2015 IEEE 54th Annual Conference on Decision and Control (CDC)
December 15-18, 2015. Osaka, Japan

A SVD approach to multivariate polynomial optimization problems

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***Abstract*— We present a novel method to compute all stationary points of optimization problems, of which the objective function and equality constraints are expressed as multivariate polynomials, in the linear algebra setting. It is shown how Stetter-Möller matrix methods can be obtained through a parameterization of the objective function, subsequently manipulated using Macaulay matrices. An algorithm is provided to extend this framework to circumvent the necessity of a Gröbner basis. The generalized eigenvalue problem is obtained through a sequence of unitary transformations and rank tests operating directly on the polynomial coefficients (data-driven). The proposed method is illustrated by means of a structured total least squares (STLS) example.**

I. Introduction

Many problems in engineering can be expressed as multivariate polynomial optimization problems with equality constraints [1], [2]. This is equivalent to finding roots of a system of polynomial equations. Some well-known methods for finding these roots include Stetter-Möller forms [3], homotopy continuation methods [4] and rational univariate representation forms [5]. In the context of optimization, moment theory allows to compute a lower bound for the global optimizer through a series of sums-of-squares relaxations using a linear matrix inequality (LMI) formulation [6].

In recent years, the polynomial root-finding problem has been reformulated in terms of linear algebra constructs [7][8][9], operating on the Macaulay matrix [10], in the Polynomial Numerical Linear Algebra framework (PNLA). Similar to the work of Stetter, finding stationary points of a polynomial optimization problem is in essence solving an eigenvalue problem.

We show that the Stetter-Möller eigenvalue problem can be constructed in the PNLA framework using a parameterization of the objective function. The main contribution of this paper is to extend upon this framework and eliminate the need of prior knowledge of the standard monomials [11], inherently linked to the rank properties of the Macaulay matrix, as they play a vital yet archaic role in current eigenvalue problem formulations. The accompanying data-driven algorithm constructs the eigenvalue problem through a series of strategically placed rank tests and using only unitary transformations in the process.

The article is structured as follows: in section II we introduce notation and revisit basic definitions in PNLA. Section III illustrates the link between standard monomials and rank properties of Macaulay matrices. Section IV explains the eigenvalue problem and how it arises from a parameterized objective function. This approach is extended in section V to eliminate the necessity of knowledge on the standard monomials. The resulting algorithm is finally tested and compared in section VI to existing state-of-the-art methods. We offer concluding remarks in section VII.

II. Notation

A. Polynomial optimization problems

We assume optimization problems with only equality constraints of the form

$$\begin{aligned} \min_{x_1,\ldots,x_n} \quad & p(x_1,\ldots,x_n) \\ \text{s.t.} \quad & c_1(x_1,\ldots,x_n)=0 \\ & \vdots \\ & c_s(x_1,\ldots,x_n)=0 \end{aligned} \tag{1}$$

where both objective function and constraints are multivariate polynomials. It is further assumed that the number of stationary points satisfying this system is finite (zero-dimensional) and distinct (i.e. multiplicities equal to 1). Such a polynomial optimization problem can be converted into solving a system of polynomial equations through the method of the Lagrange multipliers, which derives from the Lagrangian

$$\mathscr{L} = p + \sum_{k=1}^{s} l_k c_k$$

a system of $n+s$ equations in $n+s$ variables:

$$f_i = \begin{cases} \dfrac{\partial \mathscr{L}}{\partial x_i} = \dfrac{\partial p}{\partial x_i} + \displaystyle\sum_{k=1}^{s} l_k \frac{\partial c_k}{\partial x_i} = 0 & 1 \le i \le n \quad (2) \\ \dfrac{\partial \mathscr{L}}{\partial l_k} = c_k = 0, \quad i = n+k & 1 \le k \le s \quad (3) \end{cases}$$

where l_k denotes the Lagrange multiplier for the k'th equality constraint. The resulting system of polynomials forms the set of first order optimality conditions.

B. Linear algebra notation

Throughout the paper, we use uppercase boldface for matrices ($\boldsymbol{I}$ for the unit matrix), lowercase boldface for vectors and lowercase for scalars and functions. All matrices, vectors and scalars are defined over $\mathbb{C}$. By $\boldsymbol{A}^{\mathrm{T}}$ we denote the transpose of $\boldsymbol{A}$, and $\boldsymbol{A}^{*}$ for its conjugate transpose. The proposed algorithm makes frequent use of invertible row

compressions for arbitrary matrices $\boldsymbol{A} \in \mathbb{C}^{m\times n}$ to perform a dimension reduction of the form

$$\boldsymbol{U}^* \boldsymbol{A} = \begin{pmatrix} \boldsymbol{A}_r \\ 0 \end{pmatrix}$$

wherein $\boldsymbol{A}_r$ has r linearly independent rows (r is thus the rank of $\boldsymbol{A}$). Similarly we use invertible column compressions

$$\boldsymbol{AV} = \begin{pmatrix} \boldsymbol{A}_c & 0 \end{pmatrix}$$

such that $\boldsymbol{A}_c$ possesses c linearly independent columns. The singular value decomposition (SVD) provides a numerically stable way to compute both types of compression, decomposing a $m \times n$ matrix $\boldsymbol{A}$ as

$$\boldsymbol{A} = \boldsymbol{USV}^*,$$

where $\boldsymbol{U}$ and $\boldsymbol{V}$ are $m \times m$ and $n \times n$ unitary matrices, respectively. The $m \times n$ matrix $\boldsymbol{S}$ is a diagonal matrix of the form

$$\boldsymbol{S} = \begin{pmatrix} \boldsymbol{S}_p & 0 \\ 0 & 0 \end{pmatrix}, \quad \boldsymbol{S}_p = \operatorname{diag}(\sigma_1, \ldots, \sigma_p),$$

with σ_i positive real and satisfying $\sigma_1 \geq \ldots \geq \sigma_p$.

C. Polynomial vector representation

In the linear algebra framework polynomial equations are converted into vector representations using a monomial ordering, in this case the degree negative lexicographic ordering. For example, the polynomial $x^2 + y^2 - y + 1$ is represented using a row vector

$$\begin{matrix} 1 & x & y & x^2 & xy & y^2 \\ (1 & 0 & -1 & 1 & 0 & 1\,) \end{matrix}$$

For more information on monomial orderings we refer to [11]. Using a Vandermonde structured vector function

$$\boldsymbol{k}_d(x,y) = \begin{pmatrix} 1 & x & y & x^2 & xy & y^2 & x^3 & \ldots & y^d \end{pmatrix}^{\mathrm{T}}$$

the polynomial evaluation of $x^2 + y^2 - y + 1$ for (x,y) can be expressed as the inner product of its vector representation with $\boldsymbol{k}_2(x,y)$.

D. The Macaulay matrix

A zero-dimensional system of multivariate polynomials can be solved in a linear algebra setting by means of the Macaulay matrix [10]. Each row of a Macaulay matrix contains a vector representation of a polynomial. Each column holds coefficients for one monomial; each monomial is designated to a column in accordance with the degree negative lexicographic ordering. For a Macaulay matrix $\boldsymbol{M}(d)$ only monomials up to degree d are considered and rows are populated by vector representations $f_1, f_2, \ldots, f_{n+s}$ shifted by all monomials of degree up to $d - d_1, d - d_2, \ldots, d - d_{n+s}$ respectively, with $d_i = deg(f_i)$, or

$$\boldsymbol{M}(d) = \begin{pmatrix} f_1 \\ x_1 f_1 \\ \vdots \\ l_s^{d-d_1} f_1 \\ f_2 \\ \vdots \\ l_s^{d-d_{n+s}} f_{n+s} \end{pmatrix}.$$

The dimensions of the Macaulay matrix increase with d as

$$\sum_{i=1}^{n+s} \binom{n+s+d-d_i}{d-d_i} \times \binom{n+s+d}{d}$$

III. Isolating the affine roots

The purpose of this section is to distill from the Macaulay matrix, of which the null space contains all projective roots by [7], a reduced Macaulay matrix containing only the affine roots within its null space. In essence, this comes down to removing all roots at infinity.

The main premise consists of splitting the projective standard monomials [11] as a basis for $\mathscr{P}_d^n / \langle F_1, \ldots, F_{n+s} \rangle$[1] into two sets, where

$$F_i(x_0, \boldsymbol{x}, \boldsymbol{l}) \equiv x_0^d f_i(\frac{x_1}{x_0}, \ldots, \frac{x_n}{x_0}, \frac{l_1}{x_0}, \ldots, \frac{l_s}{x_0})$$

with $d = \deg(f)$. Variables $(x_1, \ldots, x_n)^{\mathrm{T}}$ and $(l_1, \ldots, l_s)^{\mathrm{T}}$ are grouped as $\boldsymbol{x}$ and $\boldsymbol{l}$, respectively. One set of standard monomials forms a basis for $\mathscr{C}^n / \langle f_1, \ldots, f_{n+s} \rangle$, with cardinality equal to the number of affine roots. Projective standard monomials are extracted in the linear algebra setting from the Macaulay matrix after regularity is reached, for which the degree of regularity and the index of regularity, denoted by d_{reg} and i_{reg} respectively, are required. When regularity sets in, a Gröbner basis [11] for $\langle f_1, \ldots, f_{n+s} \rangle$ can be isolated in the row space of $\boldsymbol{M}(d)$ whenever $d \geq d_{reg}$. A Gröbner basis for $\langle f_1, \ldots, f_{n+s} \rangle$ shares the same affine roots, but possesses no roots at infinity. The maximum degree of the Gröbner basis equations is equal to i_{reg}, the same degree for which the Hilbert function becomes the Hilbert polynomial.

In [12], a numerical algorithm acting upon $\boldsymbol{M}(d_{reg})$ is presented to find the projective standard monomials, at the expense of many costly SVD computations. By building a set of linearly independent columns of $\boldsymbol{M}(d_{reg})$ starting from the rightmost column to the leftmost, one recognizes that standard monomials in the linear algebra setting are interwoven with the rank properties of $\boldsymbol{M}(d_{reg})$. The remaining (linearly dependent) columns correspond to the projective standard monomials. For zero-dimensional systems, the emergence of a Gröbner basis in $\boldsymbol{M}(d_{reg})$ can be observed by the absence of projective standard monomials in the degree block for i_{reg}. Furthermore, all affine standard monomials are of degree lower than i_{reg}. This provides a rank test criterion to detect

[1] $\mathscr{P}_d^n$ denotes the polynomial ring of multivariate homogeneous polynomials of degree d in n variables.

when regularity sets in. The null space of $\boldsymbol{M}(d_{reg})$ can be modeled as

$$\begin{pmatrix}\boldsymbol{M}_1 & \boldsymbol{M}_2 & \boldsymbol{M}_3\end{pmatrix}\begin{matrix}n_1\\n_\infty\\n_2\end{matrix}\begin{pmatrix}\boldsymbol{X} & 0 & \boldsymbol{P}\\ 0 & 0 & \boldsymbol{Q}\\ 0 & \boldsymbol{Y} & \boldsymbol{R}\end{pmatrix}=0 \tag{4}$$

where $\boldsymbol{M}_1,\boldsymbol{M}_2,\boldsymbol{M}_3$ group together all monomials in degree smaller than i_{reg}, equal to i_{reg} and larger than i_{reg} respectively. $\boldsymbol{Y}$ forms a numerical basis for all roots at infinity with column dimension n_∞. The number of affine roots is computed as $n_a = n_1 + n_2$.

When i_{reg} and d_{reg} are known, it is possible to filter out a Macaulay matrix from $\boldsymbol{M}(d_{reg})$, where only information about the affine roots is retained. We compute the row compression of $\boldsymbol{M}_3$, or $\boldsymbol{M}_{3,p_\infty}$, with

$$p_\infty = \binom{n+s+d_{reg}}{n+s} - \binom{n+s+i_{reg}}{n+s} - n_\infty$$

the rank of $\boldsymbol{M}_3$, equal to the number of monomials of degree larger than i_{reg} minus the number of roots at infinity. When applied to $\boldsymbol{M}(d_{reg})$, we obtain[2]

$$\begin{aligned}\boldsymbol{U}_\infty^*\boldsymbol{M}(d_{reg}) &= \boldsymbol{U}_\infty^*\begin{pmatrix}\boldsymbol{M}_1 & \boldsymbol{M}_2 & \boldsymbol{M}_3\end{pmatrix}\\ &= \begin{pmatrix}\boldsymbol{M}_{1,\infty} & \boldsymbol{M}_{2,\infty} & \boldsymbol{M}_{3,p_\infty}\\ \boldsymbol{M}_{1,a} & \boldsymbol{M}_{2,a} & 0\end{pmatrix}\end{aligned} \tag{5}$$

We derive from (4) that the null space linked to the affine roots has a left annihilator

$$\begin{pmatrix}\boldsymbol{M}_{1,a} & \boldsymbol{M}_{2,a}\end{pmatrix}\begin{pmatrix}\boldsymbol{X} & \boldsymbol{P}\\ 0 & \boldsymbol{Q}\end{pmatrix}=0$$

which can be further (row) compressed to $\boldsymbol{M}_a$ of dimension $p_a \times (p_a + n_a)$ with

$$p_a = \binom{n+s+i_{reg}}{n+s} - n_a$$

IV. Case I: standard monomials known

We now show that combining the reduced Macaulay matrix $\boldsymbol{M}_a$ with a parameterization of the objective function in (1), expressed as

$$p(\boldsymbol{x}) - \lambda \tag{6}$$

will lead to the Stetter-Möller eigenvalue problem. The Stetter-Möller eigenvalue problem relies on computing the remainders (i.e. linear combination of affine standard monomials, obtained through division by a Gröbner basis) of the affine standard monomials shifted, i.e. multiplied, by $p(\boldsymbol{x})$. As a result we may obtain polynomials of degree larger than i_{reg}. This issue is resolved using the reduced Macaulay matrix $\boldsymbol{M}_a$, itself a representation of a system of polynomials, and we may construct a Macaulay matrix $\boldsymbol{M}_a(d)$ as long as $d \geq i_{reg}$. Let

$$d_{aug} = deg(p) + i_{reg} - 1$$

be the augmented degree, then no multiplication of any affine standard monomial with $p(\boldsymbol{x})$ will yield any equation of degree larger than d_{aug}.

We thus obtain a matrix pencil

$$\begin{pmatrix}\boldsymbol{M}_{aug}\\ \boldsymbol{L}_{aug}\end{pmatrix} - \lambda\begin{pmatrix}0\\ \boldsymbol{R}_{aug}\end{pmatrix}$$

where $\boldsymbol{M}_{aug} = \boldsymbol{M}_a(d_{aug})$. The rows of $\boldsymbol{P}_{aug}$ are vector representations of the affine standard monomials multiplied by p. Designating the vector representation of the product of p with each of the affine standard monomials to a particular row of $\boldsymbol{P}_{aug}$ demands the placement of a 1-coefficient in the same row in the column of $\boldsymbol{R}_{aug}$ that corresponds to that standard monomial, in order to respect (6).

Because columns of $\boldsymbol{M}_{aug}$ not associated to affine standard monomials are linearly independent, they can be used in conjunction to left unitary transformations to introduce zeros in matching columns of $\boldsymbol{P}_{aug}$. By grouping columns representing the affine standard monomials as $\boldsymbol{M}_{aug,1}$, we obtain

$$\begin{pmatrix}\boldsymbol{M}_{aug,1} & \boldsymbol{M}_{aug,2}\\ \boldsymbol{L}_{aug,1} & \boldsymbol{L}_{aug,2}\end{pmatrix} - \lambda\begin{pmatrix}0 & 0\\ \boldsymbol{I}_{n_a} & 0\end{pmatrix}$$

The full column rank of $\boldsymbol{M}_{aug,2}$ can then be exploited to cancel out matrix entries in $\boldsymbol{L}_{aug,2}$ using some unitary matrix $\boldsymbol{U}$. This is mathematically equivalent to computing the sought after remainders; while strictly speaking the rows of $\boldsymbol{L}_{aug,1}$ after cancellation of $\boldsymbol{L}_{aug,2}$ are a linear combination thereof, left unitary transformations do not alter the solutions of the final eigenvalue problem. Left-multiplication by $\boldsymbol{U}^*$ gives

$$\begin{pmatrix}\times & \times\\ \boldsymbol{A} & 0\end{pmatrix} - \lambda\begin{pmatrix}\times & 0\\ \boldsymbol{B} & 0\end{pmatrix}$$

yielding the $n_a \times n_a$ eigenvalue problem $\boldsymbol{A} = \lambda\boldsymbol{B}$.

V. Case II: standard monomials unknown

In the previous section, all affine standard monomials were known. Objectively speaking, the relevant output of the eigenvector problem is often limited to the first $q = n + s + 1$ eigenvector components, assuming that all first degree monomials are affine standard monomials. Such an assumption is reasonable; in the opposite case a variable can be expressed in terms of the other variables and eliminated by substitution. The key insight is that we are free to replace the remaining affine standard monomials by linear combinations thereof, and that they are closely intertwined with the rank properties of $\boldsymbol{M}_a$.

The proposed method will act upon the columns of $\boldsymbol{M}_a$ and expose the rank p_a. In order to keep the zero and first degree monomials intact in the column structure of $\boldsymbol{M}_a$, we do not operate on their respective columns. Partition $\boldsymbol{M}_a$ as

$$\begin{matrix}q & \bar{n}_a + p_a\end{matrix}\\ \begin{pmatrix}\boldsymbol{M}_{a,1} & \boldsymbol{M}_{a,2}\end{pmatrix}$$

where $\bar{n}_a = n_a - q$. By computing a column compression of $\boldsymbol{M}_{a,2}$

$$\boldsymbol{M}_{a,2}\boldsymbol{V}_a = \begin{matrix}\bar{n}_a & p_a\end{matrix}\\ \begin{pmatrix}0 & \boldsymbol{E}\end{pmatrix} \tag{7}$$

[2] We have chosen the notation $\boldsymbol{M}_{1,\infty}, \boldsymbol{M}_{2,\infty}$ here to distinguish between selecting the first p_∞ rows of $\boldsymbol{U}_\infty^*\boldsymbol{M}_1$ and $\boldsymbol{U}_\infty^*\boldsymbol{M}_2$ respectively, and the notation for a row compression, as in the case of $\boldsymbol{M}_{3,p_\infty}$.

the rank is exposed in the rightmost p_a columns. Based off this compression, a right unitary matrix $\boldsymbol{T} = diag(\boldsymbol{I}_q, \boldsymbol{V}_a)$ transforms $\boldsymbol{M}_a$ into

$$\boldsymbol{M}_a \begin{pmatrix} \boldsymbol{I}_q & \\ & \boldsymbol{V}_a \end{pmatrix} = \begin{matrix} q & \bar{n}_a & p_a \end{matrix} \begin{pmatrix} \boldsymbol{M}_{a,1} & 0 & \boldsymbol{E} \end{pmatrix}$$

Considering the affine standard monomials are a mere portrayal of the linear dependencies among the columns of $\boldsymbol{M}_a$, the aim is to circumvent any prior knowledge by exploiting the clear separation of the rank in the newly acquired matrix pencil

$$\begin{pmatrix} \boldsymbol{M}_{a,1} & 0 & \boldsymbol{E} \\ \boldsymbol{L}_{11} & \boldsymbol{L}_{12} & \boldsymbol{L}_{13} \\ \boldsymbol{L}_{21} & \boldsymbol{L}_{22} & \boldsymbol{L}_{23} \end{pmatrix} \boldsymbol{T}^* - \lambda \begin{pmatrix} 0 & 0 & 0 \\ \boldsymbol{I}_q & 0 & 0 \\ 0 & \boldsymbol{I}_{\bar{n}_a} & 0 \end{pmatrix} \boldsymbol{T}^* \tag{8}$$

The back-transformation $\boldsymbol{T}^*$ aids in understanding what values belong in the unknown matrices $\boldsymbol{L}_{ij}$ using (6). The block row made up by $\boldsymbol{L}_{1,j}, 1 \leq j \leq 3$ holds the remainders of the objective function shifted by the zero and first degree monomials, transformed by $\boldsymbol{T}$, in accordance to the pivots in the linear part of the matrix pencil, shown as $\boldsymbol{I}_q$.

The block row $\boldsymbol{L}_{2j}, 1 \leq j \leq 3$ requires additional work. Let us partition $\boldsymbol{V}_a$ as

$$\boldsymbol{V}_a = \begin{matrix} \bar{n}_a & p_a \end{matrix} \begin{pmatrix} \boldsymbol{V}_{a,1} & \boldsymbol{V}_{a,2} \end{pmatrix}$$

then the linear part of the matrix pencil in (8) can be written in full as

$$\begin{matrix} q & \bar{n}_a & p_a \end{matrix} \begin{pmatrix} 0 & 0 & 0 \\ \boldsymbol{I}_q & 0 & 0 \\ 0 & \boldsymbol{I}_{\bar{n}_a} & 0 \end{pmatrix} \boldsymbol{T}^* = \begin{matrix} q & \bar{n}_a + p_a \end{matrix} \begin{pmatrix} 0 & 0 \\ \boldsymbol{I}_q & 0 \\ 0 & \boldsymbol{V}_{a,1}^* \end{pmatrix} \tag{9}$$

Thus, in order to fulfill (6), this implies we must add vector representations of $p(\boldsymbol{x})$ shifted by polynomials $h_i(\boldsymbol{x}, \boldsymbol{l}), 1 \leq i \leq \bar{n}_a$ constructed as linear combinations of monomials between degrees 2 and i_{reg}. The coefficient of each monomial term of $h_i(\boldsymbol{x}, \boldsymbol{l})$ is given in accordance to the value in the i'th row of $V_{a,1}^*$ occupying the column associated to that term.

To arrive at a generalized eigenvalue problem we must traverse similar steps as we did in the case of known basis monomials, with some slight differences. Since the shift functions include polynomials of degree i_{reg}, the augmented degree now equals $\deg(p) + i_{reg}$. After the introduction of zeros into columns corresponding to monomials of degree larger than i_{reg}, the intermediate remainders can be brought in the form (8) using $\boldsymbol{T}$. Finally, the values of $\boldsymbol{L}_{13}$ and $\boldsymbol{L}_{23}$ are annihilated by left unitary transformations using the fact that $\boldsymbol{E}$ is of full column rank, yielding the modified (square) matrix pencil

$$\begin{matrix} & q & \bar{n}_a & p_a \\ p_a \\ q \\ \bar{n}_a \end{matrix} \begin{pmatrix} \boldsymbol{M}_{a,1} & 0 & \boldsymbol{E} \\ \boldsymbol{A}_{11} & \boldsymbol{A}_{12} & 0 \\ \boldsymbol{A}_{21} & \boldsymbol{A}_{22} & 0 \end{pmatrix} - \lambda \begin{matrix} \\ q \\ \bar{n}_a \\ p_a \end{matrix} \begin{pmatrix} 0 & 0 & 0 \\ \boldsymbol{B}_{11} & \boldsymbol{B}_{12} & 0 \\ \boldsymbol{B}_{21} & \boldsymbol{B}_{22} & 0 \end{pmatrix}$$

The finite eigenvalues can be singled out by extraction of the remainders, or

$$\begin{pmatrix} \boldsymbol{A}_{11} & \boldsymbol{A}_{12} \\ \boldsymbol{A}_{21} & \boldsymbol{A}_{22} \end{pmatrix} x = \lambda \begin{pmatrix} \boldsymbol{B}_{11} & \boldsymbol{B}_{12} \\ \boldsymbol{B}_{21} & \boldsymbol{B}_{22} \end{pmatrix} x \tag{10}$$

with problem dimension n_a.

The steps described in sections III and V are combined and summarized in Algorithm 1.

Data: $p, c_1, \ldots, c_s$, d_{init}
Result: $\boldsymbol{A} - \lambda \boldsymbol{B}$
compute Lagrange conditions $f_1, \ldots, f_{n+s}$;
$d \longleftarrow d_{init}$;
do
  construct $\boldsymbol{M}(d)$;
  for $i = d$ **downto** 2 **do**
    $\mathscr{M}_{i+1} = \text{span}(\begin{bmatrix} \boldsymbol{M}_{i+1} & \ldots & \boldsymbol{M}_d \end{bmatrix})$;
    $\boldsymbol{M}_i^p \longleftarrow \mathscr{M}_{i+1}^{\perp} \backslash \boldsymbol{M}_i$;
    if $\boldsymbol{M}_i^p$ *full column rank* **then**
      $i_{reg} \longleftarrow i$;
      $d_{reg} \longleftarrow d$;
    end
  end
while *regularity not reached*;
construct $\boldsymbol{M}(d_{reg})$;
$(\boldsymbol{U}_\infty, p_\infty) \longleftarrow svd(\begin{bmatrix} \boldsymbol{M}_{i_{reg}+1} & \ldots & \boldsymbol{M}_{d_{reg}} \end{bmatrix})$;
compute $\boldsymbol{M}_a$ using (5);
$(\boldsymbol{U}_a, \boldsymbol{S}_a, \boldsymbol{V}_a) \longleftarrow svd(\boldsymbol{M}_a)$;
reorder columns of $\boldsymbol{V}_a$ right to left;
row compress $\boldsymbol{M}_a$;
$\boldsymbol{T} \longleftarrow blkdiag(\boldsymbol{I}_{n+s+1}, \boldsymbol{V}_a)$;
$\boldsymbol{L}_1 \longleftarrow$ vector representations of $\begin{bmatrix} 1 & x_1 & \ldots & l_s \end{bmatrix}^{\mathrm{T}} \cdot p$;
$\boldsymbol{C} \longleftarrow$ columns of $\boldsymbol{V}_a$ forming null space $\boldsymbol{M}_a$;
$h_i \longleftarrow \boldsymbol{C}^*$ contains vector representations;
$\boldsymbol{L}_2 \longleftarrow$ vector representations of $\begin{bmatrix} h_1 & h_2 & \ldots \end{bmatrix}^{\mathrm{T}} \cdot p$;
$\boldsymbol{L} \longleftarrow \begin{bmatrix} \boldsymbol{L}_1^{\mathrm{T}} & \boldsymbol{L}_2^{\mathrm{T}} \end{bmatrix}^{\mathrm{T}}$;
$d_{aug} \longleftarrow deg(p) + i_{reg}$;
$\boldsymbol{M}_{aug} \longleftarrow \boldsymbol{M}_a(d_{aug})$;
$\boldsymbol{U}_1 \longleftarrow$ delete coefficients of columns beyond i_{reg} in $\boldsymbol{L}$;
$\boldsymbol{B} \longleftarrow n_a \times n_a$ lower-right submatrix of $\boldsymbol{U}_1^*$;
right multiply $\boldsymbol{L}$ with $\boldsymbol{T}$;
$(\boldsymbol{A}, \boldsymbol{U}_2) \longleftarrow$ delete coefficients in p_a last columns of $\boldsymbol{L}$;
$\boldsymbol{B} \longleftarrow$ left-multiply $\boldsymbol{B}$ with $n_a \times n_a$ lower-right submatrix of $\boldsymbol{U}_2^*$;

Algorithm 1: SVD-based polynomial global optimization

VI. Experiments

We illustrate our method by considering a 3×3 structured total least squares (STLS) problem. Finding a Hankel matrix of rank $n-1$ as an approximation to a given Hankel matrix based off a time series of length $2n-1$ has been tackled by various algorithms [13], [14] and amounts to solving a polynomial root-finding problem. All simulations were done in MATLAB. Results are compared with the output of the

GloptiPoly3 package [15] (relaxation order 2) and verified by a polynomial homotopy continuation method (PHCpack [16]).

The input is a time series which consists of five samples, ordered in a 3×3 Hankel matrix A of full rank. A nonlinear generalization of the SVD to solve the STLS problem is given in [17], [18], also known as the Riemannian SVD, and is essentially a system of multivariate polynomial equations. Since we are searching for a low-rank approximation of A or rank 2, let $\boldsymbol{v} = \begin{bmatrix} v_1 & v_2 & v_3 \end{bmatrix}^{\mathrm{T}}$ be the basis for the null space of the approximating Hankel structured matrix B, then the optimization problem is

$$\begin{aligned} \min \quad & \frac{1}{2}\boldsymbol{e}^{\mathrm{T}}\boldsymbol{e} \\ \text{s.t.} \quad & \boldsymbol{A}\boldsymbol{v} = \boldsymbol{T}_v\boldsymbol{e} \\ & \boldsymbol{v}^{\mathrm{T}}\boldsymbol{v} = 1 \end{aligned}$$

We introduce Lagrange multipliers $\boldsymbol{l} = \begin{bmatrix} l_1 & l_2 & l_3 \end{bmatrix}^{\mathrm{T}}$ for the first equality constraint shown as a matrix equation, and an additional variable l_4 for the normalization constraint. The matrix $\boldsymbol{T}_v$ is constructed as

$$\begin{pmatrix} v_1 & v_1 & v_3 & & \\ & v_1 & v_2 & v_3 & \\ & & v_1 & v_2 & v_3 \end{pmatrix}$$

From the derivation of the Lagrangian, we can decrease the number of variables using the equality $\boldsymbol{e} = \boldsymbol{T}_v^{\mathrm{T}}\boldsymbol{l}$. The optimization problem then turns into the root-finding problem

$$\boldsymbol{A}\boldsymbol{v} = \boldsymbol{T}_v\boldsymbol{T}_v^{\mathrm{T}}\boldsymbol{l}, \quad \boldsymbol{A}^{\mathrm{T}}\boldsymbol{l} = \boldsymbol{T}_l\boldsymbol{T}_l^{\mathrm{T}}\boldsymbol{v}, \quad \boldsymbol{v}^{\mathrm{T}}\boldsymbol{v} = 1$$

The polynomial objective function $(\boldsymbol{l}^{\mathrm{T}}\boldsymbol{T}_v\boldsymbol{T}_v^{\mathrm{T}}\boldsymbol{l})/2$ grades the eigenvalues in the proposed method such that the best low-rank matrix approximation for $\boldsymbol{A}$ can be isolated using the inverse power method. In this example we find the best rank-2 Hankel approximation for

$$\boldsymbol{A} = \begin{pmatrix} 7 & -2 & 5 \\ -2 & 5 & 6 \\ 5 & 6 & -1 \end{pmatrix}$$

The proposed algorithm reaches regularity for the values $d_{reg} = 13$ and $i_{reg} = 7$, with $\boldsymbol{M}(d)$ a 148 512 by 77 520 matrix. Starting from the maximum degree of the Riemannian SVD equations, equal to 3, the number of rank tests traversed equals $(d_{reg} - i_{reg} + 1) + \sum_{k=3}^{d_{reg}-1}(k-2)$ based on the assumption of first degree basis monomials, or in total 66 rank tests. An estimate for d_{reg} is proposed in [8] using

$$d_{reg} = \sum_{i=1} \deg(f_i) + 1.$$

Applied to our example, this yields an estimate of 14 for d_{reg}, thus only 8 rank tests are required to find i_{reg}. The matrix dimensions of M_a are equal to 1637×1716, with 78 affine roots, also predicted by the size of the normal set computed using Maple's `NormalSet` commando. Care must be taken to avoid eigenvalues of multiplicity higher than 1. For example, if a solution $\boldsymbol{v}$ satisfies the Riemannian equations, so does $-\boldsymbol{v}$. Such twin solutions belong to the same eigenspace but contribute linearly independent eigenvectors given the monomial structure, and linear combinations generally do not fulfill the Lagrange conditions of the problem. For this reason we slightly adapt the original function to

$$p = \boldsymbol{l}^{\mathrm{T}}\boldsymbol{T}_v\boldsymbol{T}_v^{\mathrm{T}}\boldsymbol{l} + Cv_3$$

where C acts to perturb the eigenvalues such that all eigenvalues occur with multiplicity 1. A sensible value for C is 5×10^{-1}.

TABLE I: STLS global minimum eigenpairs ($C = 5 \times 10^{-1}$) compared to GloptiPoly3 (GP)

	1	2	GP
λ	1.7815e1	1.8620e1	1.7815e1
$\lambda - C \cdot v_3$	1.8218e1	1.8218e1	1.8218e1
l_1	−1.8837	1.8837	−1.8922
l_2	−2.5889	2.5889	−2.6187
l_3	4.3375	−4.3375	4.3160
v_1	3.4942e−1	−3.4942e−1	3.4965e−1
v_2	4.8021e−1	−4.8021e−1	4.7764e−1
v_3	−8.0456e−1	8.0456e−1	−8.0598e−1

The objective function is multiplied by polynomials of degree i_{reg}, such that the augmentation degree is equal to $i_{reg} + \deg(p)$, or 11. After traversing the steps outlined in algorithm 1, the square matrix pencil from (10) with dimension 78 is obtained.

The global minimizer is found from the smallest eigenvalue, results are shown in Table I. It is clear from Table I and Fig. 1 that real roots in the STLS optimization problem come in pairs, sharing the same eigenvalue unless we employ the eigenvalue trick. In this case, the eigenvalue 1.8218e1 with multiplicity 2 is pulled apart into two distinct eigenvalues $\{1.7815\text{e}1, 1.8620\text{e}1\}$, and the eigenvectors are correctly visualized on the unit sphere in the $\mathbb{R}^3$ vector space.

The modified objective function ensures global optimality for the GloptiPoly3 solution, the solution however varies with C. Unlike the presented method, the Gloptypoly3 package allows for additional inequality constraints and is able to restrict to solutions belonging to the real variety. As the relaxation order increases, the dimensions of the moment matrices increase due to the combinatorial explosion of monomials, also manifested in the SVD method. However, good estimates are retrieved for low relaxation orders. This in contrast to the dependency of the SVD method upon the regularity parameters i_{reg} and d_{reg}, for which no simple rules exist in order to compute them, making the SVD method in its current form computationally expensive compared to others.

All (real) stationary points obtained from the eigenvalue problem are shown in Fig. 1, indicating their position on the unit sphere. This graphical representation shows that stationary points can be classified as either maxima, minima or saddle points present on the mapped objective function

$$J(v) = \frac{1}{2}\boldsymbol{v}^{\mathrm{T}}\boldsymbol{A}^{\mathrm{T}}(\boldsymbol{T}_v\boldsymbol{T}_v^{\mathrm{T}})^{-1}\boldsymbol{A}\boldsymbol{v}$$

which is nonlinear in $\boldsymbol{v}$ but equivalent to the polynomial objective function used in the optimization problem. Three different stationary points are visible in the middle of the unit sphere snapshot of Fig. 1. The red arrow shown coincides with the global minimum $\boldsymbol{v}_{opt}$, the blue arrow points to a maximal solution and the black arrow indicates a saddle point.

The optimal rank-2 Hankel approximation of $\boldsymbol{A}$, with $\boldsymbol{v}_{opt}$ spanning its null space, is given by

$$\begin{pmatrix} 7.6582 & -0.1908 & 3.2120 \\ -0.1908 & 3.2120 & 1.8342 \\ 3.2120 & 1.8342 & 2.4897 \end{pmatrix}.$$

VII. Conclusions and Future Works

The gap between Macaulay matrices and the work of Stetter has been bridged, omitting the need for symbolic computations. The role played by standard monomials in the Stetter-Möller eigenvalue problem has been entirely replaced by linear algebra concepts. This opens the way for numerically robust algorithms in which rank test decisions play a vital role. The dimensions of the matrix structures involved increase rapidly with the number of problem variables and equality constraints imposed. Efficient methods exploiting the quasi-Toeplitz structure and sparsity will yield great improvements in computational time requirements. On a more fundamental level, the idea of operating on the column structure of Macaulay matrices should be further explored to replace the Macaulay matrix with a more condensed data structure limiting the influence of combinatorial explosion. Alongside algorithmic improvements, the challenge to limit optimization to real-valued stationary points remains a topic for future research.

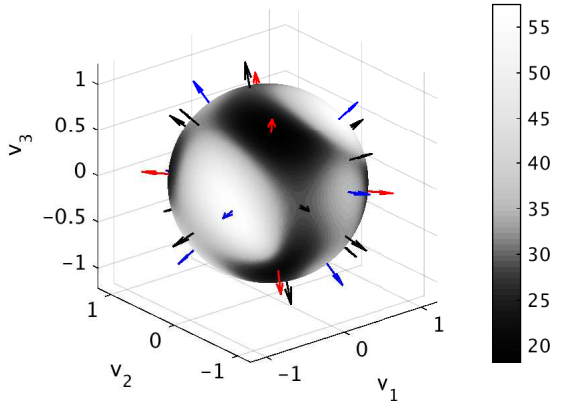

Fig. 1: Markers indicate the position of stationary points lying on the unit sphere for a 3×3 STLS problem. Stationary points can be categorized as minima (red), maxima (blue) or saddle points (black). The global optimum $(v_1, v_2, v_3) = (3.4942\text{e}{-1}, 4.8021\text{e}{-1}, -8.0456\text{e}{-1})$ is shown in the middle alongside one maximum and one saddle point.

Acknowledgments

We wish to thank Dr. Kim Batselier and the reviewers for their remarks on the manuscript. Antoine Vandermeersch is a research assistant at the KU Leuven. Bart De Moor is a full professor at the KU Leuven, Belgium. Research supported by Research Council KUL: CoE PFV/10/002 (OPTEC); PhD/Postdoc grants, Flemish Government: IOF: IOF/KP/SCORES4CHEM; iMinds Medical Information Technologies SBO 2015, Belgian Federal Science Policy Office: IUAP P7/19 (DYSCO, Dynamical systems, control and optimization, 2012-2017).

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