

Weighted/Structured Total Least Squares Problems and Polynomial System Solving

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Abstract. Weighted and Structured Total Least Squares (W/STLS) problems are generalizations of Total Least Squares with additional weighting and/or structure constraints. W/STLS are found at the heart of several mathematical engineering techniques, such as statistics and systems theory, and are typically solved by local optimization methods, having the drawback that one cannot guarantee global optimality of the retrieved solution. This paper employs the Riemannian SVD formulation to write the W/STLS problem as a system of polynomial equations. Using a novel matrix technique for solving systems of polynomial equations, the globally optimal solution of the W/STLS problem is retrieved.

1 Introduction

In the generic case, the solution of the approximation of a given data matrix by one of lower rank is well-studied and is computed by the Singular Value Decomposition [1]. However, several applications require additional constraints, such as element-wise weighting or imposing matrix structure, leading to so-called Weighted and/or Structured Total Least Squares problems [2, 3]. W/STLS problems have numerous applications in mathematical engineering, such as machine learning [4], systems and control theory [5], information retrieval [6] and statistics [7] among others.

The Riemannian SVD (RSVD) was proposed in [2, 3] to solve the W/STLS problem, and is essentially a nonlinear generalization of the well-known Singular Value Decomposition, constituting a system of polynomial equations. Fueled by the increase in computing power and the development of Groebner basis algorithms [8], polynomial system solving has witnessed an increased research interest in recent years. In this paper a matrix method is employed to solve the W/STLS problem, translating the problem of finding the solution to a system of polynomial equations into a linear algebra question, while guaranteeing that the globally optimal solution is retrieved.

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The paper is organized as follows: In Section 2, the mathematical formulation of the STLS problem is reviewed, leading to the Riemannian SVD formulation which phrases the task as the solution of a system of polynomial equations. Section 3 reviews a linear algebra method for solving systems of polynomial equations. In Section 4 this method is applied to a simple 3×3 STLS problem.

2 STLS as a System of Polynomials

Consider a given data matrix A which is of full rank and is to be approximated by a low-rank matrix B . Additionally, when A has a specific matrix structure (*e.g.*, Hankel, Toeplitz, Sylvester), which is to be preserved in its approximation B , the so-called Structured Total Least Squares problem is phrased as

$$\min_{B,v} \|A - B\|_F^2 \quad \text{s.t.} \quad Bv = 0, \quad B \text{ structured}, \quad (1)$$

where the constraint $Bv = 0$ ensures the rank-deficiency of B and the second constraint preserves the matrix structure of A in the approximation B . The Lagrange multipliers method provides the conditions for optimality as the RSVD equations [2, 3] in the unknowns v and l

$$\begin{cases} Av &= T_v T_v^T l, \\ A^T l &= T_l T_l^T v, \\ v^T v &= 1, \end{cases} \quad (2)$$

where T_l and T_v are matrices containing the elements of l (the Lagrange multipliers) and v , respectively, and capture the required matrix structure. Section 4 contains an example of T_l and T_v in the case of 3×3 Hankel STLS. For the element-wise WTLS problem the same derivation can be made, leading to a similar system of RSVD equations. The low-rank approximation B can be determined from the solutions of v and l as described in [2, 3].

Although very fast solution methods have been developed to solve (1), most current methods tackle this from a local optimization point of view. The main drawback is that one cannot ensure that the globally optimal solution is obtained, as the recovered solution is typically very dependent on the starting point of the search algorithm. Observe that the critical points of (1) are obtained from a system of polynomial equations (2). By solving the RSVD equations as a system of polynomial equations, one can guarantee to find all solutions. However, most techniques for solving systems of polynomial equations employ symbolic computations and are hence known to have severe difficulties with floating-point arithmetic.

In the following, a novel method for solving systems of polynomial equations is reviewed, which employs only matrix computations, such as null space computations and eigenvalue decompositions. The advantages of this method are twofold: it is guaranteed that all solutions of the system of equations are found — and hence the global optimum in the case of an optimization problem — and since matrix computations are used, the numerical aspects can be studied in the well-established numerical linear algebra framework.

3 Matrix Method for Solving Systems of Polynomials

In this section a brief overview of the method developed in [9] and [10] is given. The description of the algorithm is restricted to the generic case in which all solutions are simple and affine, *i.e.*, there are no solutions at infinity and no multiplicities. A description of the non-generic case can be found in the aforementioned works, however the full exposition is beyond the scope of this paper.

The algorithm proceeds in three steps. First, the system of polynomial equations is represented as a matrix-vector multiplication of a coefficient matrix M with a monomial vector k , leading to the equation $Mk = 0$. Second, a numerical basis for the null space of M is computed, which reveals the number of solutions. The third step formulates a (generalized) eigenvalue problem from the selection of certain rows in the computed null space of M which returns the numerical values of the solutions as the eigenvalues.

Consider a system of n polynomial equations in n unknowns

$$f_i(x_1, \dots, x_n) = 0, \quad i = 1, \dots, n \quad (3)$$

having total degrees d_1, \dots, d_n . By denoting $k(d_o)$ as a vector containing all monomials of degrees 0 up to $d_o = \max_i(d_i)$, each equation $f_i = 0$ can be represented as the inner product $m_i^T(d_o)k(d_o) = 0$ of a coefficient vector $m_i(d_o)$ multiplied with a vector of monomials $k(d_o)$. For example, the equation $x_1^2 + 3x_1x_2 - 2x_2 + 5 = 0$ can be written in this way as

$$\begin{pmatrix} 5 & 0 & -2 & 1 & 3 & 0 \end{pmatrix} \begin{pmatrix} 1 & x_1 & x_2 & x_1^2 & x_1x_2 & x_2^2 \end{pmatrix}^T = 0. \quad (4)$$

Note that when not all equations are of the same degree d_o , some equations do not entirely fill up the coefficient vectors. Such equations can be ‘shifted’ by multiplying them with monomials of degrees 0 up to $d_i - d_o$ so as to generate ‘new’ equations. Observe that adjoining these ‘new’ equations does not change the solution set of the input system, as they correspond to $\sigma f_i = \sigma 0 = 0$, where σ represents a monomial. By stacking all the coefficient vectors m_i obtained in this way, the Macaulay matrix $M(d_o)$ is constructed. The system (3) is hence represented as the matrix equation $M(d_o)k(d_o) = 0$. To ensure that all necessary information regarding the solutions of the polynomial system is contained in this matrix-vector representation, the degree at which the coefficient matrix and corresponding monomial vectors are constructed needs to be $d^* = \sum_i d_i - n + 1$ as prescribed by [11]. Remark that all possible shifts up to d^* of the input equations (3) are to be included.

After the suitably sized coefficient matrix $M = M(d_o)$ is constructed, it is easy to see that the dimension of the null space of M corresponds to the number of solutions m_B : by evaluating the (for the time being unknown) numerical values of the solutions in the monomial vector $k = k(d_o)$, one finds m_B independent vectors $k^{(i)}$, with $i = 1, \dots, m_B$ which (by definition) live in the null space of M . By stacking all these vectors $k^{(i)}$, with $i = 1, \dots, m_B$ together, a generalized Vandermonde structured matrix $K = \begin{pmatrix} k^{(1)} & \dots & k^{(m_B)} \end{pmatrix}$ is obtained, which is called the canonical null space of M .

The generalized Vandermonde structure of K defines a shift invariant structure: multiplication with a monomial maps the low-degree rows onto high-degree rows. This effect can be captured using row-selection matrices S_1 and S_2 as $S_1KD = S_2K$ (already suggesting an eigenvalue problem), where S_1 selects the low-degree rows in K which are mapped by multiplication with a user-chosen shift monomial to high-degree rows selected by S_2 , and D is a diagonal matrix containing the user-chosen shift monomial evaluated at the m_B solutions. Unfortunately, the canonical null space K containing the desired information of the solutions is unknown, instead a numerical basis for the null space of M can be computed, denoted Z (*e.g.*, by SVD, rank-revealing QR, or the Motzkin algorithm described below). One has $K = ZV$ which defines V as a nonsingular transformation of the canonical null space. The root-finding problem is hence reduced to the generalized eigenvalue problem

$$S_1Z(VDV^{-1}) = S_2Z, \quad (5)$$

where S_1 selects the first m_B linearly independent rows of Z and S_2 selects the corresponding shifted rows, and where D contains the eigenvalues which are the evaluations of the m_B solutions in the user-chosen shift monomial. The eigenvectors in V can be employed to reconstruct the canonical null space as $K = ZV$, revealing the mutual matching between the solution components.

Null space construction exploiting the sparsity of M is highly desirable since the matrix size can become very large. An algorithm inspired by Motzkin elimination [12] is presented here which constructs the null space of M by iterating over its rows. Let $b^T \in \mathbb{R}^{1 \times n}$ denote a row of $M \in \mathbb{R}^{m \times n}$ for which the null space $W \in \mathbb{R}^{n \times (n-1)}$ is sought. The left-most non-zero element in b^T is used as a pivot to generate pair-wise eliminations which define columns in W lying in the null space of b^T . Zero elements in b^T give rise to unit column vectors in W .

The operation of the algorithm on a single row of $M \in \mathbb{R}^{m \times n}$ is illustrated by means of a small example. Consider the row vector $b^T = (0 \ 3 \ 0 \ 1 \ 2)$. By inspection of the zero pattern and making pair-wise combinations of the pivot 3 with the remaining non-zero elements, the null space of b^T is easily found as

$$b^T W = (0 \ \mathbf{3} \ 0 \ 1 \ 2) \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1/3 & 0 & -2/3 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \quad (6)$$

The null space of a matrix $M \in \mathbb{R}^{m \times n}$ is now constructed as a product of sparse matrices as follows. In the first step, one constructs the null space of the first row of M , *i.e.*, a_1^T , as W_1 . In the next step, the second row of M , *i.e.*, a_2^T , is considered and multiplied by W_1 to obtain $b_2^T = a_2^T W_1$. The row-algorithm is then repeated for b_2^T , leading to W_2 . The remaining rows a_k^T for $k = 3, \dots, m$ of M are processed in the same way: the Motzkin row-algorithm is performed on $b_k^T = a_k^T W_1 W_2 \cdots W_{k-1}$, and the null space of M is ultimately found as

$$Z = \prod_{i=1}^m W_i. \quad (7)$$

4 Numerical Experiment: 3×3 STLS Problem

In this section a 3×3 Hankel STLS problem is solved as a system of polynomial equations as described in Section 3 and correctly retrieves the globally optimal low-rank approximation. All simulations are performed in MATLAB. Numerical results are confirmed by the polynomial homotopy continuation method PHC-pack [13] and Gröbner Basis computations performed in Maple.

Consider the 3×3 full-rank Hankel matrix

$$A = \begin{bmatrix} 7 & -2 & 5 \\ -2 & 5 & 6 \\ 5 & 6 & -1 \end{bmatrix}, \quad (8)$$

which is to be approximated by a Hankel matrix B of rank 2. Let $v = [v_1 \ v_2 \ v_3]^T$ and $l = [l_1 \ l_2 \ l_3]^T$. In the RSVD equations (2), the matrices T_v and T_l imposing the Hankel structure constraint are defined as

$$T_v = \begin{bmatrix} v_1 & v_2 & v_3 & & \\ & v_1 & v_2 & v_3 & \\ & & v_1 & v_2 & v_3 \end{bmatrix} \quad \text{and} \quad T_l = \begin{bmatrix} l_1 & l_2 & l_3 & & \\ & l_1 & l_2 & l_3 & \\ & & l_1 & l_2 & l_3 \end{bmatrix}. \quad (9)$$

The best low-rank approximation of A is reconstructed from the pair of (v, l) vectors which minimize the objective criterion $J(v) = v^T A^T (T_v T_v^T)^{-1} A v$, from which equation the dependence of J on l has been eliminated.

The coefficient matrix M is constructed for (2) and a basis for the null space of M is computed. The root-counting technique reveals there are 39 affine solutions. In Figure 1 the STLS cost function $J(v)$ and the 13 (real) critical points are represented. The optimal rank-2 Hankel matrix approximation of A is retrieved as prescribed in [2, 3] as

$$B = \begin{bmatrix} 7.6582 & -0.1908 & 3.2120 \\ -0.1908 & 3.2120 & 1.8342 \\ 3.2120 & 1.8342 & 2.4897 \end{bmatrix}. \quad (10)$$

5 Conclusions

The W/STLS problem has been solved using the Riemannian SVD by means of a linear algebra method, while guaranteeing global optimality. Although the encountered matrix sizes are prohibiting the application to large-scale problems, the presented framework allows applied mathematicians and engineers to study polynomial equations without requiring advanced algebraic geometry knowledge.

Ongoing work is focusing on how structure and sparsity of the coefficient matrix can be exploited in order to develop effective and efficient algorithms, *e.g.*, as indicated in the Motzkin algorithm presented in Section 3.

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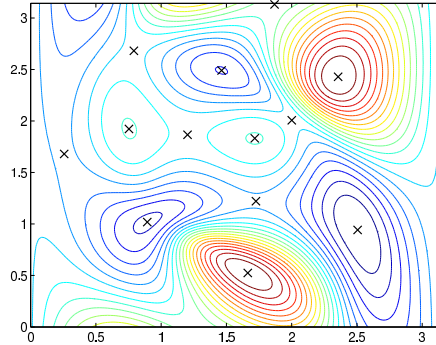


Fig. 1: Plot of the 3×3 Hankel STLS minimization problem $J(v) = v^T A^T (T_v T_v^T)^{-1} A v$ showing several local optima and the retrieved roots. The proposed method correctly identifies all 13 roots (\times) and guarantees global optimality of the solution. The x and y axes depict the spherical coordinates of v , i.e., $x = \tan^{-1} v_2/v_1$ and $y = \cos^{-1} v_3$.

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