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Optimization of Polynomials in Non-Commuting Variables

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Introduction

Optimization problems involving polynomial data arise across many sciences, e.g., in control theory [Che10, HG05, Sch06], operations research [Sho90, Nie09], statistics and probability [Las09], combinatorics and graph theory [LS91, AL12], computer science [PM81], and elsewhere. They are however difficult to solve. For example, very simple instances of polynomial optimization problems (POPs) are known to be NP hard. Because of their importance, various algorithms have been devised to approximately solve POPs. Traditionally techniques have drawn from operations research, computer science, and numerical analysis. Since the boom in semidefinite programming (SDP) in the 1990s, newer techniques for solving POPs are based on sums of squares concepts taken from real algebraic geometry and inspired by moment theory from probability and functional analysis. There are now many excellent packages available for solving POPs based on these methods, such as GloptiPoly [HLL09], SOSTOOLS [PPSP05], SparsePOP [WKK$^+$09], or YALMIP [Löf04].

In this book, our focus is on polynomial optimization problems in matrix unknowns, i.e., non-commutative POPs or NCPOPs for short. Many applied problems, for example, those in all the textbook classics in control theory [SIG97], have matrices as variables, and the formulas naturally involve polynomials in matrices. These polynomials depend only on the system layout and do not change with the size of the matrices involved; such problems are "dimension-free." Analyzing them is in the realm of *free analysis* [KVV14] and *free real algebraic geometry* (free RAG) [BPT13].

The booming area of free analysis provides an analytic framework for dealing with quantities with the highest degree of non-commutativity, such as large (random) matrices. Free RAG is its branch that studies positivity of polynomials in freely non-commuting (nc) matrix variables. In recent years, free RAG has found many applications of which we mention only a small selection. NCPOPs are ubiquitous.

Pironio, Navascués, and Acín [NPA08, PNA10] give applications to quantum theory and quantum information science and also consider computational aspects of NCPOPs. In quantum theory, NCPOPs are used to produce upper bounds on the maximal violation of Bell inequalities [PV09]. These inequalities provide a method to investigate *entanglement*, one of the most peculiar features of quantum mechanics, which allows two parties to be correlated in a non-classical way. In the same spirit, in [DLTW08], the authors investigate the quantum moment problem and entangled multi-prover games using NCPOPs. NCPOPs can also be used in quantum chemistry to compute atomic and molecular ground state energies, etc. A famous open problem due to Tsirelson [JNP$^+$11, Fri12] asks whether every quantum mechanical system can be modeled in finite-dimensional spaces. Tsirelson's problem is equivalent to two big questions in operator algebras, Kirchberg's conjecture [Kir93] and Connes' embedding conjecture [Con76]. The latter of these has a natural reformulation as a question on NCPOPs [KS08a, BDKS14, Oza04]. Closely related to Tsirelson's problem is a question about the right model for non-local quantum correlations. Without details, there are two widely accepted models, one with a tensor product structure of operators and one where only commutativity between operators located at different sites is assumed. A variant of Tsirelson's problem would imply that both models describe the same set of quantum correlations. Whereas for the latter model one can apply sums of hermitian squares (SOHS) to check for positivity, as it is done by Pironio, Navascués, and Acín [NPA08, PNA10], the former model is more difficult due to the tensor product structure. Mančinska and Roberson [MR14] and Sikora and Varvitsiotis [SV15] showed that bipartite quantum correlations from the tensor model can be written as projection of an affine section of the completely positive semidefinite cone introduced by Laurent and Piovesan [LP15]. Formally, it is the cone of Gram matrices of tuples of positive semidefinite matrices. But this cone can also be derived by dualizing a certain cone of nc polynomials with positive trace, bringing NCPOPs back into the picture; see also [BLP15].

Helton et al. in [HMdOP08] survey applications and connections to control and systems engineering. Free RAG and NCPOPs are employed to enforce convexity in classes of dimension-free problems. Cimprič [Cim10] uses NCPOPs to investigate PDEs and eigenvalues of polynomial partial differential operators. Inspired by randomized algorithms in machine learning, Recht and Re [RR12] investigate the arithmetic-geometric mean inequality for matrices with the aid of NCPOPs.

Finally, we mention an application of NCPOPs to statistical physics. The Bessis-Moussa-Villani (BMV) conjecture [BMV75] (now a theorem of Stahl [Sta13]) arose from an attempt to simplify the calculation of partition functions of quantum mechanical systems. It states that for any two symmetric matrices A,B, where B is positive semidefinite, the function $t \mapsto \operatorname{tr}(e^{A-tB})$ is the Laplace transform of a positive Borel measure with real support. This permits the calculation of explicit upper and lower bounds of energy levels in multiple particle systems. The BMV conjecture is intimately related with positivity of certain symmetric nc polynomials [KS08b, Bur11].

We developed `NCSOStools` [CKP11] as a consequence of this recent flurry of interest in free RAG. `NCSOStools` [CKP11] is an open-source Matlab toolbox for handling NCPOPs. It solves unconstrained and constrained NCPOPs, either optimizing for eigenvalues or trace of an nc polynomial objective function, by converting them to a standard SDP which is then solved using one of the existing solvers such as SeDuMi [Stu99], SDPT3 [TTT99], or SDPA [YFK03]. As a side product, our toolbox implements symbolic computation with nc variables in Matlab. This book presents the theoretical underpinnings needed for all the algorithms we implemented with examples computed in `NCSOStools` [CKP11].

Organization of the Book

The book is organized as follows. Chapter 1 collects all the background material from algebra, functional analysis, and mathematical optimization needed throughout the book. On the algebraic side, we introduce non-commutative polynomials, commutators, sums of hermitian squares, quadratic modules, and semialgebraic sets from free RAG. Then we discuss the nc moment problem and its solution via flatness and the Gelfand-Naimark-Segal (GNS) construction. Finally, the chapter concludes with a discussion of SDP.

Our basic tool to minimize the eigenvalues of an nc polynomial is based on SOHS. In fact, by Helton's sums of squares theorem [Hel02], an nc polynomial is positive semidefinite if and only if it is an SOHS. Chapter 2 explains how to test if a given nc polynomial is an SOHS. This is based on an appropriate variant of the Gram matrix method; an nc polynomial is an SOHS if and only if the associated SDP is feasible. What is new and in sharp contrast to the commutative case is the complexity of the constructed SDP. Namely, its order is linear in the size of the input data. This is obtained from a careful analysis of the nc Newton polytope and the so-called Newton chip method.

Observe that a matrix has nonnegative trace if and only if it is a sum of a positive semidefinite matrix (a hermitian square) and a trace zero matrix (a commutator). Motivated by this simple observation, we propose a sum of hermitian squares and commutators certificate for trace positivity of nc polynomials. These certificates are analyzed in Chap. 3. We provide tracial analogs of the Gram matrix method and the Newton polytope.

In Chap. 4, we turn to optimization of nc polynomials. We present unconstrained and constrained optimizations. Uncostrained optimization is a single SDP, while we give a Lasserre-type [Las01] relaxation scheme for constrained optimization. This includes a study of exactness based on the Curto-Fialkow [CF96, CF98] flatness results generalized to the non-commutative setting. Special attention is given to special cases of convex constraint sets, i.e., nc balls and nc polydiscs. Their constrained optimization reduces to a single SDP.

Finally, Chap. 5 presents tracial optimization of nc polynomials and tracial analogs of the results in Chap. 4.

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