i := p_i = \sum_{j=1}^n X_j^i$$

the power sums, we obtain $\Delta = \prod_{i < j} (x_i - x_j)$ equals (up to a scalar) the determinant of the Vandermonde matrix. The form defined above Δ which is the product over all reflections (i, j) of \mathfrak{S}_n equals therefore up to a scalar the Jacobian of Ψ .

Building on the notions of invariant theory outlined here we now can outline how to use the observation that the polynomial ring is a module over the invariant ring in the context of sums of squares formulations.

4.2 Invariant theory and sums of squares

In Section 3 where we focused on representation theory, we already saw how to apply Schur's Lemma to obtain simplifications for sums of squares computations. We shall explain how to combine the techniques developed with Schur's Lemma with results from invariant theory in the situation of symmetric sums of squares. Note that an invariant polynomial which can be expressed as a sum of squares in the ring $\mathbb{R}[X_1, \ldots, X_n]$ will not necessarily have a sum of squares decomposition in invariant polynomials, i.e.,

$$\mathbb{R}[X_1,\ldots,X_n]^G \bigcap \sum \mathbb{R}[X_1,\ldots,X_n]^2 \neq \sum (\mathbb{R}[X_1,\ldots,X_n]^G)^2,$$

as can be seen in the following example.

A symmetric sum of squares is not a sum of symmetric squares

Consider the symmetric sums of squares polynomial $f = X_1^2 + X_2^2 + ... + X_n^2$. Up to scalar multiplication there is only one symmetric polynomial of degree 1, namely $e_1 := X_1 + X_2 + ... + X_n$. Clearly, if n > 1 we have $\alpha \cdot e_1^2 \neq f$ for every $\alpha \in \mathbb{R}$.

The above example suggests that it is at first sight not clear which algebraic property in the ring $\mathbb{R}[X]^G$ certifies that a given invariant polynomial is a sum of squares of elements in $\mathbb{R}[X]$. However, we have seen that $\mathbb{R}[X]$ is a finitely generated module over the invariant ring. This observation allows for a refined version of Theorem 9. Following the presentation in [19], we focus here mainly on finite reflection groups, since, as we have seen, their representation theory is particularly nice. However, these results can be generalized to all finite groups using the Hironaka decomposition with appropriate adaptations. We begin with the following observation which makes use of the decomposition

$$\mathbb{R}[X_1,\ldots,X_n] \simeq \mathbb{R}[X_1,\ldots,X_n]^G \otimes \mathbb{R}[X_1,\ldots,X_n]_G$$

provided in Theorem 15. Since the covariant algebra is isomorphic to the regular representation of G, we can pick a basis $S := \{s_1, \ldots, s_{|G|}\}$. Relatively to this basis we now construct a matrix polynomial with entries

$$H_{u,v}^S := \mathcal{R}_G(s_u \cdot s_v)$$
, where $1 \le u, v \le |G|$.

Since now every entry $\mathcal{R}_G(s_u \cdot s_v)$ is by construction G-invariant we can express the entries in terms of the π_1, \ldots, π_n , i.e., we obtain a matrix polynomial in new variables z_1, \ldots, z_n

$$H^S(z_1,\ldots,z_n) \in \mathbb{R}[z_1,\ldots,z_n]^{|G|\times|G|}$$
.

Given any matrix-polynomial $L(z_1, \ldots, z_n) \in \mathbb{R}[z_1, \ldots, z_n]^{n \times m}$, we can construct a square matrix polynomial $M = L^T L$. We say that a $n \times n$ matrix polynomial M is a *sum of squares matrix polynomial* if it can be obtained in this way. With this notion at hand one can deduce from the decomposition in Theorem 15 the following algebraic certificate for an invariant polynomial to be a sum of squares.

Proposition 2 Let G be a finite reflection group and let f be an invariant polynomial. Consider the polynomial $g \in \mathbb{R}[z_1, \ldots, z_n]$ with $g(\pi_1, \ldots, \pi_n) = f$. Then f is a sum of squares if and only if g admits a representation of the form

$$g = \text{Tr}(M \cdot H^S)$$
.

where M is a sum of squares matrix polynomial.

The above construction works for every basis of the covariant algebra. But since we know that the group representation on the covariant algebra is the regular representation one can pick a basis that decomposes this covariant algebra into irreducible representations. We note this explicitly in the following Proposition.

Proposition 3 *Let G be a finite reflection group, and let*

$$\mathbb{R}[X_1,\ldots,X_n]_G = \bigoplus_{i\in I} \eta_i \theta^{(i)}$$

be the isotypic decomposition of the covariant algebra. Denote $\ell = |I|$. Then there are polynomials $s_{11}, \ldots, s_{\ell \eta_{\ell}} \in \mathbb{R}[X_1, \ldots, X_n]_G$ such that any $f \in \mathbb{R}[X_1, \ldots, X_n]$ can be written as

$$f = \sum_{i \in I} \sum_{j=1}^{\eta_i} \sum_{\sigma \in G} g_{ij,\sigma} \sigma s_{ij},$$

where $g_{ij,\sigma} \in \mathbb{R}[X_1,\ldots,X_n]^G$.

Note that the summation index η_i equals the multiplicity of the corresponding irreducible representation in the isotypic decomposition, which in turn equals the dimension of the irreducible representation.

Definition 13 With the notation used above, we can construct a matrix polynomial $H^{\theta_i} \in \mathbb{R}[z_1, \dots, z_n]^{\eta_i \times \eta_i}$ for every irreducible representation $\theta^{(i)}$ of G via

$$H_{u,v}^{\theta_i} = \mathcal{R}_G(s_{i,u} \cdot s_{i,v}), \text{ where } 1 \leq u, v \leq \eta_i.$$

Combining the above definition with the results from Schur's lemma we immediately get the following.

Theorem 18 Let G be a finite reflection group with $\mathbb{R}[X_1, \dots, X_n]^G \simeq \mathbb{R}[\pi_1, \dots, \pi_n]$, then we have

$$\Sigma \mathbb{R}[X_1,\ldots,X_n]^2 \cap \mathbb{R}[X_1,\ldots,X_n]^G = \left\{ g \in \mathbb{R}[\pi_1,\ldots,\pi_n] : g = \sum_{j=1}^l \operatorname{Tr}(H^{\vartheta_j} \cdot A_j) \right\},\,$$

where $A_i \in \mathbb{R}[\pi_1, \dots, \pi_n]^{\eta_j \times \eta_j}$ is a sum of squares matrix polynomial.

Although the above Theorem 18 is not too different in spirit from Theorem 9, it allows to transfer the decision if an invariant polynomial is a sum of squares into the invariant ring. Furthermore, this in turn allows for a more global approach. Indeed, Theorem 9 was stated for polynomials of a given degree 2d and relied in the decomposition of the space $\mathbb{R}[X_1,\ldots,X_n]_{\leq d}$. The use of the covariant algebra implicitly also directly yields a decomposition of the space $\mathbb{R}[X_1,\ldots,X_n]_{\leq d}$. Therefore, understanding the decomposition of the covariant algebra also provides important quantitative information. More precisely: we denote the dimension of the \mathbb{R} -vector space of G-invariant forms of degree d by $N_G(d)$, and write h_k^{ϑ} for the multiplicity of an irreducible representation θ in $(\mathbb{R}[X_1,\ldots,X_n]_G^{\theta})_{\leq k}$, i.e., for the multiplicity of θ in the isotypic decomposition of the subspace of polynomials of degree at most k in the covariant algebra. Then we get the following quantitative information necessary for applying Theorem 9 directly.

Proposition 4 Let G be a finite reflection group and θ be an irreducible representation. Then the multiplicity of the corresponding irreducible representation in the G-module $(\mathbb{R}[X_1,\ldots,X_n]_G^\theta)_{\leq k}$ equals

$$\sum_{k=0}^{d} N_G(d-k) \cdot h_k^{\vartheta}.$$

We are going to explore this theorem and its consequences a bit more in detail in the case of symmetric polynomials in the next Subsection and in the situation of a regular triangle in the next example, which is made more general in [19].

Sums of squares invariant by the dihedral group D_3

Consider the dihedral group D_3 of order 6 acting on the plane as a reflection group. The corresponding invariant ring is generated by the two polynomials $\pi_1 = X_1^2 + X_2^2$ and $\pi_2 = X_2^3 - 3X_1X_2^2$. The group has three irreducible representations, two of which are one dimensional and one of which is two dimensional. We find that the corresponding covariant algebra $\mathbb{R}[x, y]_{D_3}$ decomposes into

$$\theta^{(1)} = \langle 1 \rangle, \quad \theta^{(2)} = \langle -X_1^3 + 3X_1X_2^2 \rangle, \quad \theta_1^{(3)} = \langle X_1, X_2 \rangle, \quad \theta_2^{(3)} = \langle X_1X_2, X_2^2 \rangle.$$

Then

$$H^{\theta^{(1)}} = (1), \ H^{\theta^{(2)}} = \left(\mathcal{R}_{D_3} (3X_1X_2^2 - X_1^3)^2 \right), H^{\theta^{(3)}} = \left(\begin{array}{cc} \mathcal{R}_{D_3} (X_1^2) & \mathcal{R}_{D_3} (X_1^2X_2) \\ \mathcal{R}_{D_3} (X_1^2X_2) & \mathcal{R}_{D_3} (X_1^2X_2) \end{array} \right),$$

and we obtain

$$H^{\theta^{(1)}} = (1), \ H^{\theta^{(2)}} = \left(\pi_1^3 - \pi_2^2\right), \ H^{\theta^{(3)}} = \begin{pmatrix} \frac{\pi_1}{2} - \frac{\pi_2^2}{2} \\ -\frac{\pi_2}{2} & \frac{\pi_1^2}{8} \end{pmatrix},$$

4.3 Symmetric sums of squares

To conclude our discussion on the representations of invariant sums of squares, we focus on the case of symmetric polynomials. This case has been studied by various authors (for example [41, 58, 57, 32]), and our presentation follows [13].

In Definition 5 we have seen how to combinatorially describe the irreducible representations of \mathfrak{S}_n with the help of Young tabloids. A classical construction of Specht realizes these irreducible representations as submodules of the polynomial ring (see [66]):

Definition 14 For $\lambda \vdash n$ let T_{λ} be a standard Young tableau of shape λ and C_1, \ldots, C_{ν} be the columns of T_{λ} . To T_{λ} we associate the monomial

$$X^{T_{\lambda}} := \prod_{i=1}^{n} X_i^{m(i)-1},$$

where m(i) is the index of the row of T_{λ} containing i. Note that for any λ -tabloid $\{T_{\lambda}\}$ the monomial $X^{T_{\lambda}}$ is well defined, and the mapping $\{T_{\lambda}\} \mapsto X^{T_{\lambda}}$ is a \mathfrak{S}_{n} -isomorphism. For any column C_{i} of T_{λ} we denote by $C_{i}(j)$ the element in the j-th row and we associate to it a Vandermonde determinant:

$$\Delta_{C_i} := \det \begin{pmatrix} X_{C_i(1)}^0 \dots X_{C_i(k)}^0 \\ \vdots & \ddots & \vdots \\ X_{C_i(1)}^{k-1} \dots X_{C_i(k)}^{k-1} \end{pmatrix} = \prod_{j < l} (X_{C_i(j)} - X_{C_i(l)}).$$

The Specht polynomial $sp_{T_{\lambda}}$ associated to T_{λ} is defined as

$$sp_{T_{\lambda}} := \prod_{i=1}^{\nu} \Delta_{C_i} = \sum_{\sigma \in CStab_{T_{\lambda}}} sgn(\sigma)\sigma(X^{T_{\lambda}}),$$

where $CStab_{T_{\lambda}}$ is the column stabilizer of T_{λ} .

By the \mathfrak{S}_n -isomorphism $\{T_{\lambda}\} \mapsto X^{T_{\lambda}}$, \mathfrak{S}_n acts on $sp_{T_{\lambda}}$ in the same way as on the polytabloid $e_{T_{\lambda}}$. If $T_{\lambda,1}, \ldots, T_{\lambda,k}$ denote all standard Young tableaux associated to λ , then the set of polynomials $sp_{T_{\lambda,1}}, \ldots, sp_{T_{\lambda,k}}$ are called the *Specht polynomials* associated to λ . We then have the following result due to Specht [66]:

Proposition 5 The Specht polynomials $sp_{T_{\lambda,1}}, \ldots, sp_{T_{\lambda,k}}$ span an \mathfrak{S}_n -submodule of $\mathbb{R}[X]$ which is isomorphic to the Specht module S^{λ} .

Using the construction of Specht polynomials we aim now to obtain a version of Theorem 18 in the case of the symmetric polynomials. For this we rely on a basis for the corresponding covariant ring. Such a basis was described by Ariki, Terasoma, and Yamada in [2] with the construction of the so-called *Higher Specht polynomials*. These polynomials generalize the Specht polynomials in such a way that they yield a concrete basis as in Proposition 3. Their definition is given by a pair of Young tableaux.

Definition 15 Let $n \in \mathbb{N}$ be a natural number.

- 1. We call a finite sequence $w = (w_1, \dots, w_n)$ of non-negative integers a word of length n.
- 2. A word of length n is called a *permutation* if the set of its non-negative integers is $\{1, \ldots, n\}$.
- 3. Given a word w and a permutation u we define the monomial associated to the pair as $X_u^w := X_{u_1}^{w_1} \cdots X_{u_n}^{w_n}$.
- 4. To a given permutation w its index denoted by i(w), is the word of length n constructed the following way: the word i(w) contains 0 exactly at the same position where 1 occurs in w. The other entries are defined recursively with the following rule: if k is in position c in the word w (that is, $w_c = k$) and k + 1 is in position d, then $i(w)_d = i(w)_c$ if d > c, and $i(w)_d = i(w)_c + 1$ otherwise.

- 5. For a partition λ of n and a standard Young tableau of shape λ , T the *word* of T denoted by w(T) is defined by collecting the entries of T from the bottom to the top in consecutive columns starting from the left.
- 6. For a pair (T,V) of standard λ -tableaux we define the monomial associated to this pair as $X_{w(V)}^{i(w(T))}$. The degree of the monomial is called the *charge of T*, denoted c(T).

An example of a monomial built from a tableau

Consider the tableau

$$T = \begin{array}{|c|c|c|}\hline 1 & 2 & 4 \\\hline 3 & 5 & \\\hline \end{array}.$$

The resulting word is given by

$$w(T) = 31524,$$

with

$$i(w(T)) = 10201.$$

Taking

$$V = \begin{array}{|c|c|c|} \hline 1 & 3 & 5 \\ \hline 2 & 4 \\ \hline \end{array}$$

we obtain the monomial $X_{w(V)}^{i(w(T))} = X_2^1 X_1^0 X_4^2 X_3^0 X_5^1 = X_2 X_4^2 X_5$ of degree c(T) = 1 + 0 + 2 + 0 + 1 = 4.

Definition 16 Let $\lambda \vdash n$ and T be a λ -tableau. Then the *Young symmetrizer* associated to T is the element in the group algebra $\mathbb{R}[\mathfrak{S}_n]$ defined to be

$$\varepsilon_T = \sum_{\sigma \in RStab_T} \sum_{\tau \in CStab_T} sgn(\tau)\tau\sigma.$$

Now let T be a standard Young tableau, and define the *higher Specht polynomial* associated with the pair (T, V) to be

$$F_V^T(X_1,\ldots,X_n) := \varepsilon_V(X_{w(V)}^{i(w(T))}).$$

The importance of these higher Specht polynomials now is summarized in the following Theorem which can be found in [2, Theorem 1].

Theorem 19 The following holds for the set of higher Specht polynomials.

- 1. The set $\mathcal{F} = \bigcup_{\lambda \vdash n} \mathcal{F}_{\lambda}$ is a basis of the covariant ring $\mathbb{R}[X]_{\mathfrak{S}_n}$ over $\mathbb{R}[X]^{\mathfrak{S}_n}$.
- 2. For any $\lambda \vdash n$ and standard λ -tableau T, the space spanned by the polynomials in

$$\mathcal{F}_{\lambda}^{T} := \{F_{V}^{T}, \text{ where } V \text{ runs over all standard } \lambda\text{-tableaux}\}$$

is an irreducible \mathfrak{S}_n -module isomorphic to the Specht module W^{λ} .

The higher Specht polynomials for \mathfrak{S}_3

Consider the group \mathfrak{S}_3 . The complete list of higher Specht polynomials is given by

$$\{1\} \text{ for } W^{(3)}$$

$$\{(X_2 - X_1), (X_3 - X_1)\}, \{X_3(X_2 - X_1), X_2(X_3 - X_1)\} \text{ for } W^{(2,1)}$$

$$\{(X_2 - X_3)(X_3 - X_1)(X_3 - X_2)\} \text{ for } W^{(1,1,1)}.$$

These correspond to the trivial representation $W^{(3)}$, the 2-dimensional Specht module $W^{(2,1)}$ and the 1-dimensional Specht module $W^{(1,1,1)}$. We thus compute

$$H_{(3)} = 1$$

$$\begin{split} H_{(2,1)} &= \begin{pmatrix} R_{\mathfrak{S}_3}((X_2 - X_1)^2) & R_{\mathfrak{S}_3}((X_2 - X_1)X_3(X_2 - X_1)) \\ R_{\mathfrak{S}_3}((X_2 - X_1)X_3(X_2 - X_1)) & R_{\mathfrak{S}_3}(X_3(X_2 - X_1)^2) \end{pmatrix} \\ &= \begin{pmatrix} \pi_2 - \frac{1}{3}\pi_1^2 & -\frac{1}{3}\pi_1^3 + \frac{4}{3}\pi_1\pi_2 - \pi_3 \\ -\frac{1}{3}\pi_1^3 + \frac{4}{3}\pi_1\pi_2 - \pi_3 & -\frac{1}{6}\pi_1^4 + \frac{2}{3}\pi_1^2\pi_2 - \frac{2}{3}\pi_1\pi_3 + \frac{1}{6}\pi_2^2 \end{pmatrix} \end{split}$$

$$H_{(1,1,1)} = R_{\mathfrak{S}_3}((X_1 - X_2)(X_1 - X_3)(X_2 - X_3))$$

$$= \frac{1}{6}(-\pi_1^6 + 9\pi_1^4\pi_2 - 8\pi_1^3\pi_3 - 21\pi_1^2\pi_2^2 + 36\pi_1\pi_2\pi_3 + 3\pi_2^3 - 18\pi_3^2)$$

Using Theorem 18 one now obtains that every symmetric sum of squares polynomial $f \in \mathbb{R}[X_1, X_2, X_3]^{\mathfrak{S}_3}$ can be written in the from

$$f = \sigma_0(\pi_1, \pi_2, \pi_3) + \sigma_1(\pi_1, \pi_2, \pi_3)H_{(1,1,1)} + Tr(M(\pi_1, \pi_2, \pi_3) \cdot H_{(2,1)}),$$

where $\sigma_0(\pi_1, \pi_2, \pi_3)$, and $\sigma_1(\pi_1, \pi_2, \pi_3)$ are sums of squares in $\mathbb{R}[\pi_1, \dots, \pi_3]$ and $M \in \mathbb{R}[\pi_1, \dots, \pi_3]^{2 \times 2}$ is a sum of squares matrix polynomial.

Furthermore, we can use the combinatorial description of the Higher Specht polynomials to gain understanding of the "complexity" of symmetric sums of squares decomposition of polynomials of fixed degree 2d. Indeed, we find that the multiplicities m_{λ} of the \mathfrak{S}_n -modules W^{λ} which appear in an isotypic decomposition $\mathbb{R}[X_1,\ldots,X_n]_{=d}$ coincide with the number of standard λ -tableaux S with charge at most d, i.e., all S with $c(S) \leq d$. This yields in particular the following observation which was first remarked in [62, Theorem 4.7.], and can be generalized to all infinite families of reflection groups [19, Theorem 3.31].

Theorem 20 Let $H_{n,2d}^{\mathfrak{S}_n}$ denote the homogeneous symmetric polynomials of degree 2d. Then the matrix size needed to decide if $f \in H_{n,2d}^{\mathfrak{S}_n}$ is a sum of squares do not depend on n once $n \geq 2d$.

A similar phenomenon was also shown in situations where \mathfrak{S}_n is not acting as a reflection group [57]. The stabilization observed in Theorem 20 makes it in particular possible to give uniform descriptions for symmetric sums of squares of a given degree. For example we have the following representation theorem of symmetric quartics which was derived in [12] with the methods presented in this section.

Theorem 21 Let $f \in H_{n,4}^{\mathfrak{S}_n}$ be a symmetric quartic. Then f is a sum of squares if and only if it can be written in the form

$$\begin{split} f^{(n)} &= \alpha_{11}\pi_1^4 + 2\alpha_{12}\pi_1^2\pi_2 + \alpha_{22}\pi_2^2 \\ &+ \beta_{11}\left(\pi_1^2\pi_2 - \pi_1^4\right) + 2\beta_{12}\left(p_{(3,1)} - \pi_1^2\pi_2\right) + \beta_{22}\left(\pi_4 - \pi_2^2\right) \\ &+ \gamma\left(\frac{1}{2}\pi_1^4 - \pi_1^2\pi_2 + \frac{n^2 - 3n + 3}{2n^2}\pi_2^2 + \frac{2n - 2}{n^2}\pi_1\pi_3 + \frac{1 - n}{2n^2}\pi_4\right), \end{split}$$

where $\pi_j = \frac{1}{n}(X_1^j + \dots X_n^j)$ for $1 \le j \le 4$ and the parameters $\alpha_{11}, \alpha_{12}, \alpha_{22}, \beta_{11}, \beta_{12}, \beta_{22}$ are chosen such that $\gamma \ge 0$ and the matrices $\begin{pmatrix} \alpha_{11} & \alpha_{12} \\ \alpha_{12} & \alpha_{22} \end{pmatrix}$ and $\begin{pmatrix} \beta_{11} & \beta_{12} \\ \beta_{12} & \beta_{22} \end{pmatrix}$ are positive semidefinite.

5 Miscellaneous approaches

So far we have been focused on ways to explore symmetries in sums of squares decompositions which are used to obtain an approximation hierarchy for polynomial optimization problems. To close our discussion, we present here some other ways to use symmetries in optimization problems. The selection we present here is non exhaustive and the presentation of the individual methods is rather short. However, we hope this overview will provide useful points of references for the reader.

5.1 Orbit spaces and polynomial optimization

The methods of invariant theory presented in Section 4 have provided that we can represent an invariant polynomial algebraically in terms of generators of the invariant ring. Indeed, Theorem 10 yields that $\mathbb{K}[X]^G$ is finitely generated and therefore is the coordinate ring of an algebraic variety. So we can associate to a choice of generators π_1, \ldots, π_m and the corresponding inclusion $\mathbb{K}[\pi_1, \ldots, \pi_m] \subseteq \mathbb{K}[X_1, \ldots, X_n]$ a morphism Π defined explicitly via

$$\Pi: \mathbb{K}^n \longrightarrow \mathbb{K}^m$$

$$x \longmapsto (\pi_1(a), \dots, \pi_m(a))$$

This map is also called the *Hilbert map*. Let $a \in \mathbb{K}^n$, then the *orbit of a* denoted by G_a is the set of points to which a is mapped to under the action of G, i.e.

$$G_a := \{g(a) | g \in G\}.$$

As the orbits G_a and G_b of two points in \mathbb{K}^n are either equal or disjoint, the action of G on \mathbb{K}^n naturally defines an equivalence relation by $a \sim b$ if and only if b = g(a)for some $g \in G$ and we can consider the set of equivalence classes, i.e., the set of all G-orbits on \mathbb{K}^n and denote this by \mathbb{K}^n/G . This set is called the *orbit space*. Notice that the Hilbert map is constant on G-orbits, so it makes sense to view it as a mapping of the orbit space. Now if have a finite group G acting on a linear space defined over an algebraically closed field, for example $\mathbb{K} = \mathbb{C}$, then the polynomial mapping defined above is surjective onto the *n* dimensional variety $V_{\Pi} \subset \mathbb{C}^m$ defined by the algebraic relations between the m polynomials π_1, \ldots, π_m . In particular, if the polynomials are algebraically independent, which is exactly the case if G is a finite reflection group, each orbit is mapped to a point in \mathbb{C}^n . Moreover if g_1, \ldots, g_k are invariant polynomials that describe an algebraic set in \mathbb{C}^n the Hilbert map sends this set to a new algebraic set in \mathbb{C}^n which is given by the polynomials $\gamma_1, \ldots, \gamma_k$ which satisfy $\gamma_i(\pi_1, \dots, \pi_m) = g_i$ for $1 \le j \le k$. Therefore, the possibility to represent invariant functions in terms of generators can reduce the complexity of the description of invariant algebraic sets.

In contrast to the algebraically closed case where the Hilbert map is surjective, if we restrict Π to \mathbb{R}^n the resulting map $\tilde{\Pi}$ may fail to be surjective.

Failure of surjectivity in the D_4 case

Let $G = D_4$ be the Dihedral group acting on \mathbb{R}^2 . Then the invariant ring $\mathbb{C}[X,Y]^{D_4}$ is generated by $\pi_1 = X^2 + Y^2$ and $\pi_2 = X^2Y^2$ and since D_4 is a reflection group π_1 and π_2 are algebraically independent. The Hilbert map thus provides a connection between the orbit space \mathbb{C}^2/D_4 and \mathbb{C}^2 . However, if we restrict the map π to \mathbb{R}^2 the image of Π is strictly contained in \mathbb{R}^2 . Indeed, we must have $\pi_1(x,y) \geq 0$ for all $(x,y) \in \mathbb{R}^2$, and thus for example $\Pi^{-1}(-1,0) \notin \mathbb{R}^2$. Hence, the restricted map Π is not surjective.

Nevertheless, the real Hilbert map

$$\Pi: \mathbb{R}^n \to \mathbb{R}^n / G \subseteq \mathbb{R}^m$$
$$a \mapsto (\pi_1(a), \dots, \pi_m(a))$$

defines an embedding of the orbit space into \mathbb{R}^m and by the Traski-Seidenberg principle of real algebraic geometry its image is a semi-algebraic subset of \mathbb{R}^m . It can be shown that the failure of the map being surjective is related to the existence

of abelian 2-subgroups of G (see [14]). Therefore, as soon as the order of the group is even, additional semi-algebraic conditions need to be imposed. For example, in the example above, every point in the image needs to satisfy

$$\Pi(\mathbb{R}^2) \subseteq \{(z_1, z_2) \in \mathbb{R}^2 : z_1 \ge 0\}$$

since $\pi_1(x, y) \ge 0$ for all $(x, y) \in \mathbb{R}^2$.

It was shown by Procesi and Schwarz [55] that the image of Π is in fact a basic semialgebraic set, i.e., there exist finitely many polynomial inequalities which are satisfied if and only if a point is in the image of the map. Moreover, in the case of compact groups, these inequalities can be obtained from the chosen fundamental invariants in a direct way:

For a polynomial p we consider the differential dp defined by $dp = \sum_{j=1}^n \frac{\partial p}{\partial x_j} dx_j$. For finite (compact) G we have a G-invariant inner product $\langle \cdot, \cdot \rangle$ which when carrying over the to the differentials yields $\langle dp, dq \rangle = \sum_{j=1}^n \frac{\partial p}{\partial x_j} \cdot \frac{\partial q}{\partial x_j}$. Since differentials of G-invariant polynomials are G-equivariant, the inner products $\langle d\pi_i, d\pi_j \rangle$ $(i, j \in \{1, \dots, m\})$ are G-invariant, and hence every entry of the symmetric matrix polynomial

$$J = (\langle d\pi_i, d\pi_j \rangle)_{1 \le i, j \le m}$$

is G-invariant. With this construction Procesi and Schwarz [55] have shown the following.

Theorem 22 Let $G \subseteq GL_n(\mathbb{R})$ be a compact matrix group, and let $\Pi = (\pi_1, \dots, \pi_m)$ be fundamental invariants of G. Then the orbit space is given by polynomial inequalities,

$$\mathbb{R}^n/G \ = \ \Pi(\mathbb{R}^n) \ = \ \{z \in \mathbb{R}^n \ : \ J(z) \geq 0, \ z \in V(I)\} \ ,$$

where $I \subseteq \mathbb{R}[z_1, \dots, z_m]$ is the ideal of relations of π_1, \dots, π_m .

This statement now allows to use invariant theory in order to rewrite an invariant optimization problem: If we consider a polynomial optimization problem of the form

$$\inf\{p(x) \text{ s.t. } g_1(x) \ge 0, \dots, g_m(x) \ge 0\},\tag{14}$$

where we assume that the polynomials p, g_1, \ldots, g_m are invariant by a group G, then by choosing π_1, \ldots, π_m which generate the invariant ring we obtain corresponding polynomials $\tilde{p}, \tilde{g}_1, \ldots \tilde{g}_m \in \mathbb{R}[\pi_1, \ldots, \pi_m]$, which might be of smaller degrees than the original polynomials. By using Theorem 22 we may now translate the optimization problem (14) to the following equivalent optimization problem:

$$\inf\{\tilde{p}(z) \text{ s.t. } z \in V(I_{\Pi}), \tilde{g}_1(z) \ge 0, \dots, \tilde{g}_m(z) \ge 0, J(z) \ge 0\}.$$
 (15)

So the Hilbert map allows us to reformulate the initial polynomial optimization problem in new polynomial functions, which potentially can be of smaller degree or involve less variables, at the price that we obtain a new set of constraints that come from the fact that the Hilbert map fails in general to be surjective.

The choice of generators matters

The matrix polynomial J, as well as the specific description of the original problem in terms of generators, depend on the choices made for the generators. Thus different choices might lead to quite different optimization problems. Consider the Motzkin polynomial $M = X_1^4 X_2^2 + X_1^2 X_2^4 - 3X_1^2 X_2^2 + 1$. We can rewrite this polynomial in terms of elementary symmetric polynomials, i.e., $\pi_1 = X_1 + X_2$ and $\pi_2 = X_1 X_2$. Then

$$\tilde{M}_e = \pi_1^2 \pi_2^2 - 2\pi_2^3 - 3\pi_2^2 + 1.$$

The corresponding matrix polynomial J_e is given by

$$J_e = \begin{pmatrix} 2 & \pi_1 \\ \pi_1 & \pi_1^2 - 2\pi_2 \end{pmatrix}.$$

Now the minimal value of M on \mathbb{R}^2 is the same as the minimal value of \tilde{M}_e in the set of points $\{(\pi_1, \pi_2) \in \mathbb{R}^2 : J_e(\pi_1, \pi_2) \geq 0\}$. On the other hand we can choose the power sum polynomials $\pi_1 = X_1 + X_2$, $\pi_2 = X_1^2 + X_2^2$ and we obtain

$$\tilde{M}_{p} = \frac{1}{4} (\pi_{1}^{4} \pi_{2} - 3\pi_{1}^{4} - 2\pi_{1}^{2} \pi_{2}^{2} + 6\pi_{1}^{2} \pi_{2} + \pi_{2}^{3} - 3\pi_{2}^{2} + 4).$$

Furthermore, we find for the corresponding matrix polynomial

$$J = \begin{pmatrix} 2 & \pi_1 \\ \pi_1 & \pi_2 \end{pmatrix}.$$

Now the minimal value of M on \mathbb{R}^2 is the same as the minimal value of \tilde{M} in the set of points $\{(\pi_1, \pi_2) \in \mathbb{R}^2 : J(\pi_1, \pi_2) \geq 0\}$.

The main advantages of the approach sketched above is that it may reduce the degrees of the polynomials describing the optimization problem and even can reduce the number of variables. Furthermore, optimal points to the equivalent optimization problem (15) correspond to entire orbits of optimal points. Therefore the number of such points may also be drastically smaller. Finally, in contrast to the methods described in the main parts of this chapter, which were designed for sums of squares approximations, this approach reduces the symmetry on the formulation and therefore allows integration with other methods for solving polynomial optimization problems. However, it was observed in [63] that the special structure of the optimization problem (15) - namely the fact that the additional constraints are expressed in terms of a *polynomial matrix inequality* $J(z) \ge 0$ - allows to use a specially adapted version of the SOS-moment hierarchy established by Hol and Scherer (and dually by Henrion and Lasserre). We briefly sketch this approach.

Orbit space formulations and moment relaxations

For a polynomial matrix G(x), define the localizing matrix as follows

$$M(G \star y)_{i,j,l,k} = L(b_i \cdot b_j \cdot G(x)_{l,k})$$
.

With this construction one can define the following moment relaxation for the orbit space formulation of a polynomial optimization problem defined in (15) for $k \in \mathbb{N}$:

$$Q_{k}^{q}: \begin{array}{c} \inf_{y} \sum_{\alpha} \tilde{p}_{\alpha} y_{\alpha} \\ M_{k}(y) \geq 0, \\ M_{k-\lceil \deg \tilde{g}_{j}/2 \rceil}(\tilde{g}_{j} y) \geq 0, \\ M_{k-m}(J \star y) \geq 0. \end{array}$$

$$(16)$$

For *k* large enough, each solution to the sequence of semi-definite programs defined in (16) provides a lower bound for the problem and moreover, under additional conditions, the sequence of relaxations converges. (see [62] for details). This relaxation approach recently has also been adapted to multiplicative group actions (see [36]).

5.2 Reduction via orbit decomposition

In the symmetry reduction techniques for sums of squares presented in this chapter, the first essential step consisted in the observation that for convex sets one can reduce easily to orbits and the second step was grounded in consequences of Schur's lemma. Approaches using the second step are however clearly limited to those situations that allow for an application of Schur's lemma. However, even in cases where sophisticated tools from representation theory will not directly apply, one can obtain substantial reductions by cleverly decomposing invariant problems according to orbits. A natural idea consists for example in turning a large symmetric problem into smaller problems, in such a way that solving these smaller problems gives at least a solution by orbit, therefore giving a full understanding of the solutions of the initial problem. Such ideas can be useful, and sometimes refined, in several situations, including in optimization and computation (see for instance [22, 33, 64]). We showcase one example of this simple, but sometimes effective, idea in the context of polynomial optimization: the orbit decomposition of SAGE signomials.

In order to motivate this situation we recall that the main key for the approximations methods used in the previous sections comes from the observation that a polynomial which can be written as a sum of squares is non-negative. Of course, one can replace this condition with other certificates of non-negativity certification. Another example of such certificates relies on SAGE functions (see [15]). A signomial is a function of the form

$$f(x) = \sum_{\alpha \in \mathcal{A}} c_{\alpha} e^{\langle \alpha, x \rangle}$$

where $\mathcal{A} \subset \mathbb{R}^n$ is a finite set. Under the change of variables $y_i = e^{x_i}$, this can be seen as a generalization of polynomial functions restricted to the positive orthant.

Suppose a signomial f can be written in the from

$$f(x) = \sum_{\alpha \in \mathcal{A}} c_{\alpha} e^{\langle \alpha, x \rangle} + de^{\langle \beta, x \rangle}$$
 (17)

 $c_{\alpha} > 0$ for $\alpha \in \mathcal{A}$ and $\beta \in \operatorname{relint}(\mathcal{A})$. Then, it follows from arithmetic-geometric mean inequality that f is non-negative on \mathbb{R}^n if and only if there exists $\nu \in R_+^{\mathcal{A}}$ such that

$$\sum_{\alpha \in \mathcal{A}} \nu_{\alpha} \alpha = \left(\sum_{\alpha \in \mathcal{A}} c_{\alpha} \right) \beta \text{ and } \sum_{\alpha \in \mathcal{A}} \nu_{\alpha} \ln \frac{\nu_{\alpha}}{e \cdot c_{\alpha}} \leq d.$$

A function of this form is called an *AGE function*, and a sum of AGE functions is called a *SAGE function*. Clearly, a SAGE function is non-negative on \mathbb{R}^n , and similarly to the sum of squares formulation one can define a *SAGE-approximation* of the polynomial optimization problem (2) via

$$f^{SAGE} = \sup\{\lambda, f - \lambda \text{ is SAGE}\} \le \inf\{f(x), x \in \mathbb{R}^n\}$$

to obtain a bound on the minimum of a given signomal function f on \mathbb{R}^n . The observation which makes this formulation computationally viable is that the task to decide if a given signomial is SAGE can be decided via *relative entropy programming* (a subclass of convex programs, see [15]).

Now, if we suppose that a signomial f as written in (17) is invariant by the action of a group G (linearly on the exponents) and denote by $\hat{\mathcal{B}}$ be a set of orbit representatives for \mathcal{B} by this action, then applications of the Reynolds operator reveal (see [48] for details) that f is SAGE if and only if for every $\beta \in \hat{\mathcal{B}}$, there exists an AGE signomial

$$h_{\beta} = \sum_{\alpha \in \mathcal{A}} c_{\beta,\alpha} e^{\langle \alpha, x \rangle} + d_{\beta} e^{\langle \beta, x \rangle}$$

such that

$$f = \sum_{\beta \in \hat{\mathcal{B}}} \sum_{\rho \in G/\operatorname{Stab}(\beta)} \rho h_{\beta},$$

where the functions h_{β} can be chosen to be invariant under the action of the stabilizer $\operatorname{Stab}_{G}(\beta)$ of β .

SAGE decomposition of a symmetric signomial

Consider the symmetric signomial

$$f = 5e^{6x} + 5e^{6y} + 5e^{6z} - e^{2x+y+z} - e^{x+2y+z} - e^{x+y+2z} + 6.$$

With the notation above we have $\hat{\mathcal{B}} = \{(1, 1, 2)\}$. The stabilizer of (1, 1, 2) is $\mathfrak{S}_2 \times \mathfrak{S}_1$ and f is SAGE if and only if there exists an AGE polynomial of the form

$$g = c_1 e^{6x} + c_2 e^{6y} + c_3 e^{6z} + c_4 - e^{x+y+2z}$$

such that

$$f = g + (1 \ 3)g + (2 \ 3)g$$
.

Moreover, since we can assume that g is invariant under the action of $\mathfrak{S}_2 \times \mathfrak{S}_1$, we can assume that $c_1 = c_2$. Identifying the coefficients we find therefore that $c_1 = c_2 = 1$, $c_3 = 3$ and $c_4 = 2$. Thus, f is SAGE if and only if

$$g = e^{6x} + e^{6y} + 3e^{6z} - e^{x+y+2z} + 1$$

is AGE, and therefore we directly arrive at a substantial reduction of the associated relative entropy program.

In fact the reduction of complexity suggested in the example above can be made precise by understanding the orbits and stabilizers of the exponents appearing in the signomial. In particular in the case of symmetric AGE functions, i.e., invariant by the group \mathfrak{S}_n , it can be shown (see [48, Theorem 5.2]) that one can expect a stabilization of complexity with n similar to Theorem 20: for some sequences of signomials, if the number of terms grows quickly, the number of variables and constraints in the corresponding relative-entropy program remains constant for n large enough. Therefore, even in a situation where we are not able to use the power of representation theory, we can turn large optimization problems involving a lot of variable and constraints into a smaller one that can be solved efficiently.

5.3 Symmetries of optimizers

We conclude this section with a rather general approach, which may be used in some situations. Again, let G be a group acting linearly on a vector space V. Given an optimization problem that is symmetric, i.e., invariant by a group G, one could expect that also the solutions exhibit symmetries. Firstly, and clearly, the set of optimal points will be closed under the action of the symmetry group. In the best case, also the optimal points themselves will be fixed by the group. If we know apriori that this is the case, we only need to look at the linear subspace of points which are invariant by G. If the action of G is not the trivial one, this subspace will be of smaller dimension thus, one obtains directly a reduction of the optimization problem. The following example is one easy and simple prototype of this idea.

A symmetric problem with a symmetric solution

Given a > 0 we want to find the maximal area of an rectangle of perimeter a. The solution is the square and one find directly that the side length is $\frac{1}{4}a$.

However, it is in general not clear what conditions on the optimization problem guarantee this property (see for example [76] for a beautiful exhibition of situations and some historical panorama). But in particular, if there is just one optimal point, this optimal point has to be invariant by the group. So, we can conclude that in particular for convex optimization problems, this approach might directly lead to a reduction of dimension. Building on this simple idea, it may also be beneficial if one knows apriori that the optimal points are fixed by some (non trivial) subgroup of G. For a subgroup $G' \subset G$ we denote by $V^{G'}$ the elements in V fixed by G'. It is a simple observation that $V^{G'}$ is a vector subspace of V which might be of smaller dimension. Thus by restricting the original optimization problem to the smaller vector space $V^{G'}$ we reduce the dimension of the problem.

We present some situations in which this approach can lead to some substantial reduction. Building on the example above, suppose that we deal with an optimization problem defined in symmetric polynomials and we thus consider the action of the symmetric group \mathfrak{S}_n on \mathbb{R}^n . The action of \mathfrak{S}_n on \mathbb{R}^n naturally decomposes the space into orbits.

Definition 17 For every $x \in \mathbb{R}^n$, the associated stabilizer subgroup $\operatorname{Stab}(x) \subseteq \mathfrak{S}_n$ is of the form

$$Stab(x) \simeq \mathfrak{S}_{\ell_1} \times \mathfrak{S}_{\ell_2} \times \cdots \times \mathfrak{S}_{\ell_k}$$

with $\ell_1 \ge \ell_2 \ge ... \ge \ell_k$. We hence define the *orbit type* of x to be

$$\Lambda(x) := (\ell_1, \ell_2, \cdots, \ell_k).$$

Then, for a given $\lambda \vdash n$ we can define

$$H_{\lambda} := \{ x \in \mathbb{K}^n : \Lambda(x) = \lambda \},$$

and

$$A_k := \{x \in \mathbb{R}^n : \text{ the orbit type of } x \text{ has length at most } k\}$$

Remark 6 For $k \in \mathbb{N}$, the set A_k as defined above is a union of k-dimensional linear (sub)spaces of \mathbb{R}^n .

Example A_1

For k = 1 we find $A_1 = \{t \cdot (1, ..., 1), t \in \mathbb{R}\}$ and in general A_d can be identified with the set of points having at most d distinct coordinates

Now we have the following (see [59, Theorem 4.5], and [72]).

Theorem 23 Let $f, g_1, \ldots, g_m \in \mathbb{R}[X]^{\mathfrak{S}_n}$ and let set

$$r := \max \{2, |(\deg f)/2|, \deg g_1, \dots, \deg g_m\}.$$

Consider the optimization problem

$$f^* = \inf_{x \in K} f(x), \text{ where } K = \{x \in \mathbb{R}^n : g_1(x) \ge 0, \dots, g_m(x) \ge 0\}.$$

If the set of optimizers is not empty it contains at least one point $x^* \in A_r$, and in fact

$$f^* = \inf_{x \in K \cap A_r} f(x)$$

Now, a very direct approach to make use of this result consists in restricting to the different sub-spaces that build up A_r individually. We consider the set $\Lambda_{r,n}$ of all partitions λ of n into exactly r parts. Then for each $\lambda \in \Lambda_{r,n}$, set

$$f^{\lambda} := f(\underbrace{T_1, \dots, T_1}_{\lambda_1}, \underbrace{T_2, \dots, T_2}_{\lambda_2}, \dots, \underbrace{T_r, \dots, T_r}_{\lambda_r}) \in \mathbb{R}[T_1, \dots, T_r].$$

Similarly, let $K^{\lambda} := \{t \in \mathbb{R}^r : g_1^{\lambda}(t) \geq 0, \dots, g_m^{\lambda}(t) \geq 0\}$. With this easy substitution the original optimization problem in n variables can be transformed into a set of new optimization problems that involve only r variables,

$$\inf_{x \in K} f(x) = \min_{\omega \in \Omega} \inf_{t \in K^{\omega}} f^{\omega}(t).$$
 (18)

Remark 7 Note that $|\Lambda_{r,n}| \le \binom{n+r}{r}$ and therefore, for fixed r, the amount of additional problems in r variables grows only polynomially in n.

The main advantage of the simple approach based on Theorem 23 consists in the possibility to use any method to solve the resulting r-dimensional polynomial optimization problems. In particular, it has been observed in [62, 19] that combining this approach with the sum of squares approach can lead to qualitative improvements of the approximation. There have been several generalizations of Theorem 23: the paper [49] provides a finer criterion than only the degree of the polynomials involved to decide on the orbit type of solutions. In [60, 61] special classes of symmetric polynomials are defined, depending on special representation of the polynomials in the power sum basis or in the basis of elementary symmetric polynomials. For these classes an approach identical to the one described above can be derived from [60, Theorem 2.6] or [61, Theorem 24]. Furthermore, it can be shown that a similar statement holds in fact for all finite reflection groups [1, 23] and even in the setup of the symmetric group not acting as a reflection group [29]. Finally, via Morse theory the fact that optimal points to special symmetric optimization problems tend to have some high symmetry also has impact on the topological complexity of the orbit space of \mathfrak{S}_n -invariant semi-algebraic sets (see [5, 7]) and a refined statement can be used to give complexity reduction in various algorithmical questions related to the topology of symmetric semi-algebraic sets (see [6, 8]). Finally, one can observe that that after the restriction to A_r in some cases the resulting system will still have some symmetries. This was for example used in [22, 75] to obtain more efficient algorithmic results for computing critical points.

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