

RESEARCH STATEMENT

My research focuses on the development and improvement of algorithms to solve algebraic optimization and control problems through the exploitation of symmetry by applying methods from computer algebra, algebraic geometry and representation theory.

Tobias Metzloff, April 2025

1 State of the Art

Optimization is the problem of determining the optimal configuration of an object. Mathematically, this means to compute the minimum of a map over an ordered field, the objective function, under given constraints, defining the feasible region. The case of optimization I consider is the one, where the objective function and the constraints are algebraic, such as elements of polynomial rings, algebraic groups or operator algebras. The polynomial optimization problem for example is nonconvex, infinite-dimensional and NP-hard. Under certain algebraic and geometric assumptions however, one can approximate the minimum: The optimization problem can be rewritten to the problem of certifying whether a polynomial is positive on the feasible region. This leads to a hierarchy of lower bounds, stemming from convex finite-dimensional optimization problems, which are solvable through numerical methods [Laso1, Paro3]. Throughout, this approach is referred to as the Lasserre hierarchy.

Since Emil Artin's solution of David Hilbert's 17-th problem in 1927, the study of positivity certificates has been essential to algebraic geometry and neighboring fields of mathematics. Examples are the "Positivstellensätze" of Krivine, Stengle, Schmüdgen, Putinar [Kri64, Ste74, Sch91, Put93], and the matrix versions due to Kojima, Hol, Scherer [Koj03, HSo5]. In the Lasserre hierarchy, positivity is replaced with having a sums-of-squares representation, the necessary condition of Putinar's Positivstellensatz. By restricting the polynomial degree of the sums of squares, one obtains a hierarchy of semi-definite lower bounds, which converge to the optimal value. The degree at each step is the order of the hierarchy. Raising the order improves the quality of the bound but increases the computational cost. Recent advances on the hierarchy are to be found in [HKL21].

In practice, these sums-of-squares representations are modeled through semi-definite programs. A semi-definite program (SDP) is an optimization problem over positive semi-definite matrices and solvable with a variety of numerical techniques, see [VB96]. The number of SDP variables, that is, the number of distinct matrix entries, grows polynomially along with the order of the Lasserre Hierarchy. Hence, techniques to reduce the cost are essential for efficiency. To achieve this, the keyword in my research is symmetry. If symmetry in the data of the problem is detected, then this can be exploited. Symmetry-adapted bases for example have seen the size of SDPs decrease and have proven to be successful in the study of optimization problems [GPo4, Valo8].

I focus on a particular kind of symmetry, which is called crystallographic, and provides optimal configurations for a variety of problems in computer science. Consider for example the hexagon in Figure 1. Hexagonal patterns are classically known to be optimal for sampling, packing, covering, and quantization in the plane [CS99, KAHo5], but also proved, or conjectured, to be optimal for energy minimization problems [PS20, BF23]. The hexagonal symmetry is captured mathematically by a structure that is called A_2 . Another relevant structure called E_8 was recently proven to give an optimal solution for the sphere packing problem and a large class of energy minimization problems in the 8-dimensional space [Via17, CKM⁺22]. From an approximation point of view, such structures describe Gaussian cubatures [LX10, MP11], a rare occurrence on multidimensional spaces. In a different direction, the triangulations associated with such symmetries are relevant in graphics and computational geometry, see for instance [CKW20].

To be able to develop, implement and apply models of these symmetric structures and the problems they arise in, a strong background in representation theory and geometry is required. Indeed, what was called "structure" above originates from the classification of the simple Lie algebras in families $A_{n-1}, B_n, C_n, D_n, E_6, E_7, E_8, F_4, G_2$, see [Bou68, Ch. VI, §4]. On a fundamental level, crystallographic symmetry is often described by two objects. The first is a group \mathcal{W} , that is, a set of invertible transformations over an n -dimensional space \mathbb{R}^n . The second is a lattice Ω , that is, a discrete additive set of points in the space \mathbb{R}^n including the origin 0 , which is stable under the group transformations. This setup is called a group action of \mathcal{W} on Ω .

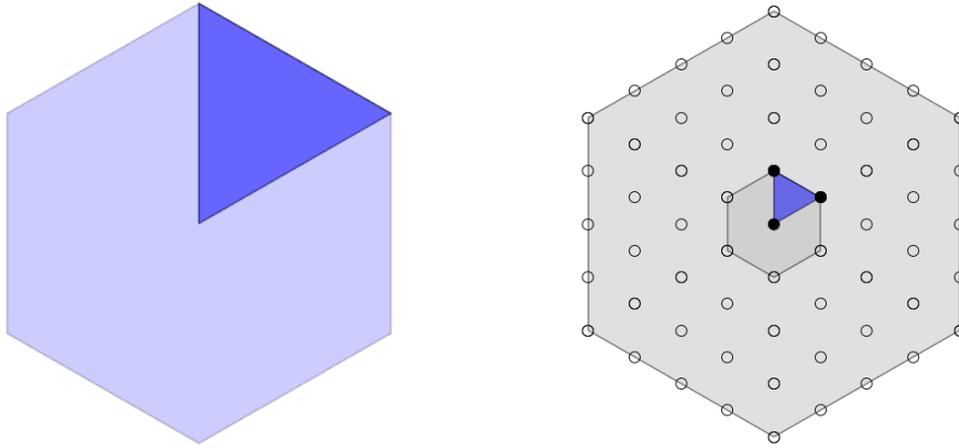


Figure 1: A hexagon in the plane is a symmetric object: Rotation of the darker shaded region on the left by an angle of $\pi/3$ allows the description of the whole hexagon while only having knowledge about a smaller subset. The rotation is a group transformation, encoded by the hexagonal lattice on the right, known as A_2 .

Polynomial optimization is a common task in this context, occurring, for example, in filter design [Dumo7], graph coloring [BDOV14], and optimal power flow [BFWo8, JM18]. One considers real-valued functions f on \mathbb{R}^n , which are square-integrable and Ω^\vee -periodic. The latter means that, whenever $\lambda \in \mathbb{R}^n$ is such that the Euclidean scalar product $\langle \mu, \lambda \rangle$ is an integer, then $f(u + \lambda) = f(u)$ for all $u \in \mathbb{R}^n$. Such functions have a Fourier expansion

$$f(u) = \sum_{\mu \in \Omega} f_\mu \exp(-2\pi i \langle \mu, u \rangle),$$

with coefficients $f_\mu \in \mathbb{R}$, see [DM85] and [CS99, Ch. 9, §2]. The task is to compute the minimum

$$f^* := \min_{u \in \mathbb{R}^n} f(u) = \min_{u \in \mathbb{R}^n} \sum_{\mu \in \Omega} f_\mu \exp(-2\pi i \langle \mu, u \rangle)$$

which is assumed in some minimizer u^* inside the periodicity domain.

If, for every transformation $s \in \mathcal{W}$ and for every lattice element $\mu \in \Omega$, the coefficients of the objective function satisfy $f_{s(\mu)} = f_\mu$, then f is called **invariant**. For the applications cited above, f can be assumed to be invariant without loss of generality and it is this property that is sought to be exploited in an optimization context.

To solve the problem of computing f^* numerically, the Lasserre hierarchy is a semi-definite relaxation technique that has been developed and improved over the past decades, see for example [Laso1, Paro3, Dumo7, JM18]. The technique boils down to approximate the objective function f through polynomials of bounded degree d over a convex cone (more precisely, through sums of squares) and leads to a hierarchy of lower bounds

$$f^{(d)} \leq f^{(d+1)} \leq f^{(d+2)} \leq \dots \leq f^*$$

with $f^{(d)}$ converging to f^* for $d \rightarrow \infty$. Computing $f^{(d)}$ is now a semi-definite program (SDP).

Exploiting symmetry in semi-definite programs has proven to be effective in the past, see [GPO4]. One also deduces from [RTJL13] that a mathematical understanding of the symmetry is fruitful, although therein the authors consider different functions with another kind of invariance. Finally, the exploitation of sign symmetry for the integer lattice has been addressed for the univariate case in [Dumo7] and more recently in [KdK23].

2 Scientific Contributions

I will now describe two symmetry reduction techniques to which I contributed, their novelty and the involved collaborations. Furthermore, I will describe the functionality of a Maple software package that I have developed for computational purposes.

My doctorate with Evelyne Hubert (Sophia Antipolis, FR) at Inria d'Université Côte d'Azur was part of the European Marie Skłodowska-Curie project POEMA, a network of 15 doctoral students with the goal to gain efficiency in optimization through moment theory and algebraic structures. My thesis [Met22] covers the contributions from Sections 2.1 and 2.2. These are based on joint work with Hubert, Philippe Moustrou (Toulouse, FR) and Cordian Riener (Tromsø, NO) that was initiated during a secondment in Tromsø, that I conducted at the beginning of my second PhD year. My role in this collaboration was to write the articles, proof the theorems and implement the algorithms under the supervision and guidance of Hubert and Riener. Moustrou provided us with an application in graph coloring, see Section 2.2.

After the PhD, I started a postdoc position at the University of Kaiserslautern-Lautern with Ulrich Thiel (Kaiserslautern, DE). During those two years, I conducted mostly independent research that has lead to one single author paper, see Section 2.3, and one joint work with Sebastian Debus (Chemnitz, DE), see Section 2.4.

2.1 Orbit Space Reductions

By Bourbaki's theorem on fundamental invariants [Bou68, Ch. VI, §3], any invariant function f can be rewritten uniquely as a polynomial in terms of so called **fundamental invariants**. This means that there are some distinguished invariants $\theta_1, \dots, \theta_n$, such that

$$f(u) = g(\theta_1(u), \dots, \theta_n(u)) =: g(\theta(u))$$

for some unique n -variate polynomial g . In particular, the optimization problem becomes

$$f^* = \min_{u \in \mathbb{R}^n} f(u) = \min_{u \in \mathbb{R}^n} g(\theta(u)) = \min_{z \in \theta(\mathbb{R}^n)} g(z).$$

When going back to the example of the hexagon in Figure 1, this rewriting strategy implies that instead of considering a function over the entire hexagon, one may reduce to a small subset, namely the darker shaded triangle. More precisely, orbit space reduction reduces the number of SDP variables in the Lasserre hierarchy by the cardinality of the group \mathcal{W} , that is, the number of transformations.

There are two problems to be overcome:

1. The polynomial g must be computed.
2. The new feasible region $\theta(\mathbb{R}^n)$, that is, the image of the space under the fundamental invariants, must be described. The latter is also called the **orbit space** of \mathcal{W} .

The computation of g becomes trivial with the theory behind symmetries. Indeed, one can use a partial ordering to show that any invariant f can be rewritten as

$$f(u) = \sum_{\mu \in \Omega^+} f_\mu \exp(-2\pi i \langle \mu, u \rangle) + \text{lower-order-terms},$$

where no two lattice elements in Ω^+ can be obtained from one another through \mathcal{W} -transformations and the lower-order-terms are obtained from the elements in Ω^+ , see [Bou68, Ch. VI, §3]. Using the definition of **generalized Chebyshev polynomials** T_μ from [HW88, MNR13, HS22] one finds the polynomial expression

$$f(u) = \sum_{\mu \in \Omega^+} f_\mu T_\mu(\theta(u)) \quad \text{and in particular} \quad g(z) = \sum_{\mu \in \Omega^+} f_\mu T_\mu(z).$$

Together with Hubert and Riener, we solved the second problem, the description of the orbit space for the lattices A_{n-1}, B_n, C_n, D_n and G_2 in [HMR24]. In this article, we use the fact that the corresponding group \mathcal{W} has a particularly nice structure, allowing the use of tools from algebraic geometry [CLO05]. Our main result is the construction of a polynomial matrix \mathbf{P} so that a point $z \in \mathbb{R}^n$ is contained in the orbit space if and only if the matrix $\mathbf{P}(z)$ is positive semi-definite. In particular, the optimization problem becomes

$$f^* = \min_{\mathbf{P}(z) \succeq 0} \sum_{\mu \in \Omega^+} f_\mu T_\mu(z).$$

[DMMV19]. Subsequently, this allowed us to compute estimates on the spectral bound for other infinite graphs that were so far studied only with different, mostly combinatorial, tools. Table 1 shows a comparison between our approach and previous best known results that used different techniques.

Note that the spectral bound is just a lower bound and not an approximation of the chromatic number. The important conclusion of our work is that the spectral bound is not sharp for some polytopes, which leaves open the problem of classifying these cases.

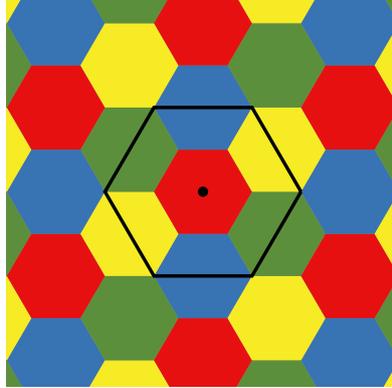


Figure 3: The graph \mathbb{R}^2 avoiding the hexagon (without the interior!) can be painted with four colors. The point in the origin \bullet , which has assigned the color red, must not share the same color with any other point on the hexagon. With a combinatorial argument, one can conclude that three colors are not sufficient [BBMP19]. This is also the conclusion from our computation in Table 1, by which the chromatic number (an integer!) is 3.57.

V	S	previous lower bound for $\chi_m(V, S)$	our estimate [HMMR24]
\mathbb{Z}^3	3-dim. crosspolytope with radius 4	7	> 6.30
\mathbb{Z}^4	4-dim. crosspolytope with radius 4	9	> 10.86
\mathbb{Z}^n	n -dim. crosspolytope with odd radius	2	2
\mathbb{Z}^n	n -dim. crosspolytope with radius 2	$2n$	$2n$
\mathbb{R}^2	hexagon	4	> 3.57
\mathbb{R}^3	rhombic dodecahedron	8	> 6.10
\mathbb{R}^4	icositetrachoron	15	> 10.02
\mathbb{R}^n	n -dim. cube	2^n	2^n

Table 1: Comparison of the previous lower bounds on the chromatic number $\chi_m(V, S)$ and our estimates on the spectral bounds (V vertices, S avoided set). The color of the table entry indicates whether our estimate is worse, better or confirms a previous one.

2.3 REDUCTION VIA SYMMETRY ADAPTED BASES AND COMPARISON

The technique in my thesis relies on first exploiting the symmetry of the trigonometric polynomial by rewriting it in terms of Chebyshev polynomials, and afterwards applying SOS reinforcements. The order can be reversed, meaning that one first applies a semi-definite relaxation and then exploits symmetry. I proposed a new complementary technique at the ISSAC'23 conference [Met23], which was published later in the Journal of Symbolic Computation [Met25].

The problem of computing f^* can be rewritten to the problem of computing the maximal $\text{Trace}(\mathbf{mat}(f) \mathbf{X})$, where $\mathbf{mat}(f)$ is an infinite matrix representation of a trigonometric polynomial and \mathbf{X} is a positive semi-definite Toeplitz matrix. Truncation at degree d leads to a Lasserre hierarchy

$$f^* \geq f^d := \min_{\mathbf{X} \in \text{Toep}_d} \text{Trace}(\mathbf{mat}(f) \mathbf{X}) \quad \text{s.t.} \quad \mathbf{X} \succeq 0, \text{Trace}(\mathbf{X}) = 1,$$

see also [Dumo7]. In the article, I equip Toep_d with a \mathcal{W} -representation and show that, if f is \mathcal{W} -invariant, one can restrict \mathbf{X} to the space of invariant Toeplitz matrices $\text{Toep}_d^{\mathcal{W}}$, which preserves the optimal value. With respect to the **isotypic decomposition** [Ser77] of Toep_d as a \mathcal{W} -module into irreducibles, one can thus compute a symmetry adapted basis in which the SDP matrices are block diagonal. This leads to smaller matrices in the Lasserre hierarchy.

For example, for a group \mathcal{W} with 3 irreducible representations, an invariant Toeplitz matrix with $7^2 = 49$ entries only has $2^2 + 2^2 + 3^2 = 17$ entries with respect to a symmetry adapted basis, that is,

$$\left(\begin{array}{cccccccc} \blacksquare & \blacksquare \\ \blacksquare & \blacksquare \\ \blacksquare & \blacksquare \\ \blacksquare & \blacksquare \\ \blacksquare & \blacksquare \\ \blacksquare & \blacksquare \\ \blacksquare & \blacksquare \end{array} \right) \rightarrow \left(\begin{array}{ccc} \left[\begin{array}{cc} \color{red}\blacksquare & \color{red}\blacksquare \\ \color{red}\blacksquare & \color{red}\blacksquare \end{array} \right] & & \\ & \left[\begin{array}{cc} \color{green}\blacksquare & \color{green}\blacksquare \\ \color{green}\blacksquare & \color{green}\blacksquare \end{array} \right] & \\ & & \left[\begin{array}{ccc} \color{blue}\blacksquare & \color{blue}\blacksquare & \color{blue}\blacksquare \\ \color{blue}\blacksquare & \color{blue}\blacksquare & \color{blue}\blacksquare \\ \color{blue}\blacksquare & \color{blue}\blacksquare & \color{blue}\blacksquare \end{array} \right] \end{array} \right).$$

I will now compare the computational cost of the two approaches discussed so far in terms of the sizes of the blocks of the SDP matrices. Denote by $|\Omega_d|$ the number of lattice elements that support trigonometric polynomials up to degree d .

- no symmetry reduction: $|\Omega_d|^2$ (1 Hermitian block).
- orbit space reduction: $\frac{|\Omega_d|^2 + n^2 |\Omega_{d-n}|^2}{|\mathcal{W}|^2}$ (2 real symmetric blocks).
- symmetry adapted bases: $\sum_{i=1}^{\#\text{irrep.}} d_i \left(m_i^{(d)} \right)^2$ (#irrep. Hermitian blocks with d_i equal subblocks).

Here, #irrep. is the number of irreducible representations of \mathcal{W} with dimension d_i and multiplicity $m_i^{(d)}$.

The observation from Table 2 is that the orbit space reduction yields smaller SDP matrices with less blocks. The downside is that the setup in the Chebyshev basis is more difficult and requires a larger minimal order of the hierarchy.

$\mathcal{W} \setminus d$	2	3	4	5	6
B_2	6, 2	10, 6	15, 12	21, 20	28, 30
	6, 3, 3, 1, 6	10, 6, 6, 3, 12	15, 10, 10, 6, 20	21, 15, 15, 10, 30	28, 21, 21, 15, 42
A_2	–	10, 3	15, 9	21, 18	28, 30
	6, 1, 6	10, 3, 12	15, 6, 20	21, 10, 30	28, 15, 42
G_2	–	6, 3	9, 6	12, 12	16, 18
	4, 2, 0, 1, 3, 3	6, 4, 1, 2, 6, 6	9, 6, 2, 4, 10, 10	12, 9, 4, 6, 15, 15	16, 12, 6, 9, 21, 21
B_3	–	13, 3	22, 9	34, 21	50, 39
	7, 3, 0, 0, 4, 1, 7, 5, 2, 1	13, 7, 1, 0, 10, 4, 17, 13, 7, 5	22, 13, 3, 1, 20, 10, 33, 27, 17, 13	34, 22, 7, 3, 35, 20, 57, 48, 33, 27	50, 34, 13, 7, 56, 35, 90, 78, 57, 48
A_3	–	–	35, 4	56, 16	84, 40
	10, 0, 5, 12, 3	20, 1, 14, 30, 12	35, 4, 30, 60, 30	56, 10, 55, 105, 60	84, 20, 91, 168, 105

Table 2: Comparison of the SDP matrix sizes. The columns are indexed by the order d of the Lasserre hierarchy. The rows are indexed by the symmetry group \mathcal{W} . The upper entry per $\mathcal{W} \setminus d$ gives the block sizes for the SPD matrices in the orbit space reduction. The lower entry gives the block sizes with respect to the symmetry adapted basis.

I did not analyze the convergence rate of either approach, but only collected some computational data so far. For three test functions, the results are shown in Table 3. The table indicates that the orbit space reduction yields better numerical results and converges faster.

d	3	4	5	6	7
OSR	−1.16667	−1.16667	−1.16667	−1.16667	−1.16667
SAB	−1.18824	−1.180240	−1.17058	−1.16970	−1.16719
OSR	−3.20499	−3.10220	−2.98718	−2.98718	−2.98718
SAB	−3.50118	−3.40372	−3.31195	−3.25383	−3.22049
OSR	−2.27496	−2.06250	−2.06250	−2.06250	−2.06250
SAB	−2.12159	−2.10672	−2.1012	−2.09959	−2.09073

Table 3: Comparison of the numerical accuracy of the two symmetry reduction techniques for three different test functions, see [HMMR24]. Note that the reduction via symmetry adapted basis (SAB) yields the same result as the dense approach. Meanwhile, the orbit space reduction (OSR) has a different solution.

2.4 MULTIPLICATIVE COINVARIANTS

The two symmetry reduction techniques I presented so far, orbit space reduction and via symmetry adapted bases, require a “setup process”. For orbit space reduction, this process is the computation of the polynomials defining the orbit space. Our article [HMR24] provides an efficient way to do that. For reduction via symmetry adapted bases on the other hand, the process involves the computation of said basis. This motivated Sebastian Debus from TU Chemnitz and myself to write an article [DM24] on the **multiplicative coinvariant space**.

I will not give the definition of a coinvariant space here, but only emphasize that the motivation behind this theoretical object is to eliminate redundant copies of irreducibles modules in computational data. Having access to a coinvariant basis allows the efficient computation of a symmetry adapted basis.

Instead of reinventing the wheel, the article with Debus draws a connection to a neighboring field of invariant theory. Our main result allows the computation of a multiplicative coinvariant basis from a so called additive one algorithmically.

3 SOFTWARE DEVELOPMENT

In order to verify the theoretical ideas preceding [HMR24, HMMR24, Met25, DM24], test the practicality and gain new insights through experiments, I began with the open source development of a Maple package entitled `GENERALIZEDCHEBYSHEV`, which is available under

<https://github.com/TobiasMetzlaff/GeneralizedChebyshev> 

From the basics, such as calculating orbits under symmetry groups, to the computation of moment matrices in the Chebyshev basis and the symmetry adapted bases, this package equips the user with tools to conduct multiplicative invariant theory in practice. The package is and will for the foreseeable future be maintained on my GitHub page.

Many software packages provide tools to compute moment matrices and SDP reductions for optimization, such as `GLOPTIPOLY`¹ or `MOMENTTOOLS`², but those only support the basis of standard monomials with permutation symmetry and make the exploitation of more general crystallographic symmetries inconvenient.

The success of the package `TSSOS`³ for sparsity exploitation, shows that specialized software is often advantageous to use in practice.

I want to emphasize some of the distinguishing features of the package.

- The generalized Chebyshev polynomials, as they appear in several applications, are obtained via a recurrence formula $|\mathcal{W}| T_\mu T_\nu = \sum_s T_{\mu+s(\nu)}$, which is, when implemented in a straightforward manner, very inefficient. Using the theory from [Bou68], their calculation is improved significantly.
- The package allows to set up SDPs for the Lasserre hierarchy in the Chebyshev basis, which is, for crystallographic symmetry reductions, the natural choice.
- Similarly, the computation of symmetry adapted bases is also enhanced through theoretical understanding of the underlying representation theory.

To summarize, although there are other computer algebra systems and softwares, which feature certain aspects of the package in a more general context with more advanced tools, `GENERALIZEDCHEBYSHEV` combines all these features in an overall more efficient manner and is tailored to connect the theory of crystallographic symmetries in a coherent way with their exploitation in optimization.

¹<https://homepages.laas.fr/henrion/software/gloptipoly3/> 

²<https://www-sop.inria.fr/members/Bernard.Mourrain/software/MomentTools/> 

³<https://wangjie212.github.io/TSSOS/dev/> 

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