SymDPoly: symmetry-adapted moment relaxations for noncommutative polynomial optimization

Rosset Denis

1 Perimeter Institute for Theoretical Physics, Waterloo, Ontario, Canada, N2L 2Y5

* physics@denisrosset.com

Abstract

Semidefinite relaxations are widely used to compute upper bounds on the objective of optimization problems involving noncommutative polynomials. Such optimization problems are prevalent in quantum information. We present an algorithm able to discover automatically and exploit the symmetries present in the problem formulation. We also provide an open source software library written in Scala (https://github.com/denisrosset/symdpoly) that computes symmetry-adapted semidefinite relaxations with interfaces to a variety of open-source and commercial semidefinite solvers. We discuss the advantages of symmetrization, namely reductions in memory use, computation time, and increase in the solution precision.

Introduction

Semidefinite programming is a prevalent tool to study quantum systems. As density matrices are semidefinite matrices of trace one, semidefinite programs naturally address questions related to unambiguous state discrimination [15], entanglement detection [14], entanglement measures [45, 51], measurement incompatibility [54] and steering [7], among other applications. Polynomial optimization problems are also frequent in quantum information. Systems of commutative polynomial equations appear in the characterization of sets of local correlations; for example in the study of network-locality [48], the study of causal structures [27], and maximal violations of Bell inequalities for given states [25]. These polynomial problems can be handled by a hierarchy of semidefinite relaxations based on sums of squares formulations [17, 26, 38, 41]. Other questions are neatly formulated as optimizations over noncommutative polynomial rings of operators. In this second setting, moment relaxations are used to characterize the quantum set of correlations [12, 41, 35], provide dimensional bounds [33, 37], quantify entanglement [31] or characterize in a robust manner quantum devices [2, 56]. Similar hierarchies were studied in their mathematical abstract setting [4, 6, 21, 36]. The complexity of those semidefinite relaxations increases rapidly with the relaxation degree. To address that problem, the symmetries of the original problem can be applied to the semidefinite relaxations and reduce the problem size. The technique was introduced in [19] in the commutative case and reviewed in [22, 26].

In quantum information, symmetry techniques have been applied to semidefinite programs: in quantum control [3] or in quantum metrology [8]. In the specific case of sums of squares relaxations, symmetry techniques were applied to self-testing [1] and translation-invariant Bell inequalities [16]. We also mention the related work in...
preparation\cite{50} applying to optimization over finite-dimensional quantum systems, based on randomized sampling rather than exact algebraic methods. As the problem sizes grow, semidefinite relaxations are not written by hand but rather constructed using software libraries. Among others, we mention the libraries YALMIP\cite{29}, GloptiPoly\cite{22}, SOSTOOLS\cite{40}, SparsePOP\cite{52} for the commutative case; NCSOStools\cite{6} and Ncpol2SDpa\cite{53} in the noncommutative case. Our implementation is particularly influenced by this last package.

In the present manuscript, we introduce symmetry-adapted moment relaxations for a variety of noncommutative optimization problems arising from quantum information scenarios, along with a software library that automates their formulation. The use of symmetries leads to huge efficiency gains in that context. Consider a semidefinite program in the canonical form that involves a matrix of size $n \times n$ on a space of affine dimension $m$. When using a primal-dual barrier method such as implemented by SDPA\cite{55}, the memory requirements scale as $O(m^2 + mn^2)$, and the CPU time per iteration scales\footnote{In the memory requirements, the $O(n^2)$ term represents the Schur complement matrix and $O(mn^2)$ is an upper bound that depends on the matrix sparsity. The scaling of the CPU time per iteration has three parts: the computation of the Schur complement in $O(mn^3 + mn^2)$, the Cholesky decomposition in $O(m^3)$ and various other contributions in $O(n^3)$.} as in $O(m^3 + n^3 + mn^3 + m^2n^2)$. Thus, any method that reduces $m$ and/or $n$ has a great impact on the memory and CPU requirements. Moreover, some recent SDP solvers only converge when the solution has no degeneracies\cite{57}, and in general, reducing the complexity can improve the precision of the solutions by 1-2 orders of magnitude, as we will see in the present manuscript.

The manuscript is divided in four parts. In Section\footnote{In the memory requirements, the $O(n^2)$ term represents the Schur complement matrix and $O(mn^2)$ is an upper bound that depends on the matrix sparsity. The scaling of the CPU time per iteration has three parts: the computation of the Schur complement in $O(mn^3 + mn^2)$, the Cholesky decomposition in $O(m^3)$ and various other contributions in $O(n^3)$.} we define formally optimization problems over noncommutative polynomials and their symmetries. In contrast to previous presentations, we emphasize the use of rewriting rules during monomial expansion. In Section\footnote{In the memory requirements, the $O(n^2)$ term represents the Schur complement matrix and $O(mn^2)$ is an upper bound that depends on the matrix sparsity. The scaling of the CPU time per iteration has three parts: the computation of the Schur complement in $O(mn^3 + mn^2)$, the Cholesky decomposition in $O(m^3)$ and various other contributions in $O(n^3)$.} we review the semidefinite hierarchies based on moment relaxations; most importantly, we express the variants due to Moroder et al.\cite{31} and Burgdorf et al.\cite{4,6} in a common framework. In Section\footnote{In the memory requirements, the $O(n^2)$ term represents the Schur complement matrix and $O(mn^2)$ is an upper bound that depends on the matrix sparsity. The scaling of the CPU time per iteration has three parts: the computation of the Schur complement in $O(mn^3 + mn^2)$, the Cholesky decomposition in $O(m^3)$ and various other contributions in $O(n^3)$.} we discuss the choices made in our implementation, including the algorithms enabling symmetric formulations. We present a practical application in Section\footnote{In the memory requirements, the $O(n^2)$ term represents the Schur complement matrix and $O(mn^2)$ is an upper bound that depends on the matrix sparsity. The scaling of the CPU time per iteration has three parts: the computation of the Schur complement in $O(mn^3 + mn^2)$, the Cholesky decomposition in $O(m^3)$ and various other contributions in $O(n^3)$.} by computing high precision bounds for the $I_{3232}$ inequality\cite{10,18,49}.

1 Optimization over noncommutative polynomials

We assume that the reader is familiar with moment relaxations, as introduced in\cite{12,34,35} for problems in quantum information. Our symmetric moment relaxations apply to optimization problems defined using noncommutative polynomials. We use a modified version of the presentation \cite{36}: first, we define the monomials involved, their rewriting rules and symmetries, before defining noncommutative polynomials over those monomials in a second step, and finally express optimization problems over those polynomials. We are not overly concerned by technicalities such as proving convergence: the optimal values and convergence properties of our hierarchies match the original formulations published in the literature.

1.1 Monomials

We consider a set of letters $\{x_1, x_2, \ldots, x_n\}$, along with an involution $\ast$ such that $(x_1)^\ast = x_1$. We collect these letters in the set $\mathfrak{x}$ along with their images under $\ast$

$$\mathfrak{x} = \{x_1, x_2, \ldots, x_n, x_1^\ast, x_2^\ast, \ldots, x_n^\ast\}.$$
We write $S$, the group of all permutations of elements $x$ that commute with the involution: we require for all $\pi \in S$, that $\pi(x_i^*) = \pi(x_i)^*$. We write $W$ the free monoid on $x$, defined as follows. A word or monomial $w \in W$ is written

$$w = w_1 w_2 \ldots w_m$$

with $m = |w|$ the length of $w$. The identity element is the empty word of zero length, denoted by $1$, and the monoid operation $\cdot$ is word concatenation, i.e. for words $v, w \in W$ written over letters as $v = v_1 \ldots v_k$ and $w = w_1 \ldots w_m$ we have

$$v \cdot w = v_1 \ldots v_k w_1 \ldots w_m.$$

The involution $*$ acts on a word $w \in W$ as

$$w^* = w_m^* w_{m-1}^* \ldots w_1^*,$$

so that $(v \cdot w)^* = w^* \cdot v^*$. Thus $W$ is a $*$-monoid \cite{14}. An element $\pi \in S_*$ acts on $w = w_1 w_2 \ldots w_m \in W$ as

$$\pi(w) = \pi(w_1) \pi(w_2) \ldots \pi(w_m), \quad \pi(1) = 1.$$

We extend our free monoid $W$ to $W^0 = W \cup \{0\}$ by the addition of a zero element. We define formally

$$0^* = 0, \quad 0 \cdot 0 = 0, \quad 0 \cdot w = 0, \quad w \cdot 0 = 0, \quad \text{for all } w \in W,$$

$$\pi(0) = 0 \quad \text{for all } \pi \in S_*, \quad \text{and } |0| = -\infty.$$

A congruence $\sim$ on $W^0$ is an equivalence relation that satisfies, for all $x, y, a, b \in W^0$,

$$(v \sim x \text{ and } w \sim y) \quad \Rightarrow \quad v^* \sim x^* \text{ and } v \cdot w \sim x \cdot y.$$ 

Given a word $w \in W^0$, we write $[w]_\sim = \{v \in W^0 : v \sim w\}$ its congruence class, and $\tilde{W} = W^0/\sim$ the set of all such congruence classes. We define a binary operation $\cdot$ on the set $\tilde{W}$ by

$$[v]_\sim \cdot [w]_\sim = [v \cdot w]_\sim \quad \text{for all } v, w \in W^0,$$

and we easily verify that $\tilde{W}$ is a $*$-monoid, the quotient monoid of $W$ by $\sim$. We define the symmetry group $S_\sim \subseteq S_*$ as containing permutations that preserve congruence

$$S_\sim = \{ \pi \in S_* : \pi(v) \sim \pi(w) \text{ for all } v, w \in W^0 \text{ such that } v \sim w \}.$$  \hspace{1cm} (1)

Then the action of $S_\sim$ on $\tilde{W}$ is well defined:

$$\pi([w]_\sim) = [\pi(w)]_\sim \quad \text{for all } \pi \in S_\sim \text{ and } w \in W^0.$$

For computational purposes, the congruence $\sim$ is represented by a set of rewriting rules $R = \{v_1 \rightarrow w_1, v_2 \rightarrow w_2, \ldots\}$, which, given a monomial $x v_i y$, applies as

$$x v_i y \rightarrow x w_i y \quad \text{for all } x, y \in W^0, (v_i \rightarrow w_i) \in R.$$

For example, these rewriting rules can encode commutation relations ($x_j x_i \rightarrow x_i x_j$ for some pairs $i, j$).

A word $u$ is in normal form if it cannot be rewritten any further. We write $N_R(u)$ the normal form obtained after repeated application of the rewriting rules $R$: we require the rewriting system to be confluent, which means that the normal form of $u$
does not depend on the order of rule application. We then define formally the congruence $\sim$ from the rewriting system $R$:

$$v \sim w \iff \mathcal{N}_R(v) = \mathcal{N}_R(w).$$

The definition (1) becomes

$$\mathcal{S}_\sim = \{ \pi \in \mathcal{S} : \mathcal{N}_R(\pi(v)) = \mathcal{N}_R(\pi(w)) \text{ for all } v, w \in \mathcal{W}^0 \text{ such that } \mathcal{N}_R(v) = \mathcal{N}_R(w) \}.$$

Confluent rewriting systems can be constructed and verified using the Knuth-Bendix completion algorithm, whose description and implementation is outside the scope of our work. We require the user of our software to provide a confluent rewriting system (confluent rules for common correlations scenarios are provided below).

We work with rewriting rules that such that $\mathcal{N}_R(w)$ has minimal length over the equivalence class of $w$. Thus, we define the length of $[w]$ as the length of $\mathcal{N}_R(w)$.

### 1.2 Rewriting rules for quantum correlation scenarios

We now give two examples of monoids $\mathcal{W}$ along with their rewriting rules $R$ and symmetry group $\mathcal{S}_\sim$.

**Binary outputs.** — Consider a two-party Bell scenario where Alice (resp. Bob) has input $x = 1, \ldots, m$ taking $m$ distinct values (respectively $y = 1, \ldots, m$) and binary outputs $a = \pm 1$ (resp. $b = \pm 1$). We write $A_x$ (resp. $B_y$) the formal variable associated with the projective measurements of Alice with eigenvalues $-1$ and $+1$ (and the same for Bob). We have

$$\mathfrak{x} = \{ A_1, \ldots, A_m, B_1, \ldots, B_m, A_1^*, \ldots, A_m^*, B_1^*, \ldots, B_m^* \} \quad (2)$$

and equivalence of monomials is defined by the rewriting rules

$$R = \{ A_x^* \rightarrow A_x, \quad B_y^* \rightarrow B_y, \quad B_y A_x \rightarrow A_x B_y, \quad A_x A_x \rightarrow 1, \quad B_y B_y \rightarrow 1 \}$$

for $x, y = 1, \ldots, m$. To simplify the computations in this self-adjoint case, we identify $A_x^* = A_x$ and $B_y^* = B_y$ directly in $\mathfrak{x}$. The symmetry group $\mathcal{S}_\sim^\mathfrak{x}$ contains the permutations preserving the partition $\{ \{ A_1, \ldots, A_m \}, \{ B_1, \ldots, B_m \} \}$.

**Multiple outputs.** — We now generalize this example to the case of $d \geq 2$ outcomes. Let Alice (respectively Bob) choose between $m$ projective measurements, each with $d$ outcomes. We write $A_{a|x}$ the formal variable associated with the projector corresponding to the output $a$ and input $x$ (respectively $B_{b|y}$ for Bob). As projectors are Hermitian, we identify $A_{a|x}^* = A_{a|x}$ and $B_{b|y}^* = B_{b|y}$ and have

$$\mathfrak{x} = \{ A_{a|x}, B_{b|y} \}$$

with the rewrite rules

$$R = \{ A_{a|x} A_{a'|x} \rightarrow A_{a|x}, \quad A_{a|x} A_{a'|x} \rightarrow 0, \quad B_{b|y} B_{b'|y} \rightarrow B_{b|y}, \quad B_{b|y} B_{b'|y} \rightarrow 0, \quad B_{b|y} A_{a|x} \rightarrow A_{a|x} B_{b|y} \}$$

for $a, a', b, b' = 1, \ldots, d$ and $x, y = 1, \ldots, m$, with $a' \neq a$, $b' \neq b$. The symmetry group $\mathcal{S}_\sim$ contains all permutations preserving the partitions $P_1$ and $P_2$:

$$P_1 = \{ \{ A_{1|1}, \ldots, A_{d|m} \}, \{ B_{1|1}, \ldots, B_{d|m} \} \},$$

$$P_2 = \{ \{ A_{1|1}, \ldots, A_{d|m} \}, \ldots, \{ A_{1|m}, \ldots, A_{d|m} \}, \{ B_{1|1}, \ldots, B_{d|1} \}, \ldots, \{ B_{1|m}, \ldots, B_{d|m} \} \}.$$  

Note that the relation $\sum_a A_{a|x} = \sum_b B_{b|y} = 1$ is not captured at the level of monomials.
1.3 Noncommutative polynomials

Given a set of letters \( x \), a list of rewrite rules \( R \), and a field \( \mathbb{K} \in \{ \mathbb{R}, \mathbb{C} \} \), we write \( \mathbb{K}[\mathbb{V}] = \{ p \} \) the set of formal sums of the form

\[
p = \sum_{[w] \in \mathbb{V}} p_{[w]}[w], \quad p_{[w]} \in \mathbb{K},
\]

where \( p_{[w]} = 0 \) for all but finitely many \( w \); in addition, we require that \( p_{[0]} = 0 \). Such formal sums are noncommutative polynomials over the monomials \( \mathbb{V} \). The degree of \( p \) is given by the largest \( |w| \)-length corresponding to a nonzero \( p_{[w]} \). Addition on \( \mathbb{K}[\mathbb{V}] \) is defined component-wise, and the multiplication is defined by having the elements of \( \mathbb{K} \) commute with the elements of \( \mathbb{V} \) (and forcing \( p_{[0]} = 0 \)). The involution acts as

\[
p^* = \sum_{[w] \in \mathbb{V}} (p_{[w]})^*[w]^*,
\]

where \( k^* \) is the complex conjugate of \( k \in \mathbb{K} \). With these definitions, \( \mathbb{K}[\mathbb{V}] \) is a *-algebra. The permutation group \( S_{\infty} \) acts naturally on \( p \):

\[
\pi(p) = \sum_{[w] \in \mathbb{V}} p_{[w]}[\pi(w)] \quad \text{for } \pi \in S_{\infty}.
\]

1.4 Optimization problems

Consider now the set \( \mathcal{B}(\mathcal{H}) \) of bounded operators on a Hilbert space \( \mathcal{H} \) defined on the field \( \mathbb{K} \), with \( \mathbb{I} \in \mathcal{B}(\mathcal{H}) \) the identity operator. Given a set of operators \( X = (X_1, \ldots, X_n) \) and a polynomial \( p \in \mathbb{K}[\mathbb{V}] \), we define the operator \( p(X) \in \mathcal{B}(\mathcal{H}) \) by replacing

\[
1 \to \mathbb{I}, \quad x_i \to X_i, \quad x_i^* \to X_i^*,
\]

in the normal form of \( p \), where \( X_i^* \) is the adjoint of \( X_i \). Note that the substitution is consistent only if the operators \( X \) satisfy the same relations \( R \) as the variables \( x \). We evaluate those polynomial on vectors \( \phi \in \mathcal{H} \) by

\[
\langle p(X) \rangle_{\phi} = \langle \phi | p(X) | \phi \rangle,
\]

noting that other choices are possible (see Section 2.4). A polynomial for which \( p = p^* \) is Hermitian, and in that case \( p(X) = p^*(X) \) is a Hermitian operator. For Hermitian \( p = p^* \), the quantity \( \langle p(X) \rangle_{\phi} \) is real; this motivates the following canonical form of a optimization problem over noncommutative polynomials.

\[
p^* = \sup_{X, \phi} \langle p(X) \rangle_{\phi} \quad (3)
\]

subject to

\[
\begin{align*}
\langle 1 \rangle_{\phi} &= 1, \\
q_i(X) &\geq 0, \quad i \in I, \\
r_j(X) &= 0, \quad j \in J, \\
s_k(X) &\geq 0, \quad k \in K,
\end{align*} \quad (4)
\]

where \( I, J \) and \( K \) are index sets, all \( q_i, s_k \) and \( p \) are Hermitian, the optimization is carried out over all states \( \phi \in \mathcal{H} \) defined on Hilbert spaces \( \mathcal{H} \) of arbitrary dimension and operators \( X = (X_1, \ldots, X_n) \in \mathcal{B}(\mathcal{H}) \) that satisfy the rewrite rules \( R \). We denote by \( q_i(X) \geq 0 \) the positive semidefiniteness of \( q_i(X) \), i.e. \( \langle \psi | q_i(X) | \psi \rangle \geq 0 \) for all \( \psi \in \mathcal{H} \) (not only for \( \psi = \phi \)).

Similarly to \([30]\) where they are called binomials, we allow efficient handling of two-term equalities \( v - w = 0 \), where \( v, w \in \mathcal{W} \), by handling them at the level of the congruence \( \sim \).
1.5 Symmetries of optimization problems

While the group \( S_\sim \) preserved the structure of the congruence \( \sim \), we define the ambient group \( G \subseteq S_\sim \) that preserves feasibility under the constraints. \( \text{G} = \{ g \in S_\sim : (X, \phi) \text{ is feasible} \implies (g(X), \phi) \text{ is feasible} \} \).

The symmetry group \( G_* \) of the optimization problem also preserves optimality:

\[ G_* = \{ g \in G : \langle p(g(X))\rangle_{\phi} = \langle p(X)\rangle_{\phi} \text{ for all } (X, \phi) \text{ is feasible} \}. \]

1.6 Signed monomials and generalized permutations

For efficiency, we generalize slightly the permutations used to build the groups \( S_\sim, S_\sim, G \) and \( G^* \). A generalized permutation \( \pi \) on \( n \) elements is defined by the sequence of images

\[ (\pi_1, \ldots, \pi_n) = (\pm \rho_1, \ldots, \pm \rho_n), \]

where \( \rho : i \mapsto \rho_i \) is a standard permutation. The generalized permutation \( \pi \) acts on the integers \( \{-n, \ldots, -1, 1, \ldots, n\} \) by

\[ \pi(i) = \text{sign}(i)\pi_{|i|}. \]

The group of the generalized permutations on \( n \) elements is also called the signed symmetric group. In the present case, we write \( S^+_{\sim} \) the signed symmetric group acting on the signed letters

\[ x^\pm = \{ \pm x_1, \ldots, \pm x_n, \pm x_1^*, \ldots, \pm x_n^* \}. \]

The signed monomials \( W^\pm \) are defined as product of letters preceded with a sign \( \omega = \pm 1 \). Given such \( w^\pm \in W^\pm \), we define \( \text{sign}(w^\pm) = \omega \) and \( \text{abs}(w^\pm) = |w^\pm| = v_1 \ldots v_m \). The action of \( \pi \in S^+_{\sim} \) on \( w^\pm \in W^\pm \) is

\[ \pi(\omega x_{i_1} \ldots x_{i_m}) = \omega \text{sign}(\pi(i_1) \ldots \pi(i_m)) x_{\pi(i_1)} \ldots x_{\pi(i_m)}. \]

We consider the equivalence classes of \( W^\pm \) under the rewriting rules \( R \), noting that \( R \) does not affect the sign: thus, elements of \( W^\pm / \sim \) are simply written \( \pm [w] \) with \( [w] \in W / \sim \). Similarly, \( S^+_{\sim} \) can be restricted to be compatible with the congruence \( \sim \), so that \( S^+_{\sim} \) acts consistently on the equivalence classes of \( W^\pm / \sim \). For example, the rewrite rule \( x_i x_i \rightarrow x_i \) is not compatible with the generalized permutation \( \pi \) that sends \( x_i \) to \( \pi(x_i) = -x_i \). However, \( \pi(x_i) = -x_i \) would be compatible with the rewrite rules for variables \( \{1, 2\} \), and generalized permutations lead to huge gains of efficiency on quantum correlation scenarios involving binary outputs. Finally, we identify \( K \)-linear combinations of signed monomials \( K[W^\pm] \) with polynomials in \( K[\tilde{W}] \) by writing

\[ p = \sum_{[w] \in W^\pm} p_{[w]} [w^\pm] = \sum_{[w^\pm]} \text{sign}([w^\pm]) p_{[w]} \text{abs}(w^\pm), \]

and the action of \( S^+_{\sim} \) on \( K[\tilde{W}] \) follows.

1.7 Example: the CHSH inequality

We consider a two-party Bell scenarios with binary inputs and outputs, i.e. \( x, y = 0, 1 \) and \( a, b = \pm 1 \). The measurements are represented by Hermitian operators \( x = \{ A_0, A_1, B_0, B_1 \} \), along with the rewriting rules \( \{1, 2\} \). The group \( S^+_{\sim} \) is generated by the generalized permutations (abusing slightly the notation)

\[ \pi_1 = (B_0, B_1, A_0, A_1), \quad \pi_2 = (A_0, A_1, B_1, B_0), \quad \pi_3 = (A_0, -A_1, B_0, B_1), \quad (5) \]
where $\pi_1$ permutes the parties, $\pi_2$ permutes the inputs of Bob, and $\pi_3$ is a conditional permutation of the outputs of Alice. The group $S_{\sim}^\pm$ is of order 128. We do not need to add explicitly the constraints
\[(1 \pm A_x) \succeq 0, \quad (1 \pm B_y) \succeq 0,\]
as $(1 \pm A_x)/2$ are both projectors: for example $(1 + A_x)/2 \sim (1 + A_x)^2/4$. Thus $G_{\sim}^\pm = S_{\sim}^\pm$.

Our goal is to maximize the value of the CHSH expression [9]
\[p_{\text{CHSH}} = [A_0B_0] + [A_0B_1] + [A_1B_0] - [A_1B_1]\]
without constraints $q_i, r_j$ or $s_k$. The expression $p_{\text{CHSH}}$ is symmetric under the group $G_{\sim}^\pm$ generated by
\[\sigma_1 = \pi_1, \quad \sigma_2 = \pi_2 \pi_3, \quad \sigma_3 = (-A_0, -A_1, -B_0, -B_1)\]
of order 16.

## 2 Moment relaxations

We now define moment relaxations of the optimization problems we just introduced. First, we present their standard formulation, before discussing their symmetrization. We conclude this section by solving a concrete example by hand.

### 2.1 Definition

Moment relaxations arise from the existence of a linear functional $L : \mathbb{K}[\tilde{W}] \to \mathbb{K}$ which satisfies
\[L([1]) = 1, \quad L(f) = L(f^*)^*, \quad L(f^* f) \succeq 0, \quad \text{for all } f \in \mathbb{K}[\tilde{W}],
\]
\[L(f^* q_i f) \succeq 0, \quad \text{for all } f \in \mathbb{K}[\tilde{W}], \quad i \in I,
\]
\[L(f r_j g) = 0, \quad \text{for all } f, g \in \mathbb{K}[\tilde{W}], \quad j \in J,
\]
\[L(s_k) \succeq 0, \quad \text{for all } k \in \mathcal{K}.
\]

Any feasible solution $(X, \phi)$ defines a linear functional
\[L_{(X, \phi)}(f) = \langle f(X) \rangle_{\phi}\]
that satisfies [6]. Moment relaxations are defined as a relaxation of the constraints [6], by considering test polynomials $f, g \in \mathbb{K}[\tilde{W}]$ such that the final expressions evaluated by $L$ involve only polynomials of maximal degree $2d$, for some $d \geq 1$:

\[\mathbb{K}[\tilde{W}]^{2d} = \{ f \in \mathbb{K}[\tilde{W}] : \deg(f) \leq 2d \}.
\]

Remark that the restriction $L : \mathbb{K}[\tilde{W}]^{2d} \to \mathbb{K}$ is fully defined by
\[L(f) = \sum_{\deg([w] \leq 2d} f_{[w]} y_{[w]}, \quad y_{[w]} \equiv L([w]),\]
as by linearity $L$ is completely characterized by the values $\vec{y} \in \mathbb{K}^{N_D}$, where $N_D$ is the number of $[w]$ of degree at most $D$.

We are now ready to express our constraints [6] in semidefinite form. The linear constraints are:
\[y_{[1]} = 1, \quad y_{[w]} = (y_{[w^*]})^*, \quad \sum_{[u][v][w]} (r_j)[v]y_{[uvw]} = 0, \quad \sum_{[w]} (s_k)[w]y_{[w]} \succeq 0, \quad (7)\]
while semidefinite constraints are given by the moment matrix $\Xi$ and the localizing matrices $\Lambda_i$:

$$\Xi = \sum_{\text{deg}([u],[v]) \leq d} y_{[u^* v]} E_{uv}^{uv} \succeq 0, \quad \Lambda_i = \sum_{\text{deg}([u],[v]) \leq d} (q_i)_{[w]} y_{[w^* w]} E_{uv}^{uv} \succeq 0,$$

with $E_{uv}$ a $N_d \times N_d$ matrix whose rows and columns indices $(r,c)$ correspond to an ordering of the monomials $[w]$ and

$$(E_{uv})_{r,c} = \begin{cases} 1 & \text{if } r = u \text{ and } c = v, \\ 0 & \text{otherwise,} \end{cases}$$

and, above, sums run over $[u],[v],[w]$ with the restriction that the $y_{[...]}$ is indexed by a monomial of degree at most $2d$; $i,j,k$ run over their respective index sets $I,J,K$. Note that, depending on the degree of $q_i$, rows and columns of the matrices $\Lambda_i$ are omitted, see [36] for details. The final semidefinite program is given by

$$\tilde{p}^* = \max_{\vec{y} \in \mathbb{C}^{N_d^2}} \sum_{\text{deg}([w]) \leq 2d} p_{[w]} y_{[w]},$$

such that the constraints (7) and (8) are satisfied, and $\tilde{p}^*$ is an upper bound on $p^*$.

### 2.2 Symmetric moment relaxations

We recall that the symmetry group $G_+^\pm$ preserves feasibility and optimality of solutions $(X,\phi)$. We now consider the impact of such symmetries on moment relaxations. For that, we note that $S_\infty$ acts on $\vec{y} = (y_{[w]})$ by

$$s(\vec{y})_{s([w])} = y_{[w]},$$

and, for signed monomials, we define formally $y_{-[w]} = -y_{[w]}$ for $[w] \in \tilde{W}$.

**Proposition 1** Let $G_+^\pm$ be the symmetry group preserving feasibility. Then we can add the following constraint to the semidefinite relaxation (9):

$$\vec{y} = g(\vec{y}), \quad \text{for all } g \in G_+^\pm.$$

**Proof** Let $(X,\phi)$ be an optimal, feasible, solution, and let $(g(X),\phi)$ be an orbit of optimal, feasible, solutions under $G_+^\pm$. Let $\vec{y}(X,\phi)$ be the solution of (9) corresponding to $(X,\phi)$; then $g(\vec{y}(X,\phi))$ is also a feasible solution of (9) with $\tilde{p}^*(\vec{y}) = \tilde{p}^*(g(\vec{y}))$. Now, the constraints of the semidefinite program (9) are convex in $\vec{y}$. So, we can replace any optimal $\vec{y}^*$ by

$$\mathcal{R}_{G_+^\pm}(\vec{y}^*) = \frac{1}{|G_+^\pm|} \sum_{g \in G_+^\pm} g(\vec{y}^*),$$

to obtain a symmetric optimal solution. By definition, $\mathcal{R}_{G_+^\pm}(\vec{y}^*)$ is invariant under $G_+^\pm$. \hfill \Box

We now restrict $\vec{y}$ to the symmetric subspace $\vec{y} = \mathcal{R}_{G_+^\pm}(\vec{y})$; thus, we have that

$$y_{[w]} = y_{C_{G_+^\pm}[w]},$$

where $C_{G_+^\pm}[w]$ is a canonical representative of $[w]$ under the symmetry group $G_+^\pm$, selected by minimality under graded lexicographic ordering. Symmetries on the moments $\vec{y}$ translate to symmetries at the level of the semidefinite matrices. We focus
on the main moment matrix $\Xi$, as the localizing matrices are usually much smaller and do not appear so frequently in practice. Remember that $\Xi$ has rows and columns indexed by the elements $\mathcal{W}$ with $\Xi_{[r], [c]} = y_{[r], [c]}$. Then

$$\Xi_{g([r]), g([c])} = y_{g([r]g([c])} = y_{g([r], [c])} = (g^{-1}([y]))_{[r], [c]} = \bar{y}_{[r], [c]} = \Xi_{[r], [c]}$$

and the matrix $\Xi$ is invariant under the simultaneous permutation of rows and columns by $G^+_x$. To cater for generalized permutations in the above, we define

$$\Xi_{r, c} = -\Xi_{-r, -c} = -\Xi_{-r, c} = \Xi_{r, -c}$$

for $r, c = 1, \ldots, N_d$. As the matrix $\Xi$ is invariant under the simultaneous action of a (signed) permutation group on its rows and columns, it can be block-diagonalized: we refer the reader to [19] for a clear explanation of the exploitation of such block structures in semidefinite programs.

### 2.3 Example

We come back to the example of Section 1.7 and consider a relaxation of degree 1. We index our moment matrix $\Xi$ using the sequence of monomials $([1], [A_0], [A_1], [B_0], [B_1])$ such that

$$\Xi = \begin{pmatrix} y_{[1]} & y_{[A_0]} & y_{[A_1]} & y_{[B_0]} & y_{[B_1]} \\ y_{[1]} & y_{[A_0A_1]} & y_{[A_0B_0]} & y_{[A_0B_1]} \\ y_{[1]} & y_{[A_1B_0]} & y_{[A_1B_1]} \\ y_{[1]} & y_{[B_0B_0]} & y_{[B_0B_1]} \end{pmatrix},$$

as the matrix is symmetric the elements of the lower triangle are conjugates of those in the upper triangle. Under symmetrization, we get that

$$y_{[A_0]} = -y_{[A_0]}, \quad y_{[A_1]} = y_{[A_1]}, \quad y_{[B_0]} = -y_{[B_0]}, \quad y_{[B_1]} = y_{[B_1]},$$

$$y_{[A_0A_1]} = -y_{[A_0A_1]}, \quad y_{[A_0B_0]} = y_{[A_0B_1]} = y_{[A_0B_1]} = -y_{[A_1B_1]},$$

and thus our semidefinite program simplifies to a program involving a single variable:

$$\hat{p}^* = \max_{x \in \mathbb{R}} 4x$$

subject to $\Xi = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & x & x \\ 1 & x & -x \\ 1 & 0 & 1 \end{pmatrix} \succeq 0.$

Finally, note that $\Xi$ can be fully diagonalized as $U^\top \Xi U = \text{diag}(1, 1 - \sqrt{2}x, 1 - \sqrt{2}x, 1 + \sqrt{2}x, 1 + \sqrt{2}x)$ using

$$U = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & -1/2 & -1/2 & 1/2 & 1/2 \\ 0 & 1/2 & -1/2 & -1/2 & 1/2 \\ 0 & 0 & \sqrt{2}/2 & 0 & \sqrt{2}/2 \\ 0 & 0 & \sqrt{2}/2 & 0 & \sqrt{2}/2 \end{pmatrix},$$

and we easily recover the bound $\hat{p}^* = 2\sqrt{2}$ on the value of the CHSH inequality.

---

2However, the same procedure can be applied on $A_i$; for $A_i$ corresponding to the constraint $q_i \geq 0$, one will need to consider the subgroup $G^+_q \subseteq G^+_x$ that leave this particular $q_i$ invariant as well.
2.4 Generalizations of the NPA hierarchy

The original NPA hierarchy \[34, 35\] employs states \(\phi \in \mathcal{H}\) and the evaluation \(\langle p(X) \rangle_{\phi} = \langle \phi | p(X) | \phi \rangle\) for the polynomial \(p\). The PPT hierarchy introduced in \[31\] instead employs density matrices \(\rho \in \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B)\) with positive partial transpose \((\rho^\top \succeq 0)\), and the evaluation rule
\[
\langle p(X) \rangle_{\rho} = \text{tr}[\rho \ p(X)].
\]

In our relaxations, it translates to the constraint that
\[
\mathcal{L}(\alpha \beta) = \mathcal{L}(\alpha \beta^*)
\]
if \(\alpha\) (resp. \(\beta\)) is a product of operators acting only on \(\mathcal{H}_A\) (resp. \(\mathcal{H}_B\)). The tracial moment hierarchy \[4–6, 36\] does not only employ states for the evaluation, but rather defines
\[
\langle p(X) \rangle = \frac{1}{d} \text{tr}[p(X)],
\]
which translates to
\[
\mathcal{L}(fg) = \mathcal{L}(gf)
\]
for arbitrary \(f, g \in \tilde{\mathcal{W}}\) due to the cyclic property of the trace. A framework for such generalizations is discussed in Section 3.5.

3 Implementation details

We built our software library in Scala, a language that provides four main advantages: it runs on the Java virtual machine (an optimal combination of portability and speed), it has a strong type system able to encode mathematical abstractions \[39\], it provides a flexible syntax well-suited to the creation of domain specific languages \[11\], and it interfaces with good libraries to represent exact number types (rational, cyclotomic or algebraic numbers). We now walk through key parts of our implementation. As the library is under active development, we refer the user to the up-to-date documentation present on the repository [https://github.com/denisrosset/sympoly].

3.1 Definition of the free algebra

We exploit the syntax of the Scala programming language. We start by defining the \(*\)-monoid \(\mathcal{W}\), by creating an object extending free.MonoidDef. As seen by the user, the variables \(x = \{x_1, x_2, \ldots, x_n, x_1^*, x_2^*, \ldots, x_n^*\}\) are represented by data classes with an arbitrary number of indices. Internally, however, we work with integers indexing all possible instances of those variables; the range of possible instances is provided by the companion object property allInstances, and all operator variables are enumerated in a variable operators. The adjoint method of each variable returns \(x_i^*\) given \(x_i\). Convenience implementations are provided by the HermitianOp and HermitianType# base classes. We use Scala pattern matching to provide readable notation. For the example of Section 1.7:

```scala
object Free extends free.MonoidDef {

  case class A(x: Int) extends HermitianOp
  object A extends HermitianType1(0 to 1)

  case class B(y: Int) extends HermitianOp

  object B extends HermitianType1(0 to 1)

  def main(args: Array[String]): Unit = {
    val a = A(1)
    val b = B(2)
    val x = a + b
    println(x)
  }

  object Free extends free.MonoidDef {
    case class A(x: Int) extends HermitianOp
    object A extends HermitianType1(0 to 1)

    case class B(y: Int) extends HermitianOp

    object B extends HermitianType1(0 to 1)

    def main(args: Array[String]): Unit = {
      val a = A(1)
      val b = B(2)
      val x = a + b
      println(x)
    }
  }
```

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object B extends HermitianType1(0 to 1)

val operators = Seq(A, B)
}

Internally, we build a table of the adjoints for all possible instances, so future processing only requires a single array lookup. Monomials are represented by a length \( n \) and an array of integer indices. By convention \( n = -1 \) represents the monomial 0. Note that the \( \text{Op} \) type is an inner type of the object \texttt{Free} written \texttt{Free.Op} (a path-dependent type), and the Scala type system will make sure that \texttt{Free.Op} instances are not mixed with variables from other rings.

### 3.2 Definition of the quotient algebra

The quotient algebra is given by the rewrite rules \( R \), expressed naturally as:

```scala
val Quotient = quotient.MonoidDef(Free) {
  case (A(x1), A(x2)) if x1 == x2 => Mono.one
  case (B(y1), B(y2)) if y1 == y2 => Mono.one
  case (B(y), A(x)) => A(x) * B(y)
  case (op1, op2) => op1 * op2
}
```

For now, we only allow rewrite rules where the left monomial is of degree two, as they apply to a majority of optimization problems in quantum information. Internally, we build an integer table \( \text{rule}(i,j) \), where \( i, j \) run over indices of the first and second variable, and the value in \( \text{rule}(i,j) \) is interpreted as follows:

| 0 | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|
| Set to 0 | Preserve | Remove both | Swap | Keep 1st, remove 2nd | Custom |

A value 5/Custom requires an additional lookup in a dictionary, but all other substitutions are fast. Monomial substitution is performed by Algorithm 1 so that equivalence classes \( \mathcal{W} \) are represented by their normal form \( \mathcal{N}_R(w) \in \mathcal{W}^0 \).

**Algorithm 1** Computation of monomial normal form

Input: length \( n \), array of integers \( (m_1, \ldots, m_n) \) representing the monomial

Output: new length \( n \) (or special flag \( n = -1 \) indicating zero monomial), new array \( (m_1, \ldots, m_n) \)

\[ i \leftarrow 1 \]

While \( i \leq n - 1 \)

If \( \text{rule}(m_i, m_{i+1}) = 0 \)

\[ n \leftarrow -1 \]

Return

ElseIf \( \text{rule}(m_i, m_{i+1}) = 1 \)

\[ i \leftarrow i + 1 \]

Else

Perform substitution at the \( i \)-th position, update length \( n \)

If \( i \neq 4 \) Then \( i \leftarrow \max(i - 1, 0) \)

End

End
3.3 Definition of symmetries

Generalized permutation of the variables are declared again using pattern matching. In our example (5):

```scala
val p1 = Free.generator {
  case A(i) => B(i)
  case B(i) => A(i)
}
val p2 = Free.generator {
  case B(0) => B(1)
  case B(1) => B(0)
  case A(i) => A(i)
}
val p3 = Free.generator {
  case A(1) => -A(1)
  case op => op // fallback, do nothing
}
```

The group $S^{±}_2$ has to be explicitly constructed by the user:

```scala
typeambientGroup = Quotient.ambientGroup(p1, p2, p3)
```

and is internally represented as a permutation group on (signed) indices of variables using a stabilizer chain, see [23].

3.4 Definition of the optimization problem

Polynomials entering in the optimization problem are defined using standard mathematical notation. For example:

```scala
def A(x: Int) = Quotient.quotient(Free.A(x))
def B(y: Int) = Quotient.quotient(Free.B(y))
val CHSH = A(0)*B(0) + A(0)*B(1) + A(1)*B(0) - A(1)*B(1)
```

Internally, polynomials are represented by the pairs $([w],p_{[w]})$ for which $p_{[w]} \neq 0$, sorted using graded reverse lexicographic order. For now, our library does not support constraints of the form $q_i(X) \succeq 0$, $r_j(X) = 0$ or $\langle s_k(X) \rangle_{\varphi} \geq 0$; thus only an objective polynomial $p$ can be provided for now. This implies that $G^{±}_2 = S^{±}_2$.

3.5 Linear evaluation: rules and canonical form

The constraints (6) applying on the linear functional $L$, with the possible addition of (11) or (12), do not apply at the level of monomials, but only when performing the final evaluation.

\begin{itemize}
  \item \textbf{Transposition equivalence under a predicate $P : x \rightarrow \{\text{true, false}\}$, that apply in place to the variables for which the predicate is true.}
  \item \textbf{Cyclic permutations under a predicate $P : x \rightarrow \{\text{true, false}\}$, that apply in place to the variables for which the predicate is true.}
\end{itemize}
Let $w = t_1 t_2 f_1 t_3 f_2 f_3 t_4$ such that the predicate $P$ is true for the variables $t_i$ and false for the variables $f_i$. Then, application of a transposition returns

$$T_P(w) = t'_1 t'_3 f_1 t'_2 f_2 f'_3 t'_4,$$

while a single application of a cyclic permutation returns

$$C_P(w) = t_2 t_3 f_1 t_4 f_2 f_3 t_1.$$

The canonical form $C(w) \in \mathcal{W}^\pm$ of a signed monomial $w \in \mathcal{W}^\pm$ is obtained by applying the rewriting rules $R$ on all iterations of

- the symmetry group $G^\pm$,
- partial transpositions $w \rightarrow \{w, T_P(w)\}$ for all transposition predicates,
- cyclic permutations $w \rightarrow \{w, C_P(w), C_P(C_P(w)), \ldots\}$ for all cyclic permutation predicates,

and keeping the minimal lexicographic representative along with its sign. In the case that $C(w) = C(-w)$, we set formally $C(w) = 0$. For the problem sizes considered, brute force evaluation is faster than algorithms exploiting the problem structure, provided the code is optimized to operate on primitive types (machine-size integers) during the enumeration. In our library, predicates are defined using pattern matching.

```scala
val partialTransposeBob = PartialTransposition(Free) {
  case A(i) => false
  case B(i) => true
}
val fullCyclic = CyclicPermutation(Free) {
  case op => true
}
```

### 3.6 Computation of the symmetry group $G^\pm$

The group $G^\pm$ is provided by the user, see Section 3.3. To construct the symmetry subgroup $G^\pm_\star$ that preserves the objective value $p \in \mathbb{K}[\mathcal{W}]$, we proceed as follow.

We construct the smallest set of signed monomials $M \subset \tilde{\mathcal{W}}^\pm$ that

- includes all monomials present in $p$,
- is invariant under action of $G^\pm$ (i.e. $w \in M \iff g(w) \in M$).

We write $S_M$ the symmetric group acting on $M$. As $G^\pm$ acts on $M$ as well, there exists a permutation group $H \subseteq S_M$, along with an isomorphism $\varphi : G^\pm \rightarrow H$ representing this action.

Explicit steps are presented in Algorithm 2. Fast algorithms based on stabilizer chains exist for the last two steps of the algorithm [23], and are implemented in GAP System [20] or our library Alasc [47].

### 3.7 Construction of the symmetrized moment matrices

We come to the final part of our method, the construction of moment matrices to be provided to the solver. We use a value $T$ as a token, where $T$ is larger than a crude upper bound on the number of final monomials, for example, $T = 2^{31} - 1$. The full
Algorithm 2 Computation of the symmetry group $G^\pm_\star$

Input: Objective polynomial $p$, set of monomials $M \subset \tilde{W}$, group $H$, isomorphism $\varphi$

Output: symmetry subgroup $G^\pm_\star$

Compute the partition $P$ of $M$ under the equivalence relation $v^\pm \sim w^\pm$ if $y_{C(v^\pm)} = y_{C(w^\pm)}$.

Compute the subgroup of $H_\star \subseteq H$ that stabilizes $P$.

Return $G^\pm_\star = \varphi^{-1}(H_\star)$.

method is presented in Algorithm 3. At the output, the matrices $C$ and $\{A_k\}$ of the SDP are recovered with:

$$C_{jk} = \begin{cases} 1 & \text{if } J_{jk} = 1 \\ 0 & \text{otherwise} \end{cases}, \quad (A_k)_{jk} = \begin{cases} \text{sign}(J_{jk}) & \text{if } |J_{jk}| = i \\ 0 & \text{otherwise} \end{cases}.$$  

Note that with our convention, the variable $y_1$ is never used and $A_1 = 0$. The variables $y_2, y_3, \ldots$ correspond to the unique moments that appear in the SDP matrix according to the map $\mu$. To get the expression of the objective in the symmetrized variables, initialize $\vec{b} \leftarrow 0 \in \mathbb{R}^{N_M}$, and for each term $p[w][w]$ appearing in the objective with real coefficient $p[w]$ and monomial $[w]$, set $b_{C(w)} \leftarrow b_{C(w)} + p[w]$.

The resulting SDP program is thus:

$$\max \quad \vec{b}^T \cdot \vec{y}$$

$$\text{over} \quad \vec{y} \in \mathbb{R}^{N_M}$$

such that

$$\chi = C - \sum_i y_i A_i \geq 0$$

where $C$ and $\{A_i\}$ are symmetric matrices in $\mathbb{R}^{n \times n}$.

4 Application: high precision bounds for the $I_{3322}$ inequality

As a test of our technique, we apply our symmetrization technique to the $I_{3322}$ inequality [10, 18, 49], in its variant symmetric under permutation of parties:

$$I_{3322} = (A_1 B_3 + A_3 B_1 - A_2 B_3 - A_3 B_2) + (A_1 B_1 - A_1 B_2 - A_2 B_1 + A_2 B_2) + A_1 + A_2 + B_1 + B_2,$$

which, in particular, is symmetric under permutation of parties, and under the signed permutation:

$$(A_1, A_2, A_3, B_1, B_2, B_3) \rightarrow (A_2, A_1, A_3, B_1, B_2, -B_3)$$

which together generate a symmetry group of order 8, which we identify as a dihedral group. We compare three approaches:

- Symmetries="no": we construct the standard NPA relaxation.
- Symmetries="partial": we symmetrize our SDP as discussed in Section 3 and then split the blocks according to the symmetric/antisymmetric subspace under permutation of parties, which is the most simple block diagonalization possible.
- Symmetries="diag": we symmetrize our SDP, and then try to split the blocks as much as possible. Unfortunately, there is no general software package to perform full block-diagonalization in exact arithmetic. Thus, we performed the block diagonalization by hand. This explains the presence of 6 blocks in our results, whereas the dihedral group of order 8 has five rational representations, and thus we should expect a decomposition in at most 5 blocks.
Algorithm 3 Computation of the symmetrized moment matrices

Input
List of generating monomials $V = (v_i), i = 1, \ldots, N_D$
Symmetry group $G^\pm$
Predicates of partial transpositions $\{P^T_i\}$, cyclic permutations $\{P^C_i\}$

Output
$J$ a matrix of integers of size $n \times n$
$\mu$ a bidirectional map between operator sequences and integer indices
$N_M$ total number of matrices $\{C,A_i\}$ in the SDP constraint

Initialize $J$ with the token value $T$
Initialize $\mu$ empty
$N_M \leftarrow 1$
For $i = 1, \ldots, n$ and $j = i, \ldots, n$
  If $J_{i,j} \neq T$
    Skip the current iteration, the current cell has already been computed
  End
  Compute the canonical $c = C(N_R(v_i^\dagger v_j))$ by enumeration (global transposition, $G^\pm$, $\{P^T_i\}, \{P^C_i\}$)
  If $c \in \{0, 1\}$
    $k \leftarrow c$
  ElseIf $\mu(c)$ is defined
    $k \leftarrow \mu(c)$
  Else
    $N_M \leftarrow N_M + 1$
    $\mu(c) \leftarrow N_M$
  End
For $(r,c) \in \{(g(i),g(j)) : g \in G^\pm\}$
  $\sigma \leftarrow \text{sign}(rc)$
  $J_{|r|,|c|} \leftarrow \sigma k$
  $J_{|c|,|r|} \leftarrow \sigma k$
End
End
We see that the biggest reductions in memory usage are provided by the reduction of the number of variables \( m \) and the quite straightforward block-diagonalization due to symmetry under permutation of parties; this is not surprising as the memory usage is in general dominated by a factor \( O(m^2) \). However, the block diagonalization has still a non negligible impact on the CPU time, as it reduces the terms in \( O(n^3) \).

Computational results using the SDPA double-double precision solver \([32]\) are reported in Table 1.

| Level | Sym.  | \# vars | SDP block sizes | CPU time (s) | Memory use (MB) |
|-------|-------|---------|-----------------|--------------|-----------------|
| 3     | no    | 867     | 88              | 73.2         | 15              |
| 3     | partial | 124     | 44.44           | 4.3          | 3               |
| 3     | diag. | 124     | 22,22,13,11,11,9 | 1.2          | 2               |
| 4     | no    | 4491    | 244             | 8416.0       | 331             |
| 4     | partial | 593     | 122,122         | 292.9        | 14              |
| 4     | diag. | 593     | 61,61,35,31,30,26 | 62.6        | 10              |

Table 1. Relaxation levels, symmetry reduction method used and resources needed to solve successfully the SDP relaxation using the SDPA double-double precision solver.

For completeness, we also computed the relaxation of level 5 using a diagonalization in 4 blocks (sizes: 162+157+157+152), which completed in 8700 [s] using SDPA in double-double precision. We also recomputed levels 2-4 in quadruple-double precision. The results are, along with the gap being the difference between the objective value of the primal and dual problem reported by the solver:

\[
I_2 \simeq 1.2509397216370581 \text{ (gap } \sim 10^{-31}),
\]

\[
I_3 \simeq 1.2508755620230350 \text{ (gap } \sim 10^{-31}),
\]

\[
I_4 \simeq 1.2508753845139768 \text{ (gap } \sim 10^{-30}),
\]

\[
I_5 \simeq 1.2508753845139766 \text{ (gap } \sim 10^{-21}).
\]

There still seems to be a gap between \( I_4 \) and \( I_5 \), but the SDPA high precision solvers only report \( \sim 17 \) digits. Using the VSDP package \([24]\), rigorous bounds can be computed for the solution of a semidefinite program. Because the symmetrization reduces the complexity of the problem, we should be able to observe an effect on the numerical precision of the obtained results. Indeed, we computed a robust solution for \( I_3 \) using VSDP and standard double precision arithmetic, to obtain:

\[
I_3^{\text{without-symmetrization}} \in [1.25087555, 1.25087557],
\]

and

\[
I_3^{\text{with-symmetrization}} \in [1.250875561, 1.250875568],
\]

and we see that symmetrization provides an additional digit of precision.

5 Conclusion

We introduced symmetry-adapted moment relaxations for optimization problems over noncommutative polynomials, with a particular emphasis on the problems arising from quantum information scenarios. We also presented a software library automating the discovery and use of the symmetries present in the problem formulation. This work is only a first step in that journey. In particular, we are looking to extend our software library in the following directions. First, the code has not been tested on problems involving non-Hermitian variables and polynomial with complex coefficients. Second,
we are lacking implementations of localizing matrices and support for general linear constraints. These additions should be pretty straightforward, except that automatic discovery of the full symmetry group could be difficult under involved combinations of constraints. Additional gains can be obtained using block diagonalization. As of today, there exists a variety of algorithms to decompose an algebra of matrices commuting with the representation of a group: the software library AREP [44] provides structured decomposition of permutation representations of solvable groups; numerical approaches can decompose arbitrary representations [30]; finally, a recent preprint proposed an algebraic method [25] based on Groebner bases. We also mention a recent promising approach using Jordan algebras [43].

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