

# Improved Approach for Optimization Problems of Determining the $C$ -numerical Range

Youping Fan \* Bernd Tibken \*\*

\*, \*\* Faculty of Electrical, Information and Media Engineering,  
University of Wuppertal, 42097 Wuppertal, Germany  
(e-mail: {fan, tibken}@uni-wuppertal.de)

**Abstract:** In quantum computing and quantum control, the investigation of the  $C$ -numerical range is of great importance. One relevant optimization problem can be represented as maximizing the trace function  $\Re(\text{tr}(UA^\dagger U^\dagger C))$  subject to the unitary matrix conditions  $U^\dagger U = I_n, UU^\dagger = I_n$ .

To solve this NP-hard problem, the Positivstellensatz from the real algebraic geometry is used to construct a dual relaxation problem, which is represented with a linear objective function subject to some matrix inequalities constraints. In general this results in some bilinear terms with respect to the decision variables in the matrix constraints. Instead of further relaxation to those bilinear terms, so that a pure linear matrix inequalities (LMIs) optimization problem is derived, we reformulate this dual structure as a generalized eigenvalue problem (GEVP) with some LMIs constraints and some linear-fractional LMIs conditions. The GEVP dual relaxation provides a tractable approach for finding high quality bounds to the hard primal problem under acceptable computational effort.

Numerical results of a benchmark example from quantum computing are presented and demonstrate that the improved approach yields much more competitive bound of the  $C$ -numerical range in comparison with other methods.

## 1. INTRODUCTION

In optimal controlling of quantum systems, to investigate the coherency transfer from a given initial state to a desired final state plays an important role. Consider the signal-relevant components of the initial state and those of the final state to be collected into two matrices  $A$  and  $C$ , respectively, which are arbitrary finite square matrices with complex or real entries. Then the inner product  $\langle C|A \rangle := \text{tr}(C^\dagger A)$  induces a metric and a Hilbert space structure, where  $\cdot^\dagger$  denotes the complex conjugate transpose of a matrix.

The overlap of points on the unitary orbit of the initial state  $A$  with the final state  $C$ , defined as

$$f(U) := \langle UAU^\dagger | C \rangle = \text{tr}(UA^\dagger U^\dagger C)$$

is actually well-known in the mathematics as the  $C$ -numerical range of  $A$  defined by

$$W_C(A) := \{ \text{tr}(UA^\dagger U^\dagger C) : U \in U(n, \mathbb{C}) \},$$

where  $U(n, \mathbb{C}) := \{ U : U \in \mathbb{C}^{n \times n}, U^\dagger U = UU^\dagger = I_n \}$ . See Li [1994]. Cheung et al. [1996] has proved that  $W_C(A)$  is compact, connected and star-shaped with respect to the point  $\frac{\text{tr}(A^\dagger)\text{tr}(C)}{n}$ .

However, the geometry of the  $C$ -numerical range can be quite complicated and is only partially understood at present. A natural measure of the size of  $W_C(A)$  is the so-called  $C$ -numerical radius of  $A$ ,

$$r_C(A) := \max_{U \in U(n, \mathbb{C})} |\text{tr}(UA^\dagger U^\dagger C)|. \quad (1)$$

The  $r_C(A)$  is the radius of the smallest disk centered at the origin containing  $W_C(A)$ . See Goldberg et al. [1977] and Horn et al. [1990], the following inequalities for  $r_C(A)$

$$\rho_C(A) \leq r_C(A) \leq \|A\|_C, \quad (2)$$

have been derived, where  $\rho_C(A)$  stands for the  $C$ -spectral radius of  $A$  defined by

$$\rho_C(A) := \max_{\pi(j)} \left| \sum_{j=1}^n \lambda_j(A) \lambda_{\pi(j)}(C) \right|, \quad (3)$$

$$\pi(j) \in \text{perm}\{1, 2, \dots, n\}$$

with  $\lambda_j(A)$ ,  $\lambda_j(C)$  denoting the eigenvalues of the matrices  $A$  and  $C$ , respectively; and  $\|A\|_C$  is the  $C$ -spectral norm of  $A$  defined by

$$\|A\|_C := \max_{V, W \in U(n, \mathbb{C})} |\text{tr}(VAWC)|. \quad (4)$$

The equality (2) is reached in case of Hermitian matrices  $A$  and  $C$ . In the general case of non-Hermitian matrices  $A$  and  $C$ ,  $r_C(A)$  is poorly limited with those lower and upper bounds, see Glaser et al. [1998].

On the other hand, in the setting of  $C$ -numerical ranges, there are some geometric optimization tasks of particular practical relevance as they determine maximal signal intensity in coherent spectroscopy, see Glaser et al. [1998], and Schulte-Herbruggen et al. [2002]. For instance, the task of minimizing the Euclidean distance between  $C$  and the unitary orbit of  $A$ . Obviously, the distance

$$\|UAU^\dagger - C\|_2^2 = \|A\|_2^2 + \|C\|_2^2 - 2\Re\{\text{tr}(UA^\dagger U^\dagger C)\}$$

reaches minimum if the overlap  $\Re \{ \text{tr}(UA^\dagger U^\dagger C) \}$  is maximum. Moreover, in the experiments like Nuclear Magnetic Resonance (NMR), some exposed points of the  $C$ -numerical range of  $A$  can be obtained. Such exposed points could be the ones which have the largest real parts. In this sense we can solve an optimization problem defined by

$$\max_{U \in U(n, \mathbb{C})} \Re \{ \text{tr}(UA^\dagger U^\dagger C) \} \quad (5)$$

for bounding the geometry of the  $C$ -numerical range.

Extending concepts of Brockett (see Brockett [1988, 1993]) from the orthogonal to the unitary group (see Glaser et al. [1998], Helmke et al. [2002], Schulte-Herbruggen [1998]), the optimization problem (5) can be treated by the gradient-flows method proposed by Helmke et al. [1994]. However, there is no guarantee that the gradient flows always reach the *global* extrema.

(5) is in fact a so-called quadratically constrained quadratic problem (QCQP). See Tibken et al. [2006a,b], it has been presented that, some convex SDP dual relaxations can be constructed to the primal QCQP (5). These dual structures are actually linear matrix inequalities (LMI) optimization problems with respect to some decision variables. By solving those LMIs, global upper bounds to the optimal value of the objective of the primal one (5) were calculated numerically. However, observing the procedure of constructing those LMIs closely, we find out, those non-convex bilinear matrix inequality constraints ever arising became just convex LMIs when one of the decision variables in the bilinear terms was held as a reasonable constant. Consequently, much "looser" dual relaxations to the primal one (5) were obtained indeed.

Hence, inspired by the idea of keeping those bilinear terms, the aim in this contribution is to construct a much tighter dual relaxation structure. We expect the duality gap can be therefor narrowed significantly and a much sharper estimation to the geometry of the  $C$ -numerical range can be obtained in general.

## 2. QCQPS AND THE DUAL RELAXATIONS

As explained in section 1, the geometric optimization tasks concerning  $W_C(A)$  can sometimes be simplified to maximizing the trace function  $\Re \{ \text{tr}(UA^\dagger U^\dagger C) \}$  over the decision variable  $U$  and  $U \in U(n, \mathbb{C})$ . After we represent the conditions with the unitary matrix equalities  $U^\dagger U = I_n$ ,  $UU^\dagger = I_n$  and  $U \in \mathbb{C}^{n \times n}$  concretely, we have

$$\begin{aligned} \gamma_O^* &:= \max_U \Re \{ \text{tr}(UA^\dagger U^\dagger C) \} \\ \text{s.t. } &U^\dagger U = I, \quad UU^\dagger = I, \quad U \in \mathbb{C}^{n \times n} \end{aligned} \quad (6)$$

where  $A, C \in \mathbb{C}^{n \times n}$  are given matrices. Notice that, in the case that the boundary of  $\{ \text{tr}(UA^\dagger U^\dagger C) : U \in U(n, \mathbb{C}) \}$  is to estimate, the constraint  $\Im \{ \text{tr}(UA^\dagger U^\dagger C) \} = 0$  should also be added to (6).

### 2.1 QCQPs in the complex and real domain

Obviously, (6) is a QCQP in terms of  $U$  in the complex domain. Since

$$\text{tr}(UA^\dagger U^\dagger C) = \text{vec}(U^T)^T (C^T \otimes A^\dagger) \text{vec}(U^\dagger) \quad (7)$$

where  $\text{vec}(\cdot)$  means to formulate a vector from a matrix columnwise, the objective function in (6) is subsequently reformulated as follows

$$\begin{aligned} &\Re \{ \text{tr}(UA^\dagger U^\dagger C) \} \\ &= \frac{1}{2} \left( \text{tr}(UA^\dagger U^\dagger C) + (\text{tr}(UA^\dagger U^\dagger C))^\dagger \right) \\ &= \text{vec}(U^T)^T \left( \frac{C^T \otimes A^\dagger + (C^T \otimes A^\dagger)^\dagger}{2} \right) \text{vec}(U^\dagger). \end{aligned} \quad (8)$$

Define that

$$\hat{x} := \text{vec}(U^\dagger) \in \mathbb{C}^{n^2}, \quad (9)$$

$$\hat{P}_0 := \frac{C^T \otimes A^\dagger + (C^T \otimes A^\dagger)^\dagger}{2} \in \mathbb{C}^{n^2 \times n^2}. \quad (10)$$

Hence we have

$$\Re \{ \text{tr}(UA^\dagger U^\dagger C) \} = \hat{x}^\dagger \hat{P}_0 \hat{x}. \quad (11)$$

The advantage of describing the objective function with  $\hat{x}$  and  $\hat{P}_0$  is that all the information about the matrices  $A, C$  is therefore contained in the unique matrix  $\hat{P}_0$  compactly.

On the other hand, the matrix conditions  $U^\dagger U = I_n$ ,  $UU^\dagger = I_n$  imply  $2n^2$  polynomial equalities in the real domain. From a computational view point, in order to *absorb* the relevant information about those  $2n^2$  polynomials and save the information for further numerical calculation, we define two sets of Hermitian matrices  $F_r = F_r^\dagger \in \mathbb{C}^{n \times n}$  and  $G_r = G_r^\dagger \in \mathbb{C}^{n \times n}$ , respectively, where  $r = 1, 2, \dots, n^2$ .

Table 1 and Table 2 show the exact definitions to  $F_r$  and  $G_r$  depending on the different indices ( $kl$ ) of the elements  $(U^\dagger U)_{kl}$  and  $(UU^\dagger)_{kl}$ , respectively, where  $k = 1, 2, \dots, n$ ,  $l = k, k+1, \dots, n$ .

Table 1. Definitions to  $F_r$  concerning the elements  $(U^\dagger U)_{kl}$ .

$(U^\dagger U)_{kk}$	$\Re \{ (U^\dagger U)_{kl} \}, k \neq l$	$\Im \{ (U^\dagger U)_{kl} \}, k \neq l$
$F_r := e_k e_k^T$	$F_r := e_k e_l^T + e_l e_k^T$	$F_r := i e_k e_l - i e_l e_k^T$
$\text{tr}(F_r) = 1$	$\text{tr}(F_r) = 0$	$\text{tr}(F_r) = 0$

Table 2. Definitions to  $G_r$  concerning the elements  $(UU^\dagger)_{kl}$ .

$(UU^\dagger)_{kk}$	$\Re \{ (UU^\dagger)_{kl} \}, k \neq l$	$\Im \{ (UU^\dagger)_{kl} \}, k \neq l$
$G_r := e_k e_k^T$	$G_r := e_k e_l^T + e_l e_k^T$	$G_r := i e_k e_l - i e_l e_k^T$
$\text{tr}(G_r) = 1$	$\text{tr}(G_r) = 0$	$\text{tr}(G_r) = 0$

Notice that, we use  $i = \sqrt{-1}$  to denote the imaginary unit.  $e_k, e_l \in \mathbb{R}^n$  denote the  $k$ -th and  $l$ -th unit column vectors with an 1 in the  $k$ -th and  $l$ -th positions, respectively.

Then due to  $U^\dagger U = I_n$  and  $UU^\dagger = I_n$ , we have

$$\text{tr}(F_r (U^\dagger U - I_n)) = 0, \quad r = 1, 2, \dots, n^2, \quad (12)$$

$$\text{tr}(G_r (UU^\dagger - I_n)) = 0, \quad r = 1, 2, \dots, n^2, \quad (13)$$

which are equivalent to

$$\text{tr}(F_r U^\dagger U) = \text{tr}(F_r), \quad r = 1, 2, \dots, n^2, \quad (14)$$

$$\text{tr}(G_r UU^\dagger) = \text{tr}(G_r), \quad r = 1, 2, \dots, n^2. \quad (15)$$

It can be proved briefly, that these  $2n^2$  equalities (14) (15) depending on  $F_r, G_r$  defined in Table (1) and (2) are equivalent with those  $2n^2$  real polynomial equalities implied by  $U^\dagger U = I_n$  and  $UU^\dagger = I_n$ . In other words, all the information necessary for presenting computationally those  $2n^2$  real polynomial equalities are saved in those matrices  $F_r, G_r, r = 1, 2, \dots, n^2$ , which are all sparse matrices.

Since

$$\text{tr}(F_r U^\dagger U) = \text{vec}(U^T)^T (I_n \otimes F_r) \text{vec}(U^\dagger), \quad (16)$$

$$\text{tr}(G_r U U^\dagger) = \text{vec}(U^T)^T (G_r^T \otimes I_n) \text{vec}(U^\dagger), \quad (17)$$

we define

$$\hat{P}_j = I_n \otimes F_r, \quad j = 1, 2, \dots, n^2, \quad (18)$$

$$\hat{P}_j = G_r^T \otimes I_n, \quad j = n^2 + 1, \dots, 2n^2, \quad (19)$$

with  $r = 1, 2, \dots, n^2$  in (18) and (19), respectively. By using the definition of  $\hat{x}$  in (9) and the definitions of  $\hat{P}_j$  above, the QCQP (6) in terms of  $U \in \mathbb{C}^{n \times n}$  is hence formulated as

$$\begin{aligned} \gamma_O^* := \max_{\hat{x}} \hat{x}^\dagger \hat{P}_0 \hat{x} \\ \text{s.t. } \hat{x}^\dagger \hat{P}_j \hat{x} = b_j \end{aligned} \quad (20)$$

where  $\hat{P}_0, \hat{P}_j \in \mathbb{C}^{n^2 \times n^2}$  are Hermitian matrices,  $b_j \in \{0, 1\}$ ,  $j = 1, 2, \dots, 2n^2$ .  $\hat{x} \in \mathbb{C}^{n^2}$  is the decision variable of the optimization problem. Define that

$$x = \begin{bmatrix} \Re(\hat{x}) \\ \Im(\hat{x}) \end{bmatrix}, \quad P_j = \begin{bmatrix} \Re(\hat{P}_j) & -\Im(\hat{P}_j) \\ \Im(\hat{P}_j) & \Re(\hat{P}_j) \end{bmatrix}, \quad (21)$$

with  $j = 0, 1, \dots, 2n^2$ . Since  $\hat{x}^\dagger \hat{P}_j \hat{x} = x^T P_j x$  with  $j = 0, 1, \dots, 2n^2$ , we obtain the standard QCQP representation for (6) in the real domain:

$$\begin{aligned} \gamma_O^* := \max x^T P_0 x \\ \text{s.t. } x^T P_j x = b_j \end{aligned} \quad (22)$$

where  $P_0, P_j \in \mathbb{R}^{2n^2 \times 2n^2}$  are symmetric matrices,  $b_j \in \{0, 1\}$ ,  $j = 1, 2, \dots, 2n^2$ .  $x \in \mathbb{R}^{2n^2}$  is the corresponding decision variable in the real domain. Since  $P_0$  is not necessarily positive semidefinite, this is the maximization of a nonconvex function over a nonconvex set.

Notice that, despite the different representations of QCQPs from (6) to (20) and (22), they are all NP-hard and numerically intractable generally; an alternative and efficient approach for solving such problems is to construct and solve their dual problems. In the following sections, it will be showed, QCQP in the standard representation (22) is however more desirable and convenient for constructing a convex dual relaxation structure to the primal one, especially when man uses theories concerning about positive polynomials and polynomials in sums of squares (SOS) decompositions.

## 2.2 Dual Relaxations to QCQPs

Referring to (22) we introduce a real number  $t$  and define a real semialgebraic set reading  $\mathcal{S}_{\mathcal{P}}$

$$\mathcal{S}_{\mathcal{P}} := \left\{ x \in \mathbb{R}^N \mid \begin{array}{l} x^T P_0 x - t \geq 0 \\ x^T P_j x - b_j = 0, j = 1, 2, \dots, m \end{array} \right\}, \quad (23)$$

where  $N = 2n^2$  and  $m = 2n^2$  in the case of (6) and (22). The feasibility of  $\mathcal{S}_{\mathcal{P}}$  can be checked up for a fixed  $t$ . Obviously, when  $t$  is bigger than the optimal value  $\gamma_O^*$  in (22), i.e.,  $t > \gamma_O^*$ , the set  $\mathcal{S}_{\mathcal{P}}$  is definitely infeasible, otherwise when  $t \leq \gamma_O^*$ , the set  $\mathcal{S}_{\mathcal{P}}$  might have some feasible solutions in terms of  $x$ . In this sense, (22) is formulated as follows

$$\begin{aligned} \gamma_O^* := \max_t t \\ \text{s.t. } \mathcal{S}_{\mathcal{P}} : \text{feasible} \end{aligned} \quad (24)$$

However, to test feasibility of a real semialgebraic set is in general intractable, especially when the set cannot be proved to be convex. But due to Stengle [1973] and Parrilo [2000], the Positivstellensatz from the real algebraic geometry can be used to construct dual structures to (24) and check infeasibility of the real semialgebraic set  $\mathcal{S}_{\mathcal{P}}$ . i.e., when the dual structures are in the form of semidefinite programs, by solving the semidefinite programs, one may obtain some certificates of infeasibility for the infeasible semialgebraic set.

The following is a dual problem to (22) or (24) with  $\gamma_D^* \geq \gamma_O^*$ .

$$\begin{aligned} \gamma_D^* := \min_t t \\ \text{s.t. } \mathcal{S}_{\mathcal{P}} : \text{infeasible} \end{aligned} \quad (25)$$

Based upon the Positivstellensatz we know, if there exist sum-of-squares (SOS) polynomials  $s_0(x), s_1(x)$  such that

$$\begin{aligned} s_0(x) + s_1(x) (x^T P_0 x - t) + \\ \sum_{j=1}^m t_j(x) (x^T P_j x - b_j) + 1 = 0, \end{aligned} \quad (26)$$

then the set  $\mathcal{S}_{\mathcal{P}}$  is infeasible. In (26)  $t_j(x)$  are arbitrary quadratic polynomials with bounded degree. This sufficient condition for infeasibility of the set  $\mathcal{S}_{\mathcal{P}}$  may be tested using semidefinite programming (SDP). In other words, one picks a fixed degree  $d$  over which to search for SOS polynomials  $s_0(x), s_1(x)$  satisfying this equality condition (26). The decision variables in those semidefinite programming are the coefficients of the polynomials  $s_0(x), s_1(x), t_j(x)$  and the parameters contained in the constraints that  $s_0(x), s_1(x)$  be SOS are imposed as positive semidefiniteness constraints. Therefore,

$$\begin{aligned} \gamma_D^* := \min_t t \\ \text{s.t. } (26) \\ s_0(x), s_1(x) : \text{SOS}, \forall x \in \mathbb{R}^N \end{aligned} \quad (27)$$

On the one hand, we assume  $s_1(x)$  and  $t_j(x)$  are all quadratic polynomial of degree  $d = 2$  and define

$$s_1(x) = x^T S_1 x + \mu \quad (28)$$

$$t_j(x) = x^T T_j x + \lambda_j, \quad j = 1, \dots, m \quad (29)$$

where  $S_1 = S_1^T \in \mathbb{R}^{N \times N}$ ,  $T_j = T_j^T \in \mathbb{R}^{N \times N}$  and  $\mu, \lambda_j \in \mathbb{R}$  with  $j = 1, 2, \dots, m$  are the decision variables to  $s_1(x)$  and  $t_j(x)$ , respectively. Concerning  $s_1(x)$ , it can be proved that

$$s_1(x) \text{ is SOS} \Leftrightarrow S_1 = S_1^T \succeq 0 \text{ and } \mu \geq 0 \quad (30)$$

which means the constraint of  $s_1(x)$  being SOS can be equivalently represented with those two positive semidefinite matrix constraints.

On the other hand, referring to  $s_0(x)$ , combining the definitions (28), (29) with (26) we obtain

$$s_0(x) = s_{00}(x) + s_{02}(x) + s_{04}(x) \quad (31)$$

with

$$s_{00}(x) = \mu t + \sum_{j=1}^m \lambda_j b_j - 1 \quad (32)$$

$$s_{02}(x) = x^T \left( tS_1 - \mu P_0 + \sum_{j=1}^m (b_j T_j - \lambda_j P_j) \right) x \quad (33)$$

$$s_{04}(x) = \text{vec}(xx^T)^T \left( -S_1 \otimes P_0 - \sum_{j=1}^m T_j \otimes P_j \right) \text{vec}(xx^T) \quad (34)$$

Obviously, with respect to  $x$ ,  $s_0(x)$  contains three homogeneous polynomials  $s_{00}(x)$ ,  $s_{02}(x)$ ,  $s_{04}(x)$  of degree 0, 2, 4, respectively. Meanwhile we define

$$s_0(x) = S_{00} + x^T S_{02} x + \omega^T S_{04} \omega, \quad (35)$$

where  $\omega$  is a vector composed of all monomials of degree 2 in the variables  $x$  and its length, denoted as  $d_\omega$ , is  $d_\omega = \frac{N(N+1)}{2}$ ;  $S_{00} \in \mathbb{R}$ ,  $S_{02} \in \mathbb{R}^{N \times N}$  and  $S_{04} \in \mathbb{R}^{d_\omega \times d_\omega}$ . Then the sufficient conditions that  $s_0(x)$  has SOS decompositions for all  $x \in \mathbb{R}^N$  can be represented with three positive semidefinite matrix constraints:

$$S_{00} \geq 0, S_{02} = S_{02}^T \succeq 0, S_{04} = S_{04}^T \succeq 0 \quad (36)$$

By matching coefficients of monomials in (31) and (35), we have following conclusions:

$$\begin{aligned} S_{00} &= \mu t + \sum_{j=1}^m \lambda_j b_j - 1 \\ S_{02} &= tS_1 - \mu P_0 + \sum_{j=1}^m (b_j T_j - \lambda_j P_j) \\ S_{04} &= S_{04}(S_1, T_j, \sigma) \end{aligned}$$

where  $S_{04}$  denotes the linear combination of matrices depending on the decision variables  $S_1, T_j$  and some  $\sigma$ . Due to Lasserre [2001], Parrilo et al. [2003a,b], Tibken et al. [2006b], for a homogeneous and possibly dense polynomial  $s_{04}(x)$  of degree 4 in  $x \in \mathbb{R}^N$ , the set of Gram matrices  $S_{04}$  with which  $s_{04}(x) = \omega^T S_{04} \omega$  for all  $x$  is an affine set. In this case,  $N_\sigma = \frac{N^2(N+1)(N-1)}{12}$  additional parameters  $\sigma_j$ ,  $j = 1, \dots, N_\sigma$  are required, which help to interpret such affine feature and build the linear combination of the matrix  $S_{04}(S_1, T_j, \sigma)$ .

Consequently we obtain the dual relaxation to (6).

$$\begin{aligned} \gamma_D^* &:= \min_{t, \mu, \lambda, \sigma, S_1, T_j} t \\ \text{s.t. } &\mu t + \sum_{j=1}^m \lambda_j b_j - 1 \geq 0 \\ &tS_1 - \mu P_0 + \sum_{j=1}^m (b_j T_j - \lambda_j P_j) \succeq 0 \\ &S_{04}(S_1, T_j, \sigma) \succeq 0 \\ &\mu \geq 0 \\ &S_1 \succeq 0 \end{aligned} \quad (37)$$

It is actually to minimize  $t$  subject to some positive semidefinite matrix constraints with respect to the decision variables  $t, \mu, \lambda, \sigma, S_1, T_j$ ,  $j = 1, 2, \dots, m$ . Since there exist some bilinear terms  $\mu t$ ,  $tS_1$  in the first two matrix constraints, (37) is actually a low non-convex rank Bilinear Matrix Inequalities (BMI) optimization problem.

Referring to the obtained BMI optimization problem (37) further relaxations to those bilinear terms could be carried out, so that those low non-convex rank bilinear matrix inequality constraints can be replaced with some pure LMIs. i.e., man can define  $\mu, S_1$  or  $T_j$  as some constant numbers or matrices, e.g. a)  $\mu = 1, S_1 = 0$  and  $T_j = 0, j = 1, 2, \dots, m$ ; b)  $\mu = 1, S_1 = 0$ , so that Lagrange dual relaxations and SDP relaxations of second order in the form of pure LMI problems are obtained, respectively, see Tibken et al. [2006a,b]. However, due to the forced relaxations to those bilinear terms, those dual structures are much looser relaxations to the primal problem generally.

### 3. GENERALIZED EIGENVALUE MINIMIZATION PROBLEM

Actually, we can reformulate (37) as

$$\begin{aligned} \gamma_D^* &:= \min_{t, \mu, \lambda, \sigma, S_1, T_j} t \\ \text{s.t. } &S_{04}(S_1, T_j, \sigma) \succeq 0 \\ &\begin{bmatrix} \mu & 0 \\ 0 & S_1 \end{bmatrix} \succeq 0 \\ &t \begin{bmatrix} \mu & 0 \\ 0 & S_1 \end{bmatrix} \succeq \begin{bmatrix} 1 - \sum_{j=1}^m \lambda_j b_j & 0 \\ 0 & \mu P_0 + \sum_{j=1}^m \lambda_j P_j \\ 0 & 0 \\ 0 & -\sum_{j=1}^m b_j T_j \end{bmatrix} \end{aligned} \quad (38)$$

where zero entries stand for zero matrices of appropriate dimension. Define

$$A := \begin{bmatrix} \mu & 0 \\ 0 & S_1 \end{bmatrix} \quad (39)$$

$$B := \begin{bmatrix} 1 - \sum_{j=1}^m \lambda_j b_j & 0 \\ 0 & \mu P_0 + \sum_{j=1}^m \lambda_j P_j - \sum_{j=1}^m b_j T_j \end{bmatrix} \quad (40)$$

which are linear combination of matrices depending on  $\mu, \lambda, S_1$  and  $T_j$ ,  $j = 1, 2, \dots, m$ . Therefore we have

$$\begin{aligned} \gamma_D^* := & \min_{\mu, \lambda, \sigma, S_1, T_j} t \\ \text{s.t. } & S_{04}(S_1, T_j, \sigma) \succeq 0 \\ & A(\mu, S_1) \succeq 0 \\ & tA(\mu, S_1) \succeq B(\mu, \lambda, T_j) \end{aligned} \quad (41)$$

which is in fact a generalized eigenvalue minimization problem (GEVP).

It is noteworthy that, in order to get the corresponding GEVP structure based upon (37), the reformulation described above is not performed trivially. The GEVP dual relaxation (41) is characterized as to minimize the generalized eigenvalue  $t$  over the decision variables  $\mu, \lambda, \sigma, S_1, T_j$  subject to the standard LMI constraint  $S_{04}(S_1, T_j, \sigma) \succeq 0$  and the linear-fractional LMI  $tA(\mu, S_1) \succeq B(\mu, \lambda, T_j)$ . The constraint  $A(\mu, S_1) \succeq 0$  is required for well-posedness of the problem in the case of solving GEVP problem. The `gev`p-solver provided by the LMI-Toolbox in MATLAB is the one we used at present which can solve such GEVP numerically well.

While the GEVP dual relaxation *keeps* the bilinear terms, no relevant information get lost. The GEVP dual relaxation can therefore lead to much narrower duality gap between the primal and the dual problem generally. Nevertheless, due to the representation of multivariate polynomials as sums of squares with Gram matrices and the complexity in the GEVP dual relaxation, large scale problems arise with a huge number of decision variables and hence we must face the computational problems of capacity and time.

#### 4. NUMERICAL EXAMPLE

In this example,  $M$  is a given  $3 \times 3$  diagonal matrix with  $M(1,1) = 1$ ,  $M(2,2) = e^{\frac{2\pi}{3}i}$  and  $M(3,3) = e^{-\frac{2\pi}{3}i}$ . The matrices  $\hat{A}$  and  $\hat{C}$  are the normalized versions of  $(e^{\frac{\pi}{3}i}M + I_3)$  and  $(M + \frac{3}{10}I_3)$ , respectively, where  $I_3$  is

the  $3 \times 3$  identity matrix. We define  $A := \hat{A} - \frac{\text{tr}(\hat{A})}{3}I_3$  and  $C := \hat{C}$ . Then referring to the given  $3 \times 3$  matrices  $A$  and  $C$ , the boundary of the image of the  $C$ -numerical range  $W_C(A)$  is generated by solving a series of the primal optimization problem as follows:

$$\begin{aligned} \gamma_O^* := & \max_{U \in \mathbb{C}^{3 \times 3}} \Re\{\text{tr}(UA^\dagger U^\dagger C)\} \\ \text{s.t. } & U^\dagger U = UU^\dagger = I_3, \\ & \Im\{\text{tr}(UA^\dagger U^\dagger C)\} = 0. \end{aligned} \quad (42)$$

Based on the method introduced in section 3 and the ones from Tibken et al. [2006a,b], we construct the corresponding different dual relaxations with the optimal values  $\gamma_D^*$  of the objectives, i.e., the GEVP dual relaxation, the Lagrangian dual relaxation and the SDP second order dual relaxation. The optimal values  $\gamma_O^*$  of the objectives of the primal ones can be bounded through those upper bounds  $\gamma_O^* \leq \gamma_D^*$ .

Since  $A$  and  $C$  are  $3 \times 3$  matrices, the corresponding space of a unitary matrix  $U$  is 18-dimensional in the real domain. It was calculated that the Lagrangian dual relaxation is an LMI with 20 decision variables, meanwhile the SDP second

order dual relaxation is also in the form of an LMI but with 11990 decision variables; the GEVP dual relaxation however contains 12162 decision variables.

The numerical results calculated by using different algorithms are illustrated in Fig. 1, Fig. 2 and Fig. 3. Note that in the figures  $\cdot^H$  denotes the Hermitian conjugates of a matrix.

Firstly, the  $C$ -spectral norm of  $A$  denoted with  $\|A\|_C$  marked with the blue dashed circle in Fig. 1 indicates actually a much rougher upper limit to the boundary of  $W_C(A)$  in this case.

Secondly, in comparison with the Lagrangian dual relaxation and the higher-order SDP dual relaxation, the GEVP dual relaxation yields much sharper upper bounds  $\gamma_D^*$  to the optimal values  $\gamma_O^*$  of the primal problems generally. The obtained GEVP structure by keeping those bilinear information performs as a tighter dual structure indeed. Especially, Fig. 2 and Fig. 3 show clearly that the optimal values of the objectives of the GEVP dual relaxation (marked with red solid curve) almost coincide with those (marked with blue dots)calculated by using the Gradient-flows-method in Glaser et al. [1998]. This fact confirms that the local extrema calculated through the local optimization algorithm, Gradient-flows-method, could also be the global extrema in this case.

Thirdly, since  $\frac{\text{tr}(A^\dagger)\text{tr}(C)}{3} = 0$ , the geometry of  $W_C(A)$  showed in Fig. 1 is indeed star-shaped and centered at the origin of the complex plane. Referring to the three points  $D_1, D_2, D_3$  in Fig. 1, we calculated the  $C$ -spectral radius of  $A$  (3) denoted with  $\rho_C(A)$  analytically, which in this case is exactly

$$\rho_C(A) = \frac{3}{\sqrt{6}\sqrt{3.27}} \approx 0.67728546147860. \quad (43)$$

Meanwhile the optimal values of the objectives of the GEVP dual relaxations about those three points are:

$$\begin{aligned} \gamma_D^*(D_1) &= 0.67728929487533, \\ \gamma_D^*(D_2) &= 0.67728881393757, \\ \gamma_D^*(D_3) &= 0.67729555427641, \end{aligned} \quad (44)$$

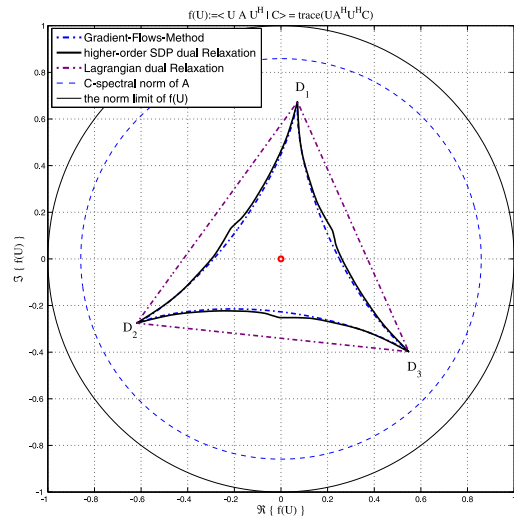


Fig. 1. Comparing results among different algorithms (I).

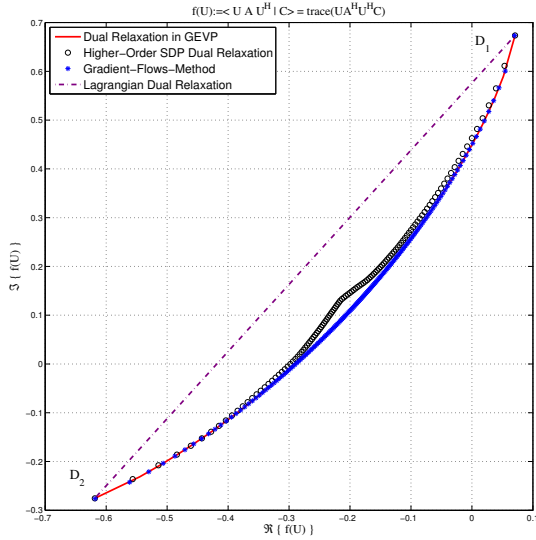


Fig. 2. Comparing results among different algorithms (II).

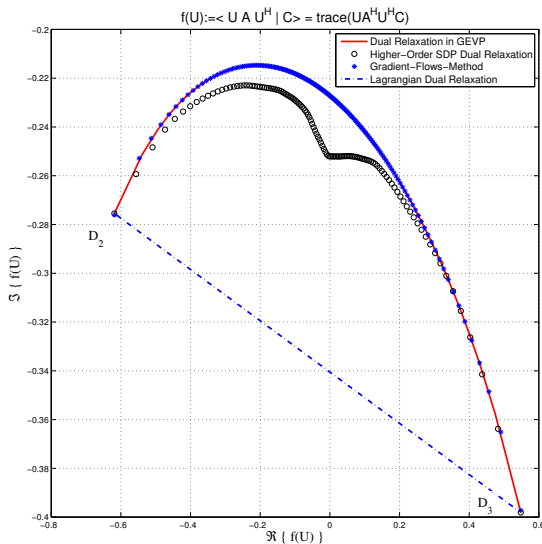


Fig. 3. Comparing results among different algorithms (III).

with the required accuracy  $1e-5$ . The numerical results indicate that the optimal values  $\gamma_O^*(D_1)$ ,  $\gamma_O^*(D_2)$ ,  $\gamma_O^*(D_3)$  of the objectives of the primal optimization problems (42) are bounded very well through the lower limit  $\rho_C(A)$  (43) and the global upper bounds  $\gamma_D^*(D_1)$ ,  $\gamma_D^*(D_2)$ ,  $\gamma_D^*(D_3)$  (44), respectively.

#### REFERENCES

R.W. Brockett. Dynamical Systems that Sort Lists, Diagonalize Matrices and Solve Linear Programming Problems. *Proc. 27th IEEE Conference on Decision and Control*, Austin, USA, pages 799–803, 1988.

R.W. Brockett. Differential Geometry and the Design of Gradient Algorithms. *Proc. Symp. Pure Math.*, Volume 54, pages 69–92, 1993.

W.S. Cheung and N.K. Tsing. The  $C$ -numerical Range of Matrices is Star-Shaped. *Lin. Multilin. Alg.*, Volume 41, pages 245–250, 1996.

S.J. Glaser, T. Schulte-Herbrüggen, M. Sieveking, O. Schedletzky, N.C. Nielsen, O.W. Sørensen and C. Griesinger. Unitary Control in Quantum Ensembles: Maximizing Signal Intensity in Coherent Spectroscopy. *Science*, Volume 280, pages 421–424, 1998.

M. Goldberg and E.G. Straus. Elementary inclusion relations for generalized numerical ranges. *Linear Algebra Application*, Volume 18, pages 1–24, 1977.

U. Helmke and J.B. Moore. *Optimization and Dynamical Systems*, Springer, Berlin, 1994.

U. Helmke, K. Hüper, J.B. Moore and T. Schulte-Herbrüggen. Gradient Flows Computing the  $C$ -numerical Range with Applications in NMR Spectroscopy. *Journal of Global Optimization*, Volume 23, No. 3-4, pages 283–308, 2002.

R.A. Horn and C.R. Johnson. *Matrix Analysis*, second ed. Cambridge University Press, Cambridge (UK), 1990.

J. B. Lasserre. *Global optimization with polynomials and the problem of moments*, SIAM J. Optim., Volume 11(3), pages 796–817, 2001.

C.K. Li.  $C$ -Numerical ranges and  $C$ -Numerical radii. *Linear and Multilinear Algebra*, Volume 37, pages 51–82, 1994.

P.A. Parrilo. Structured Semidefinite Programs and Semi-algebraic Geometry Methods in Robustness and Optimization. Ph. D. Thesis at California Institute of Technology Pasadena, California, 2000.

P.A. Parrilo and Bernd Sturmfels. Minimizing Polynomial Functions. *Algorithmic and Quantitative real algebraic geometry, DIMACS Series in Discrete Mathematics and Theoretical Computer Science*, Volume 60, AMS, pages 83–99, 2003.

P.A. Parrilo and S. Lall. Semidefinite Programming Relaxations and Algebraic Optimization in Control. *European Journal of Control*, Volume 9, No.2-3, pages 307–321, 2003.

T. Schulte-Herbrüggen. *Aspects and Prospects of High-Resolution Nuclear Magnetic Resonance*, Ph.D. Thesis at Eidgenössische Technische Hochschule Zürich, Zürich, 1998.

T. Schulte-Herbrüggen, K. Hüper, U. Helmke and S.J. Glaser. Geometry of Quantum Computing by Hamiltonian Dynamics of Spin Ensembles. *Applications of Geometric Algebra in Computer Science and Engineering*, Birkhäuser, Boston, pages 271–283, 2002.

G. Stengle. A Nullstellensatz and a Positivstellensatz in Semialgebraic Geometry. *J. Math. Ann.*, Volume 207, pages 87–97, 1973.

B. Tibken, Y.P. Fan, T. Schulte-Herbrüggen, S.J. Glaser. Optimization Approach for Quadratically Constrained Quadratic Programs with Application to Determining  $C$ -Numerical Ranges. *the 17th International Symposium on Mathematical Theory of Networks and Systems*, Kyoto, Japan, pages 1179–1184, July 2006.

B. Tibken, Y.P. Fan, S.J. Glaser, T. Schulte-Herbrüggen. Semidefinite Programming Relaxations Applied to Determining Upper Bounds of  $C$ -Numerical Ranges. *the Joint 2006 IEEE CCA/CACSD/ISIC multi-conference*, Munich, Germany, pages 2601–2606, October 2006.