Chapter 5
Trace Optimization of Polynomials in Non-commuting Variables

5.1 Introduction

In Chap. 3 trace-positivity together with the question how to detect it was explored in details. Due to hardness of the decision problem "Is a given nc polynomial f trace-positive?" we proposed a relaxation of the problem, i.e., we are asking if f is cyclically equivalent to SOHS. The tracial Gram matrix method based on the tracial Newton polytope was proposed (see Sects. 3.3 and 3.4) to efficiently detect such polynomials.

In this chapter we turn our attention to trace optimization of nc polynomials. We are interested in computing the smallest number the trace of a given nc polynomial can attain or approaches over a given nc semialgebraic set of symmetric matrices. This is in general a very difficult question, so we employ approximation tools again and present a *tracial* Lasserre relaxation scheme [Las01, Las09]. It yields again a hierarchy of semidefinite programming problems resulting in an increasing sequence of lower bounds for the optimum value. Finally we also shortly discuss the extraction of optimizers.

5.2 Unconstrained Trace Optimization

The purpose of this section is twofold. First we formulate the unconstrained trace optimization problem and second we present a Lasserre type of approximation hierarchy consisting of semidefinite programming problems. We also explore the duality properties.

Let $f \in \mathbb{R}\langle \underline{X} \rangle$ be given. We are interested in the *trace-minimum* of f, that is,

$$\operatorname{tr}_{\min}(f) := \inf\{\operatorname{tr} f(\underline{A}) \mid \underline{A} \in \mathbb{S}^n\}. \qquad (\mathrm{Tr}_{\min})$$

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This is a hard problem. For instance, a good understanding of trace-positive polynomials is likely to lead to a solution of the Connes' embedding conjecture [Con76], an outstanding open problem from operator algebras; see [KS08]. Another way to see the hardness is due to a result of Ji [Ji13] who proved that deciding whether the quantum chromatic number of a graph is at most three is NP-hard. This problem in turn is a conic optimization problem which is dual to an optimization problem over certain trace-positive polynomials, see [LP15] for details.

We can rewrite ($\mathrm{Tr}_{\min}$) as

$$\mathrm{tr}_{\min}(f) = \sup\{a \mid \mathrm{tr}\,(f-a)(\underline{A}) \geq 0,\ \forall \underline{A} \in \mathbb{S}^n\}. \qquad (\mathrm{Tr}_{\min'})$$

We again assume $\sup \varnothing = -\infty$. Nc polynomials from Θ^2 are trace-positive therefore it is natural to consider the following relaxation of ($\mathrm{Tr}_{\min'}$):

$$\mathrm{tr}_{\Theta^2}(f) := \sup\{a \mid f - a \in \Theta^2_{2d}\}, \qquad (\mathrm{Tr}_{\mathrm{sohs}})$$

where $2d = \mathrm{cdeg} f$ (if $\mathrm{cdeg} f$ is an odd number, then $\mathrm{tr}_{\min}(f) = \mathrm{tr}_{\Theta^2}(f) = -\infty$, hence we do not need to consider this case).

Remark 5.1. Since we are only interested in the trace of nc polynomials $f \in \mathbb{R}\langle \underline{X} \rangle$, when evaluated on elements from $\mathbb{S}^n$, $\mathscr{D}_S$, or $\mathscr{D}_S^{\mathrm{II}_1}$ we use that $\mathrm{tr} f(\underline{A}) = \mathrm{tr} f^*(\underline{A})$ for all $\underline{A}$; hence there is no harm in replacing f by its symmetrization $\frac{1}{2}(f + f^*)$. Thus we will focus in this chapter on *symmetric* nc polynomials.

Lemma 5.2. *Let* $f \in \mathrm{Sym}\,\mathbb{R}\langle \underline{X} \rangle$. *Then* $\mathrm{tr}_{\Theta^2}(f) \leq \mathrm{tr}_{\min}(f)$.

Proof. Indeed, if $a \in \mathbb{R}$ is such that $f - a \in \Theta^2$, then $0 \leq \mathrm{tr}\,(f-a) = \mathrm{tr} f - \mathrm{tr}\, a = \mathrm{tr} f - a$, hence $\mathrm{tr} f \geq a$. ∎

In general we do not have equality in Lemma 5.2. For instance, the Motzkin polynomial f satisfies $\mathrm{tr}_{\min}(f) = 0$ and $\mathrm{tr}_{\Theta^2}(f) = \sup \varnothing := -\infty$, see [KS08] and Example 5.14. Nevertheless, $\mathrm{tr}_{\Theta^2}(f)$ gives a solid approximation of $\mathrm{tr}_{\min}(f)$ for most of the examples and is easier to compute. It is obtained by solving an instance of SDP.

Suppose $f \in \mathrm{Sym}\,\mathbb{R}\langle \underline{X} \rangle$ is of degree $\leq 2d$ (with constant term f_1). Let $\mathbf{W}_d$ be a vector of all words up to degree d with first entry equal to 1. Then ($\mathrm{Tr}_{\mathrm{sohs}}$) rewrites into

$$\begin{array}{lrcl} \sup & f_1 - \langle E_{1,1} \mid F \rangle & & \\ \text{s. t.} & f - f_1 & \overset{\text{cyc}}{\sim} & \mathbf{W}_d^*(G - \langle E_{1,1} \mid F \rangle E_{1,1})\mathbf{W}_d \\ & F & \succeq & 0. \end{array} \qquad (\mathrm{Tr}_{\mathrm{SDP}})$$

Here $E_{1,1}$ is again the matrix with all entries 0 except for the $(1,1)$-entry which is 1. The cyclic equivalence translates into a set of linear constraints, cf. Proposition 1.51.

In general ($\mathrm{Tr}_{\mathrm{SDP}}$) does not satisfy the Slater condition. Nevertheless:

Theorem 5.3. (Tr$_{\text{SDP}}$) *satisfies strong duality.*

Proof. The proof is essentially the same as that of Theorem 4.1 so is omitted. We only mention an important ingredient is the closedness of the cone Θ^2 which is a trivial corollary of Proposition 1.58. ■

Repeating the Lagrangian procedure from (4.1)–(4.4) we obtain the dual to (Tr$_{\text{SDP}}$):

$$\begin{aligned} L_{\Theta^2}(f) &= \inf L(f) \\ &\quad \text{s.t. } L(1) = 1 \\ &\qquad\quad L \in (\Theta^2_{2d})^{\vee} \end{aligned}$$

Following Remark 1.64 we rewrite this problem into an explicit semidefinite programming problem:

$$\begin{aligned} L_{\Theta^2}(f) &= \inf \langle H_L \,|\, G_f \rangle \\ &\quad \text{s.t. } (H_L)_{u,v} = (H_L)_{w,z} \text{ for all } u^*v \overset{\text{cyc}}{\sim} w^*z, \\ &\qquad (H_L)_{1,1} = 1, \\ &\qquad\quad H_L \succeq 0. \end{aligned} \tag{Tr$_{\text{DSDP}}$}$$

Recall that H_L from the SDP above is a tracial Hankel matrix. It is of order $\sigma(d)$. By Theorem 5.3, we have $\operatorname{tr}_{\Theta^2}(f) = L_{\Theta^2}(f)$. The question is, does $\operatorname{tr}_{\Theta^2}(f) = L_{\Theta^2}(f) = \operatorname{tr}_{\min}(f)$ hold? This is true for the case of unconstrained eigenvalue optimization (see Theorem 5.3), while in the unconstrained trace optimization it only holds under additional assumptions. We show that if the optimum solution of (Tr$_{\text{DSDP}}$) satisfies a flatness condition (see Definitions 1.47 and 1.49), then the answer to the question is affirmative. In particular, the proposed Θ^2-relaxation is then exact. Furthermore, in this case we can even extract global trace-minimizers of f.

Theorem 5.4. *If the optimizer H_L^{opt} of* (Tr$_{\text{DSDP}}$) *satisfies the* flatness condition*, i.e., the linear functional underlying H_L^{opt} is 1-flat, then the Θ^2-relaxation is exact:*

$$\operatorname{tr}_{\Theta^2}(f) = L_{\Theta^2}(f) = \operatorname{tr}_{\min}(f).$$

Proof. The first equality is strong duality shown in Theorem 5.3. For the second equality, if the linear functional L^{opt} corresponding to H_L^{opt} satisfies the flatness condition, then by Theorem 1.71 there exist finitely many n-tuples $\underline{A}^{(j)}$ of symmetric matrices and positive scalars $\lambda_j > 0$ with $\sum_j \lambda_j = 1$ such that

$$L^{\text{opt}}(f) = \sum_j \lambda_j \operatorname{tr} f(\underline{A}^{(j)}).$$

Hence $L_{\Theta^2}(f) = L^{\text{opt}}(f) \leq \operatorname{tr}_{\min}(f)$ and equality follows from weak duality. ■

5.3 Constrained Trace Optimization

In this section we present the tracial version of Lasserre's relaxation scheme to minimize the trace of an nc polynomial.

Let $S \subseteq \operatorname{Sym}\mathbb{R}\langle \underline{X} \rangle$ be finite and let $f \in \operatorname{Sym}\mathbb{R}\langle \underline{X} \rangle$. We are interested in the smallest trace the polynomial f attains on $\mathscr{D}_S$, i.e.,

$$\operatorname{tr}_{\min}(f,S) := \inf\left\{\operatorname{tr} f(\underline{A}) \mid \underline{A} \in \mathscr{D}_S\right\}. \qquad (\text{Constr-Tr}_{\min})$$

Hence $\operatorname{tr}_{\min}(f,S)$ is the greatest lower bound on the trace of $f(\underline{A})$ for tuples of symmetric matrices $\underline{A} \in \mathscr{D}_S$, i.e., $\operatorname{tr}(f(\underline{A}) - \operatorname{tr}_{\min}(f,S)\underline{A}) \geq 0$ for all $\underline{A} \in \mathscr{D}_S$, and $\operatorname{tr}_{\min}(f,S)$ is the largest real number with this property.

We introduce $\operatorname{tr}^{\mathrm{II}_1}_{\min}(f,S) \in \mathbb{R}$ as the trace-minimum of f on $\mathscr{D}_S^{\mathrm{II}_1}$. Since $\mathscr{D}_S^{\mathrm{II}_1} \supseteq \mathscr{D}_S$, we have $\operatorname{tr}^{\mathrm{II}_1}_{\min}(f,S) \leq \operatorname{tr}_{\min}(f,S)$. As mentioned in Remark 1.61 (see also Proposition 1.63), $\operatorname{tr}^{\mathrm{II}_1}_{\min}(f,S)$ is more approachable than $\operatorname{tr}_{\min}(f,S)$. In fact, in this section we shall present Lasserre's relaxation scheme producing a sequence of computable lower bounds $\operatorname{tr}^{(s)}_{\Theta^2}(f,S)$ monotonically converging to $\operatorname{tr}^{\mathrm{II}_1}_{\min}(f,S)$. Here, as always, the constraint set S is assumed to produce an archimedean quadratic module M_S. From Proposition 1.62 we can bound $\operatorname{tr}^{\mathrm{II}_1}_{\min}(f,S)$ from below by

$$\begin{aligned} \operatorname{tr}^{(s)}_{\Theta^2}(f,S) := \sup\ & \lambda \\ \text{s.t. } & f - \lambda \in \Theta^2_{S,2s}, \end{aligned} \qquad (\text{Constr-Tr}^{(s)}_{\mathrm{SDP}})$$

for $2s \geq \operatorname{cdeg} f$. For $2s < \operatorname{cdeg} f$, (Constr-Tr$^{(s)}_{\mathrm{SDP}}$) is infeasible.

For each *fixed* s, (Constr-Tr$^{(s)}_{\mathrm{SDP}}$) is an SDP (see Proposition 5.7 below) and leads to the tracial version of the Lasserre relaxation scheme.

Corollary 5.5. *Let* $S \subseteq \operatorname{Sym}\mathbb{R}\langle \underline{X} \rangle$, *and let* $f \in \operatorname{Sym}\mathbb{R}\langle \underline{X} \rangle$. *If* M_S *is archimedean, then*

$$\operatorname{tr}^{(s)}_{\Theta^2}(f,S) \underset{s\to\infty}{\longrightarrow} \operatorname{tr}^{\mathrm{II}_1}_{\min}(f,S). \qquad (5.1)$$

The sequence $\operatorname{tr}^{(s)}_{\Theta^2}(f,S)$ *is monotonically increasing and bounded from above, but the convergence in* (5.1) *is not finite in general.*

Proof. This follows from Proposition 1.63. For each $m \in \mathbb{N}$, there is $s(m) \in \mathbb{N}$ with

$$f - \operatorname{tr}^{\mathrm{II}_1}_{\min}(f,S) + \frac{1}{m} \in \Theta^2_{S,2s(m)}.$$

In particular,

$$\operatorname{tr}^{(s(m))}_{\Theta^2}(f) \geq \operatorname{tr}^{\mathrm{II}_1}_{\min}(f,S) - \frac{1}{m}.$$

Since also

$$\operatorname{tr}_{\Theta^2}^{(s(m))}(f) \le \operatorname{tr}_{\min}^{\mathrm{II}_1}(f,S),$$

we obtain

$$\lim_{s\to\infty} \operatorname{tr}_{\Theta^2}^{(s)}(f,S) = \lim_{m\to\infty} \operatorname{tr}_{\Theta^2}^{(s(m))}(f) = \operatorname{tr}_{\min}^{\mathrm{II}_1}(f,S).$$

■

Example 5.6. For a simple example with non-finite convergence, consider

$$p = (1-X^2)(1-Y^2) + (1-Y^2)(1-X^2),$$

and

$$S = \{1-X^2, 1-Y^2\}.$$

Then $\operatorname{tr}_{\min}^{\mathrm{II}_1}(p,S) = 0$, but $p \notin \Theta_S^2$ [KS08, Example 4.3]. The first few lower bounds for $\operatorname{tr}_{\min}^{\mathrm{II}_1}(p,S)$ are in the second column of Table 5.1.

Generally we are interested in $\operatorname{tr}_{\min}^{\mathrm{II}_1}(f,S)$, but there is no good procedure or algorithm for computing it. Therefore we stick to $\operatorname{tr}_{\Theta^2}^{(s)}(f,S)$ since its computational feasibility comes from the fact that verifying whether $f \in \Theta_{S,2s}^2$ is a semidefinite programming feasibility problem when S is finite.

Proposition 5.7. *Let* $f = \sum_w f_w w \in \operatorname{Sym}\mathbb{R}\langle \underline{X} \rangle$ *and* $S = \{g_1, \ldots, g_t\} \subseteq \operatorname{Sym}\mathbb{R}\langle \underline{X} \rangle$ *with* $g_i = \sum_{w \in \langle \underline{X} \rangle_{\deg g_i}} g_w^i w$*. Then* $f \in \Theta_{S,2s}^2$ *if and only if there exists a positive semidefinite matrix* A *of order* $\sigma(s)$ *and positive semidefinite matrices* B^i *of order* $\sigma(s_i)$ *(recall that* $s_i = \lfloor s - \deg(g_i)/2 \rfloor$*) such that for all* $w \in \langle \underline{X} \rangle_{2s}$*,*

$$f_w = \sum_{\substack{u,v \in \langle \underline{X} \rangle_s \\ u^* v \overset{\mathrm{cyc}}{\sim} w}} A_{u,v} + \sum_i \sum_{\substack{u,v \in \langle \underline{X} \rangle_{s_i}, z \in \langle \underline{X} \rangle_{\deg g_i} \\ u^* z v \overset{\mathrm{cyc}}{\sim} w}} g_z^i B_{u,v}^i. \tag{5.2}$$

Proof. We start with the "only if" part. Suppose $f \in \Theta_{S,2s}^2$, hence there exist nc polynomials $a_i = \sum_{w \in \langle \underline{X} \rangle_s} a_w^i w$ and $b_{i,j} = \sum_{w \in \langle \underline{X} \rangle_{s_i}} b_w^{i,j} w$ such that $f \overset{\mathrm{cyc}}{\sim} \sum_i a_i^* a_i + \sum_{i,j} b_{i,j}^* g_i b_{i,j}$. In particular this means that for every $w \in \langle \underline{X} \rangle_{2s}$ the following must hold:

$$\begin{aligned} f_w &= \sum_i \sum_{\substack{u,v \in \langle \underline{X} \rangle_s \\ u^* v \overset{\mathrm{cyc}}{\sim} w}} a_u^i a_v^i + \sum_{i,j} \sum_{\substack{u,v \in \langle \underline{X} \rangle_{s_i}, z \in \langle \underline{X} \rangle_{\deg g_i} \\ u^* z v \overset{\mathrm{cyc}}{\sim} w}} b_u^{i,j} b_v^{i,j} g_z^i \\ &= \sum_{\substack{u,v \in \langle \underline{X} \rangle_s \\ u^* v \overset{\mathrm{cyc}}{\sim} w}} \sum_i a_u^i a_v^i + \sum_i \sum_{\substack{u,v \in \langle \underline{X} \rangle_{s_i}, z \in \langle \underline{X} \rangle_{\deg g_i} \\ u^* z v \overset{\mathrm{cyc}}{\sim} w}} g_z^i \sum_j b_u^{i,j} b_v^{i,j}. \end{aligned}$$

If we define a matrix A of order $\sigma(s)$ and matrices B^i of order $\sigma(s_i)$ by $A_{u,v} = \sum_i a^i_u a^i_v$ and $B^i_{u,v} = \sum_j b^{i,j}_u b^{i,j}_v$, then these matrices are positive semidefinite and satisfy (5.2).

To prove the "if" part we use that A and B^i are positive semidefinite, therefore we can find (column) vectors A_i and $B_{i,j}$ such that $A = \sum_i A_i A_i^T$ and $B^i = \sum_j B_{i,j} B_{i,j}^T$. These vectors yield nc polynomials $a_i = A_i^T \mathbf{W}_{\sigma(s)}$ and $b_{i,j} = B_{i,j}^T \mathbf{W}_{\sigma(s_i)}$, which give a certificate for $f \in \Theta^2_{S,2s}$. ■

Remark 5.8. The last part of the proof of Proposition 5.7 explains how to construct the certificate for $f \in \Theta^2_{S,2s}$. First we solve the semidefinite feasibility problem in the variables $A \in \mathbb{S}^+_{\sigma(s)}$, $B^i \in \mathbb{S}^+_{\sigma(s_i)}$ subject to constraints (5.2). Then we use the Cholesky or eigenvalue decomposition to compute column vectors $A_i \in \mathbb{R}^{\sigma(s)}$ and $B_{i,j} \in \mathbb{R}^{\sigma(s_i)}$ which yield desired polynomial certificates $a_i \in \mathbb{R}\langle \underline{X} \rangle_s$ and $b_{i,j} \in \mathbb{R}\langle \underline{X} \rangle_{s_i}$.

By Proposition 5.7, (Constr-Tr$^{(s)}_{\mathrm{SDP}}$) is an SDP. It can be explicitly presented as

$$
\begin{aligned}
\operatorname{tr}^{(s)}_{\Theta^2}(f,S) = \sup\ & f_1 - A_{1,1} - \textstyle\sum_i g^i_1 B^i_{1,1} \\
\text{s.t. } & f_w = \sum_{\substack{u,v \in \langle \underline{X} \rangle_s \\ u^* v \overset{\mathrm{cyc}}{\sim} w}} A_{u,v} + \sum_i \sum_{\substack{u,v \in \langle \underline{X} \rangle_{s_i}, z \in \langle \underline{X} \rangle_{\deg g_i} \\ u^* z v \overset{\mathrm{cyc}}{\sim} w}} g^i_z B^i_{u,v} \\
& \quad \text{for all } 1 \neq w \in \langle \underline{X} \rangle_{2s}, \\
& A \in \mathbb{S}^+_{\sigma(s)}, \quad B^i \in \mathbb{S}^+_{\sigma(s_i)},
\end{aligned}
\qquad (\text{Constr-Tr}^{(s)}_{\mathrm{SDP}'})
$$

where we use $s_i = \lfloor s - \deg(g_i)/2 \rfloor$.

Lemma 5.9. *The dual semidefinite program to* (Constr-Tr$^{(s)}_{\mathrm{SDP}}$) *and* (Constr-Tr$^{(s)}_{\mathrm{SDP}'}$) *is*

$$
\begin{aligned}
L^{(s)}_{\Theta^2}(f,S) = \inf\ & L(f) \\
\text{s.t. } & L : \mathbb{R}\langle \underline{X} \rangle_{2s} \to \mathbb{R} \ \text{ is linear and symmetric}, \\
& L(1) = 1, \\
& L(pq - qp) = 0, \ \text{ for all } p,q \in \mathbb{R}\langle \underline{X} \rangle_s, \\
& L(q^* q) \geq 0, \ \text{ for all } q \in \mathbb{R}\langle \underline{X} \rangle_s, \\
& L(h^* g_i h) \geq 0, \ \text{ for all } i \text{ and all } h \in \mathbb{R}\langle \underline{X} \rangle_{s_i}, \\
& \qquad \text{where } s_i = \lfloor s - \deg(g_i)/2 \rfloor.
\end{aligned}
\qquad (\text{Constr-Tr}^{(s)}_{\mathrm{DSDP}})
$$

Proof. For this proof it is beneficial to adopt a functional analytic viewpoint of (Constr-Tr$^{(s)}_{\mathrm{SDP}}$) and (Constr-Tr$^{(s)}_{\mathrm{SDP}'}$).

We have the following chain of reasoning, similar to (4.1)–(4.4) (recall $2s \geq \lceil \operatorname{cdeg} f \rceil$):

$$
\begin{aligned}
\sup\{\lambda \mid f - \lambda \in \Theta^2_{S,2s}\} &= \sup\ \left\{\lambda \mid f - \lambda \in \overline{\Theta^2_{S,2s}}\right\} \\
&= \sup\ \left\{\lambda \mid \forall L \in \left(\Theta^2_{S,2s}\right)^{\vee} : L(f - \lambda) \geq 0\right\}
\end{aligned}
\qquad (5.3)
$$

$$= \sup \left\{\lambda \mid \forall L \in \left(\Theta^2_{S,2s}\right)^{\vee} \text{ with } L(1) = 1 : L(f) \geq \lambda\right\} \quad (5.4)$$

$$= \inf \left\{L(f) \mid L \in \left(\Theta^2_{S,2s}\right)^{\vee} \text{ with } L(1) = 1\right\}. \quad (5.5)$$

(Recall that $\left(\Theta^2_{S,2s}\right)^{\vee}$ is the set of all linear functionals $\mathbb{R}\langle \underline{X}\rangle_{2s} \to \mathbb{R}$ nonnegative on $\Theta^2_{S,2s}$.) The last equality is trivial. We next give the reasoning behind the third equality. Clearly, "$\leq$" holds since every λ feasible for the right-hand side of (5.3) is also feasible for the right-hand side of (5.4). To see the reverse inequality we consider an arbitrary λ feasible for (5.4). Note that $\lambda \leq f_1 = \tilde{L}(f)$, where $\tilde{L} \in \left(\Theta^2_{S,2s}\right)^{\vee}$ maps every polynomial into its constant term. We shall prove that $L(f-\lambda) \geq 0$ for every $L \in \left(\Theta^2_{S,2s}\right)^{\vee}$. Consider an arbitrary $L \in \left(\Theta^2_{S,2s}\right)^{\vee}$ and define $\hat{L} = \frac{L+\varepsilon}{L(1)+\varepsilon}$ for some $\varepsilon > 0$. Then $\hat{L}(1) = 1$ and $\hat{L} \in \left(\Theta^2_{S,2s}\right)^{\vee}$, therefore $\hat{L}(f-\lambda) \geq 0$, whence $L(f-\lambda) \geq \varepsilon(\lambda - 1)$. Since ε was arbitrary we get $L(f-\lambda) \geq 0$.

The problem $\inf\{L(f) \mid L \in \left(\Theta^2_{S,2s}\right)^{\vee}$ with $L(1) = 1\}$ is an SDP, and this is easily seen to be equivalent to the problem (Constr-$\mathrm{Tr}^{(s)}_{\mathrm{DSDP}}$) given above. Indeed, if $L \in \left(\Theta^2_{S,2s}\right)^{\vee}$, $L(1) = 1$, then L must be nonnegative on the terms (1.18) and on every commutator, therefore L is feasible for the constraints in (Constr-$\mathrm{Tr}^{(s)}_{\mathrm{DSDP}}$). ■

Proposition 5.10. *Suppose $\mathscr{D}_S$ contains an ε-neighborhood of 0. Then the SDP (Constr-$\mathrm{Tr}^{(s)}_{\mathrm{DSDP}}$) admits Slater points.*

Proof. Since the constructed linear functional in the proof of Proposition 4.9 is tracial, the same proof can be applied here and is thus omitted. ■

Remark 5.11. As in the eigenvalue case, having Slater points for (Constr-$\mathrm{Tr}^{(s)}_{\mathrm{DSDP}}$) is important for the duality theory. In particular, there is no duality gap, so for every $s \geq 1$

$$L^{(s)}_{\Theta^2}(f,S) = \mathrm{tr}^{(s)}_{\Theta^2}(f,S)$$

and

$$L_{\Theta^2}(f,S) := \lim_{s\to\infty} L^{(s)}_{\Theta^2}(f,S) = \mathrm{tr}^{\mathrm{II}_1}_{\min}(f,S).$$

Algorithms to compute the lower bounds $\mathrm{tr}^{(s)}_{\Theta^2}(f,S) = L^{(s)}_{\Theta^2}(f,S)$ for $\mathrm{tr}^{\mathrm{II}_1}_{\min}(f,S)$ and $\mathrm{tr}_{\min}(f,S)$ are implemented in `NCSOStools` [CKP11] . We demonstrate it on a few examples at the end of the chapter.

5.4 Flatness and Extracting Optimizers

In this section we assume $S \subseteq \mathrm{Sym}\,\mathbb{R}\langle \underline{X} \rangle$ is finite, and $f \in \mathrm{Sym}\,\mathbb{R}\langle \underline{X} \rangle_{2d}$. Let M_S be archimedean. In this case $\mathscr{D}_S^{\mathrm{II}_1}$ is bounded and hence $\mathrm{tr}_{\min}^{\mathrm{II}_1}(f,S) > -\infty$. Since M_S is archimedean, for s big enough (Constr-$\mathrm{Tr}_{\mathrm{SDP}}^{(s)}$) will be feasible.

Like in constrained eigenvalue optimization, flatness is a sufficient condition for finite convergence of the bounds $\mathrm{tr}_{\Theta^2}^{(s)}(f,S) = L_{\Theta^2}^{(s)}(f,S)$ and exactness of the relaxed solution; it also enables the extraction of optimizers.

We first recall a variant of Theorem 1.71 adapted to this setting.

Theorem 5.12. *Suppose L^{opt} is an optimal solution of (Constr-$\mathrm{Tr}_{\mathrm{DSDP}}^{(s)}$) for some $s \geq d+\delta$ that is δ-flat. Then there are finitely many n-tuples $\underline{A}^{(j)}$ of symmetric matrices in $\mathscr{D}_S$ and positive scalars $\lambda_j > 0$ with $\sum_j \lambda_j = 1$ such that*

$$L^{\mathrm{opt}}(f) = \sum_j \lambda_j \mathrm{tr} f(\underline{A}^{(j)}). \tag{5.6}$$

In particular, $\mathrm{tr}_{\min}(f,S) = \mathrm{tr}_{\min}^{\mathrm{II}_1}(f,S) = L_{\Theta^2}^{(s)}(f,S) = \mathrm{tr}_{\Theta^2}^{(s)}(f,S)$.

We propose Algorithm 5.1 to find solutions of (Constr-$\mathrm{Tr}_{\mathrm{DSDP}}^{(s)}$) for $s \geq d+\delta$ which are δ-flat enabling us to extract a minimizer of (Constr-$\mathrm{Tr}_{\mathrm{SDP}}^{(s)}$). It is a variant of Algorithm 4.2 and performs surprisingly well; e.g., it finds flat solutions in all tested situations where finite convergence was numerically detected (i.e., at least two consequent bounds were equal).

Algorithm 5.1: Randomized algorithm to find flat solutions for problem (Constr-$\mathrm{Tr}_{\mathrm{DSDP}}^{(s)}$)

Input: $f \in \mathrm{Sym}\,\mathbb{R}\langle \underline{X} \rangle$ with $\deg f = 2d$, $S = \{g_1,\ldots,g_t\}$,
  $\delta = \lceil \max_i \deg(g_i)/2 \rceil$, $\delta_{\max}$;

$L_{\mathrm{flat}} = 0$;
for $s = d+\delta, d+\delta+1, \ldots, d+\delta+d_{\max}$ **do**
  Compute $L^{(s)}$ – the optimal solution for (Constr-$\mathrm{Tr}_{\mathrm{DSDP}}^{(s)}$);
  if $L^{(s)}$ *is δ-flat* **then**
    $L_{\mathrm{flat}} = L^{(s)}$. **Stop**;
  end
  Compute $L_{\mathrm{rand}}^{(s)}$;
  if $L_{\mathrm{rand}}^{(s)}$ is *δ-flat* **then**
    $L_{\mathrm{flat}} = L_{\mathrm{rand}}^{(s)}$. **Stop**;
  end
end
Output: L_{flat};

In Step 7 we solve the SDP which is obtained from (Constr-$\text{Tr}^{(s)}_{\text{DSDP}}$) by fixing the upper left-hand corner of the Hankel matrix to be equal to the upper left-hand corner of the Hankel matrix of $L^{(s)}$ and by taking a full random objective function—like in (Constr-$\text{Eig}^{(s)}_{\text{RAND}}$). We repeat this step several (e.g. 10) times. In our experiments, this algorithm very often returns flat solutions if the module $\Theta^2_{S,2d}$ is archimedean. On the other hand, there is little theoretical evidence supporting this performance.

We repeat Steps 1–3 at most $\delta_{\max}+1$ times, where $\delta_{\max}$ is for computational complexity reasons chosen so that $d+\delta+\delta_{\max}$ is at most 10, when we have two nc variables, and is at most 8 if we have three nc variables. Otherwise the complexity of the underlying SDP exceeds the capability of our current hardware. We implemented Steps 1–3 from 5.1 in the `NCSOStools` function `NCtraceOptRand`.

In [KP16] we report numerical results obtained by running Algorithm 5.1 on random polynomials. We generated random polynomials as in Sect. 4.3.2 and we check for δ-flatness by computing ranks much like in Sect. 4.3.2. In all cases we took the tolerance to be $\min\{30\cdot \texttt{err}_{\texttt{flat}}, 10^{-3}\}$.

With this tolerance we can observe (as in Sect. 4.3.2) that in almost all tested (random) cases Algorithm 5.1 returned a flat optimal solution already after the first step, i.e., for $s=d+\delta$; see [KP16, Table 4] for concrete results.

Once we have a flat optimum solution for (Tr_{DSDP}) or (Constr-$\text{Tr}^{(s)}_{\text{DSDP}}$) we can extract optimizers, i.e., compute an n-tuple of symmetric matrices $\underline{A}$, which is in $\mathscr{D}_S$ when we consider the constrained case, such that $\text{tr}(\underline{A})$ is equal to $\text{tr}_{\min}(f)$ and $\text{tr}_{\min}(f,S)$, respectively, by running Algorithm 1.2.

5.5 Implementation

We can compute the unconstrained and constrained trace optimum exactly only for very simple and nice examples. For all other cases we shall use numerical algorithms. The software package `NCSOStools` contains `NCcycMin` to compute the unconstrained trace optimum (i.e., $\text{tr}_{\Theta^2}(f) = L_{\Theta^2}(f)$) and `NCcycOpt` to extract the related optimizers if the dual optimal solution is 1-flat. Likewise we have `NCtraceOpt` to compute $\text{tr}^{(s)}_{\Theta^2}(f,S)$ and `NCtraceOptRand` to compute flat solutions together with $\text{tr}^{\text{II}_1}_{\min}(f,S)$ when a flat solution is found. In this case we also extract optimizers by running Algorithm 1.2.

Example 5.13. Let

$$\begin{aligned} f = {} & 3+X_1^2+2X_1^3+2X_1^4+X_1^6-4X_1^4X_2+X_1^4X_2^2+4X_1^3X_2+2X_1^3X_2^2-2X_1^3X_2^3 \\ & +2X_1^2X_2-X_1^2X_2^2+8X_1X_2X_1X_2+2X_1^2X_2^3-4X_1X_2+4X_1X_2^2+6X_1X_2^4-2X_2 \\ & +X_2^2-4X_2^3+2X_2^4+2X_2^6. \end{aligned}$$

The minimum of f on $\mathbb{R}^2$ is 1.0797. Using `NCcycMin` we obtain the floating point trace-minimum $\operatorname{tr}_{\Theta^2}(f) = 0.2842$ for f which is different from the commutative minimum. In particular, the minimizers will not be scalar matrices. The dual optimal solution for ($\mathrm{Tr}_{\mathrm{DSDP}}$) is of rank 4 and 1-flat. Thus the matrix representation of the multiplication operators A_i is given by 4×4 matrices (see the proof of Theorem 1.69 and Algorithm 1.1):

$$A_1 = \begin{bmatrix} -1.0761 & 0.5319 & 0.1015 & 0.2590 \\ 0.5319 & 0.4333 & -0.3092 & 0.2008 \\ 0.1015 & -0.3092 & -0.2633 & 0.9231 \\ 0.2590 & 0.2008 & 0.9231 & -0.3020 \end{bmatrix},$$

$$A_2 = \begin{bmatrix} 0.7107 & 0.2130 & 0.7090 & 0.4415 \\ 0.2130 & 0.2087 & 0.3878 & -0.9321 \\ 0.7090 & 0.3878 & -0.5016 & -0.0757 \\ 0.4415 & -0.9321 & -0.0757 & 0.1393 \end{bmatrix}.$$

The Artin–Wedderburn decomposition for the matrix $*$-algebra $\mathscr{A}$ generated by A_1, A_2 gives in this case only one block. Using `NCcycOpt`, which essentially implements Algorithm 1.2 leads to the trace-minimizer

$$\hat{A}_1 = \begin{bmatrix} -1.0397 & -0.0000 & 0.1024 & 0.6363 \\ -0.0000 & -1.0397 & -0.6363 & 0.1024 \\ 0.1024 & -0.6363 & 0.4356 & -0.0000 \\ 0.6363 & 0.1024 & -0.0000 & 0.4356 \end{bmatrix},$$

$$\hat{A}_2 = \begin{bmatrix} -0.4246 & 0.0000 & -0.1377 & -0.8559 \\ 0.0000 & -0.4246 & 0.8559 & -0.1377 \\ -0.1377 & 0.8559 & 0.7031 & 0.0000 \\ -0.8559 & -0.1377 & 0.0000 & 0.7031 \end{bmatrix}.$$

The reader can easily verify that $\operatorname{tr}(f(\hat{A}_1, \hat{A}_2)) = 0.2842$.

Note that $\mathscr{A}$ is (as a real $*$-algebra) isomorphic to $M_2(\mathbb{C})$. For instance,

$$A \approx \tilde{A} = \begin{bmatrix} -1.0397 & 0.6363 + 0.1024\mathrm{i} \\ 0.6363 - 0.1024\mathrm{i} & 0.4356 \end{bmatrix},$$

$$B \approx \tilde{B} = \begin{bmatrix} -0.4246 & -0.8559 - 0.1377\mathrm{i} \\ -0.8559 + 0.1377\mathrm{i} & 0.7031 \end{bmatrix}.$$

In this case it is possible to find a unitary matrix $U \in \mathbb{C}^{2\times 2}$ with $A' = U^*\tilde{A}U \in \mathbb{R}^{2\times 2}$ and $B' = U^*\tilde{B}U \in \mathbb{R}^{2\times 2}$, e.g.,

$$U = \begin{bmatrix} 0.9803 + 0.1576\mathrm{i} & 0.1176 + 0.0189\mathrm{i} \\ 0.1191 & -0.9929 \end{bmatrix},$$

$$A' = \begin{bmatrix} -0.8663 & -0.8007 \\ -0.8007 & 0.2622 \end{bmatrix}, \quad B' = \begin{bmatrix} -0.6136 & 0.7089 \\ 0.7089 & 0.8921 \end{bmatrix}.$$

Then $(A', B') \in \left(\mathbb{S}^{2\times 2}\right)^2$ is also a trace-minimizer for f.

Example 5.14. We demonstrate our software for constrained trace optimization for the set $S = \{1 - X^2, 1 - Y^2\}$ with the polynomial

$$p = (1 - X^2)(1 - Y^2) + (1 - Y^2)(1 - X^2)$$

from Example 5.6, and a non-commutative version of the Motzkin polynomial from Example 4.25,

$$q = XY^4X + YX^4Y - 3XY^2X + 1.$$

It is obvious (see Example 5.6 and [KS08, Example 4.3]) that $\mathrm{tr}^{\mathrm{II}_1}_{\min}(p, S) = 0$. Similarly, $\mathrm{tr}^{\mathrm{II}_1}_{\min}(q, S) = 0$ (see [KS08, Example 4.4]). We use NCSOStools as follows:

```
>> NCvars x y
>> S = {1 - x^2, 1 - y^2};
>> p = (1-x^2)*(1-y^2)+(1-y^2)*(1-x^2);
>> q = x*y^4*x+y*x^4*y-3*x*y^2*x+1;
```

To compute the sequence of lower bounds $\mathrm{tr}^{(s)}_{\Theta^2}(p, S)$ for $\mathrm{tr}^{\mathrm{II}_1}_{\min}(p, S)$ we call

```
>> [opt,decom_sohs,decom_S,base] = NCtraceOpt(p,S,2*s);
```

with $s = 2, 3, 4, 5$. Similarly we obtain bounds for q. Results are reported in Table 5.1.

We can see that the sequence of bounds $\mathrm{tr}^{(s)}_{\Theta^2}(p, S)$ of p increases and does not reach the limit for $s \le 5$. Actually, it never reaches $\mathrm{tr}^{\mathrm{II}_1}_{\min}(p, S)$; see Example 5.6. On the other hand, the sequence of bounds for q is finite and reaches the optimal value already for $s = 3$ ($\mathrm{tr}^{(2)}_{\Theta^2}(q, S)$ is not defined).

Table 5.1 Lower bounds $\mathrm{tr}^{(s)}_{\Theta^2}(f, S)$ for p and q over $S = \{1 - X^2, 1 - Y^2\}$

s	$\mathrm{tr}^{(s)}_{\Theta^2}(p, S)$	$\mathrm{tr}^{(s)}_{\Theta^2}(q, S)$
2	−0.2500	n.d.
3	−0.0178	0
4	−0.0031	0
5	−0.0010	0

Table 5.2 Lower bounds $\operatorname{tr}^{(s)}_{\Theta^2}(p,S)$, $\operatorname{tr}^{(s)}_{\Theta^2}(q,S)$, and $\operatorname{tr}^{(s)}_{\Theta^2}(r,S)$ over $S = \{1-X, 1-Y, 1+X, 1+Y\}$

s	$\operatorname{tr}^{(s)}_{\Theta^2}(p,S)$	$\operatorname{tr}^{(s)}_{\Theta^2}(q,S)$	$\operatorname{tr}^{(s)}_{\Theta^2}(r,S)$
2	−2.0000	n.d.	−1.0000
3	−0.2500	−0.0261	−1.0000
4	−0.0178	0.0000	−1.0000
5	−0.0031	0.0000	−1.0000

Example 5.15. Let p,q be as in Example 5.14 and let $r = XYX$. Let us define $S = \{1-X, 1-Y, 1+X, 1+Y\}$. The resulting sequences from the relaxation are in Table 5.2 and show that there is again no convergence in the first four steps for p, while for q we get convergence at $s = 4$ and for r we get the optimal value immediately (at $s = 2$).

To compute, e.g., $\operatorname{tr}^{(5)}_{\Theta^2}(p,S)$ we need to solve (Constr-$\operatorname{Tr}^{(s)}_{\mathrm{SDP}'}$) which has 3739 linear constraints and five positive semidefinite constraints with matrix variables of order 63, 31, 31, 31, 31.

Example 5.16. Let us consider $p = XY$, $q = 1 + X(Y-2) + Y(X-2)$, $f = p^*q + q^*p$ and $S = \{4 - X^2, 4 - Y^2\}$. If we use NCSOStools and call

```
>> NCvars x y
>> p = x*y;q = 1+x*(y-2)+y*(x-2);f = p'*q+q'*p;
>> S = {4-x^2,4-y^2};
>> [opt_2,decom_1,dec_S1,base1] = NCtraceOpt(f,S,4);
>> [opt_3,decom_2,dec_S2,base2] = NCtraceOpt(f,S,6);
>> [opt_4,decom_3,dec_S3,base3] = NCtraceOpt(f,S,8);
```

we obtain `opt_2` $= \operatorname{tr}^{(2)}_{\Theta^2}(f,S) = -8$ and `opt_3` $= \operatorname{tr}^{(3)}_{\Theta^2}(f,S) = \operatorname{tr}^{(4)}_{\Theta^2}(f,S) = -5.2165$. This was checked numerically but running `NCtraceOptRand` did not finish with a numerical proof of 1-flat solutions, so we cannot claim that $\operatorname{tr}^{\mathrm{II}_1}_{\min}(f,S)$ is equal to -5.2165.

It is easy to see that the (commutative) minimum of f on $\mathscr{D}_S \cap \mathbb{R}^2 = [-2,2]^2$ is -4.5.

Example 5.17. Let us compute the trace-minimum of $f = 2 - X^2 + XY^2X - Y^2$ over the semialgebraic set defined by $S = \{4 - X^2 - Y^2, XY + YX - 2\}$.

```
>> NCvars x y
>> f = 2 - x^2 + x*y^2*x - y^2;
>> S={4-x^2-y^2,x*y+y*x-2};
>> [X,fX,tr_val,flat,err_flat]=NCtraceOptRand(f,S,4);
```

Firstly we see that `flat` $= 1$ which means that the method has found a flat optimal solution with `err_flat`$\approx 4 \cdot 10^{-8}$. This gives a matrix X of size 2×16; each row represents one symmetric 4×4 matrix,

$$A = \text{reshape}(X(1,:),4,4) = \begin{bmatrix} -0.0000 & 1.4044 & -0.1666 & -0.0000 \\ 1.4044 & 0.0000 & 0.0000 & 1.1329 \\ -0.1666 & 0.0000 & -0.0000 & -0.8465 \\ -0.0000 & 1.1329 & -0.8465 & 0.0000 \end{bmatrix}$$

$$B = \text{reshape}(X(2,:),5,5) = \begin{bmatrix} -0.0000 & 0.8465 & 1.1329 & 0.0000 \\ 0.8465 & 0.0000 & 0.0000 & -0.1666 \\ 1.1329 & 0.0000 & 0.0000 & -1.4044 \\ 0.0000 & -0.1666 & -1.4044 & 0.0000 \end{bmatrix}$$

such that A and B are from $\mathscr{D}_S(4)$ and

$$fX = f(A,B) = \begin{bmatrix} -1.0000 & 0.0000 & 0.0000 & -0.0000 \\ 0.0000 & -1.0000 & 0.0000 & 0.0000 \\ 0.0000 & 0.0000 & -1.0000 & 0.0000 \\ -0.0000 & 0.0000 & 0.0000 & -1.0000 \end{bmatrix}$$

with (normalized) trace equal to `trace_val` $= -1$.

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