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Total Linear Least Squares with Inequality Constraints

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Abstract

We discuss total linear least squares problems with inequality constraints on the solution vector. It is shown that the Karush-Kuhn-Tucker conditions for the corresponding optimization problem are a generalized linear complementarity problem. The optimization problem coincides with the minimization of a quadratic objective function subject to quadratic and/or nonnegativity constraints. An interpretation is given in terms of the concept of *oriented energy* (the field of values of a matrix). An algorithm for solving the generalized linear complementarity problem can be used as a preprocessor in a general solution scheme. It provides additional geometrical insight in the solution set. Other results include a Langrangean derivation of total linear least squares and least squares with nonnegativity constraints. The results are illustrated with several numerical examples.

Keywords: (Generalized) linear complementarity, constrained optimization, Lagrangean equations, Karush-Kuhn-Tucker conditions, linear least squares, quadratic eigenvalue problem, field of values.

1 Introduction

Solving sets of linear equations is a basic issue in many applications. The *total linear least squares* approach (**TLLS**) has been introduced recently in the numerical analysis literature [6] as an alternative for least squares estimation schemes in the case that all data are corrupted by additive noise. The generic problem reduces to the following:

TLLS Problem:
Given a real $m \times n$ matrix A with $m > n$ and $rank(A) = n$. Find the matrix B of rank $n-1$ that minimizes $\|A - B\|_F^2$ where $\|.\|_F$ is the Frobenius norm of a matrix. The total least squares solution is the non-trivial vector x that satisfies $Bx = 0$.

An interpretation of **TLLS** is that the noisy data, while not satisfying a linear relation, are modified with minimal effort, as measured by the Frobeniusnorm, in a 'nearby' matrix B which is rank deficient so that its columns are linearly related. The solution to the **TLLS** problem can be determined from the singular value decomposition of the matrix A. Generically, the matrix B is a rank one modification of the matrix A as will be shown in section 2.

A *linear least squares* approach for determining a linear relation between the columns of A consists of first specifying a certain column of A, say the n-th one a_n, and writing it as a right hand side in the approximate equation:

$$A_n y \approx a_n$$

where A_n is an $m \times (n-1)$ matrix obtained from A by omission of its n-th column. Then solve the optimization problem:

LLS Problem:

$$min_{\ over\ \ all\ \ y \in \Re^{n-1}} \|a_n - A_n y\|^2$$

In the generic case the matrix A is of full column rank. The solution is then given by

$$y = (A_n^t A_n)^{-1} A_n^t a_n \tag{1}$$

We call the vector

$$x = \begin{pmatrix} y \\ -1 \end{pmatrix}$$

a least squares solution. Obviously, there are n such least squares solutions (one for each column of A) and the relation of these n least squares solutions with the **TLLS** solution has been analysed in [4]. There, we have proved the following result:

Lemma 1
Up to a non-zero scalar, the k-th least squares solution is given by the k-th column of the matrix $(A^t A)^{-1}$. *The norm squared of the residual* $\|a_n - A_n y\|_2^2$ *is the inverse of the* (k,k)*-th element of* $(A^t A)^{-1}$.

The geometrical interpretation of the **LLS** approach is as follows: The column vector a_n is orthogonally projected onto the column space of the matrix A_n. Hence, the **LLS** solution represents also a rank one modification of the data, but only one of the columns of A is modified as opposed to all columns in the **TLLS** approach. Obviously, in a lot of practical situations, the **TLLS** approach, while computationally more involved, is conceptually more natural than the **LLS** approach because typically, *all* measured data are corrupted by additive noise. Hence, there is a fundamental trade off between **TLLS** and **LLS**: While the geometrical interpretation of **TLLS** is more natural (all data are modified), the computation of the solution is equivalent with an eigenvalue problem (or singular value decomposition). The **LLS** solution however only requires the solution of a set of linear equations, which in principle can be done in a finite number of steps.

Frequently, the solution to either a linear or total linear least squares problem is required to satisfy additional restrictions, such as nonnegativity and inequality constraints (see [1] for references related to the least squares problem with inequality constraints). The main purpose of this paper is the analysis and solution of the **TLLS** problem when inequality constraints are imposed on the solution vector. We shall consider both *nonnegativity constraints*

$$x \geq 0 \tag{2}$$

and *inequality constraints*:

$$x \geq a \qquad a \neq 0 \tag{3}$$

As we'll see, the price to be paid for nonnegativity is quite heavy: If the solution to the unconstrained problem is itself not nonnegative, imposing nonnegativity constraints will cause the rejection of one or more columns of A as being irrelevant in the solution. Nevertheless, in some applications, it's precisely this property of radical rejection of certain measurements that is appealing. Consider the following example: Assume that the matrix $m \times n$ matrix A contains a *library* of n *templates* (e.g. spectra in the frequency domain) and that the $m \times 1$ vector b contains a measured signal. One wants to find the relative contribution of each template in the measured signal. Obviously, one could then solve

$$Ax \approx b \qquad x \geq 0$$

The '$\approx$'-sign refers to the fact that with practical data, the equation only holds approximately, or in other words, that the data should first be modified in order to find an exact solution. If one assumes that only the right hand side b is corrupted by noise, the problem should be solved in a **LLS** sense. If however the templates themselves are also noisy, we have a **TLLS** problem with nonnegativity constraints.

The main result of this paper is the fact that in the solution of the TLLS problem with and without constraints, the matrix B can be eliminated. It is always a rank one modification of the matrix A, which can be derived from the solution of the following quadratic programming problem with linear and quadratic constraints:

$$min_{\ over\ \ all\ \ x \in \mathbb{R}^n}\ x^t A^t A x \tag{4}$$

subject to

$$x^t x = 1 \tag{5}$$

and either (2) or (3).
The Karush-Kuhn-Tucker conditions of the optimization problem (4)-(5)-(2) form a *generalized linear complementarity problem*, the solution set of which has a special structure. This generalization of the 'classical' linear complementarity problem (LCP) has been introduced in [9]. A earlier similar version can be found in [2]. The problem can be phrased as follows:

GLCP:
Given a real $m \times n$ matrix Z. Find all real vectors q such that

$$Zq = 0 \qquad (orthogonality) \tag{6}$$

$$q \geq 0 \qquad (nonnegativity) \tag{7}$$

$$\sum \prod q_i = 0 \qquad (complementarity) \tag{8}$$

The last constraint is to be understood as follows: The sum of certain specified products of components of q should be zero. Because all components of q are nonnegative, this implies that each of the terms in the sum must be zero and hence, that in each term, at least one factor is zero. In the simple case that for instance n is even and q is divided into two $n/2$-vectors q_1 and q_2 as $q^t = (\ q_1^t\ \ q_2^t\ )$ and the complementarity condition is $q_1^t q_2 = 0$, the zero pattern of q_1 will be complementary to the zero pattern of q_2.
Observe that the solution set to the problem without the complementarity condition is a polyhedral cone. With the complementarity condition, it is easy to see that the solution set becomes a union of 'smaller' polyhedral cones. The reason is that in the polyhedral solution cone of the problem without complementarity constraints, not all vertices satisfy the complementarity conditions. If a vector does not satisfy the complementarity conditions, no nonnegative combination of another vector with that vector can satisfy these conditions. Hence, vertices of the original polyhedral solution cone that do not satisfy the complementarity condition, can be disregarded. Another condition that determines the geometrical composition of the solution set, is the so-called *cross-complementarity* of a pair vectors. Let p and q be two vectors that are solutions to the **GLCP** and consider a nonnegative combination $p\alpha + q\beta$ where $\alpha, \beta \geq 0$. If for all values of α and β, the vector $p\alpha + q\beta$ is a solution to the **GLCP**, the pair of vectors p and q is said to be *cross-complementary*.
In the example above, where n was even, consider two nonnegative vectors p and q partitioned as $p^t = (\ p_1^t\ \ p_2^t\ )$ and $q^t = (\ q_1^t\ \ q_2^t\ )$. Assume that they satisfy the complementarity condition $p_1^t p_2 = 0$ and $q_1^t q_2 = 0$. Then, it is easy to show that they are crosscomplementary iff $p_1^t q_2 = 0$ and $p_2^t q_1 = 0$.
In [9] we have developed an algorithm that finds all solutions to the **GLCP** and even

a complete geometrical description of the solution set, which in general is a collection of polyhedral cones. This algorithm will be used in the present paper to solve the Karush-Kuhn-Tucker conditions of (4)-(5)-(2).

This paper is organised as follows: In section 2, we shall briefly summarize the Lagrangean approach to solve optimization problems (Karush-Kuhn-Tucker conditions). As an illustration, we present a proof of the unconstrained **TLLS** solution and of the **LLS** result with nonnegativity constraints.
In section 3, we apply the Lagrangean approach to the solution of the **TLLS** problem with nonnegativity constraints. A combinatorial solution scheme is discussed in section 4 while a **GLCP** solution is presented in section 5. In section 6, we take a closer look at the **TLLS** problem with an inequality constraint of the form $x \geq a$. In section 7, we illustrate our results with some numerical examples.

2 Constrained optimization

Let $x \in \Re^n$ be a vector of variables. Consider the general problem of minimizing a scalar function $f(x)$ subject to the constraints

$$g_i(x) \geq 0 \qquad i = 1, \ldots, r_1 \tag{9}$$

$$g_i(x) = 0 \qquad i = r_1 + 1, \ldots, r_2 \tag{10}$$

where $r_1 \leq r_2$. Define nonnegative slack variables $\xi_i^2, i = 1, \ldots, r_2$, which convert the inequality constraints into equality constraints:

$$g_i(x) - \xi_i^2 = 0 \qquad i = 1, \ldots, r_1 \tag{11}$$

The Lagrangean function for this problem is

$$\begin{aligned} & L(x,\ \xi_i\ (i = 1, \ldots, p),\ \lambda_j\ (j = 1, \ldots, m)) \\ & = f(x) - \sum_{i=1}^{r_1} \lambda_i (g_i(x) - \xi_i^2) - \sum_{i=r_1+1}^{r_2} \lambda_i g_i(x) \end{aligned} \tag{12}$$

Let $s^t = (\xi_1\ \ \xi_2\ \ \ldots\ \ \xi_{r_1})$ be the vector of slack variables and $l^t = (\ \lambda_1\ \ \ldots\ \ \lambda_{r_2}\ )$ be the vector of *Lagrange multipliers*. The Karush-Kuhn-Tucker conditions necessary for x^* and l^* to be a stationary point of the minimization problem can be summarized as follows:

KKT-conditions for minimization

$$\begin{aligned} \frac{\delta f}{\delta x_k}(x^*) - \sum_{i=1}^{r_2} \lambda_i^* \frac{\delta g_i}{\delta x_k}(x^*) &= 0 && k = 1, \ldots, n \\ \lambda_i^* g_i(x^*) &= 0 && i = 1, \ldots, r_1 \\ g_i(x^*) &\geq 0 && i = 1, \ldots, r_1 \\ g_i(x^*) &= 0 && i = r_1 + 1, \ldots, r_2 \\ l^* &\geq 0 \end{aligned}$$

It is assumed that the functions g_i and f are differentiable at x^*.
If instead of minimimizing one wants to maximize the objective function, then we simply require $l \leq 0$. In general, the Karush-Kuhn-Tucker conditions are necessary only.

Example 1: Total linear least squares

Let's prove the *total linear least squares* result without nonnegativity constraints using the Lagrangean approach. Hereto, we reformulate the **TLLS** problem as one of minimizing over all vectors $x \in \Re^n$ and all matrices $B \in \Re^{m \times n}$ the Frobenius norm $\|A - B\|_F^2$ subject to

$$Bx = 0 \tag{13}$$
$$x^t x = 1 \tag{14}$$

The first constraint ensures the rank deficiency of B, if $x \neq 0$, which is ensured by the second constraint. The Lagrangean function is here

$$L(B, x) = \sum_{i=1}^{m} \sum_{j=1}^{n} (a_{ij} - b_{ij})^2 - \lambda(x^t x - 1) - \sum_{i=1}^{m} \lambda_i b_i^t x \tag{15}$$

where b_i^t is the i-th row of the matrix B. Differentation with respect to b_{ij} results in [1]:

$$-(a_{ij} - b_{ij}) - \lambda_i x_j = 0 \tag{16}$$

while differentiation with respect to x_k results in

$$-x\lambda - \sum_{i=1}^{m} \lambda_i b_{ik} = 0 \tag{17}$$

Let $l^t = (\ \lambda_1 \ \ \ldots \ \lambda_m\ )$. We then have the following equations necessary for a vector x to be a solution to the **KKT-conditions**.

$$B = A + lx^t \tag{18}$$
$$B^t l = -x\lambda \tag{19}$$
$$Bx = 0 \tag{20}$$
$$x^t x = 1 \tag{21}$$

The first equation indicates that the optimal matrix B is a rank one modification of the matrix A. It follows from (21) that

$$\|A - B\|_F^2 = \|lx^t\|_F^2 = \|l\|^2 \tag{22}$$

[1] With a slight abuse of notation, we have absorbed the factor 2 in the scalars λ_i

Premultiplying (19) with x^t, (20) with l^t and using (21) results in $\lambda = 0$. Hence, it is easily found that

$$Ax = (\frac{-l}{\sigma})\sigma \tag{23}$$

$$A^t(\frac{-l}{\sigma}) = x\sigma \tag{24}$$

where $\sigma = \sqrt{l^t l}$. It's an easy exercise to show that this relation can only be satisfied if (x, σ, l) is a singular triplet of the matrix A. From (22) it follows that it has to be the singular triplet corresponding to the smallest singular value. As a matter of fact, we have just proved that the unconstrained *total least squares* solution vector x is the solution to the optimization problem (4)-(5).
The scalar $x^t A^t A x$ determined by a certain unit vector x has been called the *oriented energy* of the matrix A in the direction x in [3]. It is a special case for Hermitian matrices of the so called *numerical range* of a complex matrix (references see [7]). The *oriented energy surface* is the collection of vectors defined by

$$\{z \in \Re^n \mid z = x(x^t A^t A x)\ ,\ x \in \Re^n\ ,\ x^t x = 1\ \} \tag{25}$$

It is well known that the stationary points of the oriented energy are precisely the right singular vectors of the matrix A. Hence, the total least squares solution vector is the direction of minimal oriented energy of the matrix A.

It's interesting to apply our Lagrangean derivation to the **TLLS** problem with other constraints. For instance, instead of solving the **TLLS** problem with the constraint (14), we might as well impose the constraint:

$$x_k = 1 \qquad 1 \leq k \leq n \tag{26}$$

It is easy to prove that in this case, the **TLLS** vector x is still given by the right singular vector of A, corresponding to the smallest singular value, but scaled in such a way that the k-th component is 1.
However, the solution of the **TLLS** problem with constraint (26) does **not** correspond to the solution of the following optimization problem:

$$min_{\,over\ \ all\ \ x \in \Re^n}\ x^t A^t A x \tag{27}$$

subject to

$$x_k = 1 \tag{28}$$

The surprised reader may wish to verify that the solution to this problem is precisely the k-th least squares solution which has been described in Lemma 1.

Example 2: Linear least squares with nonnegativity constraints

The connection between a linear least squares problem with nonnegativity constraints on the one hand and complementarity problems on the other hand is well known, since the former is a special case of so called *quadratic programming* problems. The Karush-Kuhn-Tucker conditions for such problems are precisely linear complementarity problems. If the solution vector y to (1) is required to be nonnegative, the Lagrangean for the least squares problem becomes:

$$L(x) = \sum_{i=1}^{m}(c_i^t y - a_{in})^2 - \sum_{i=1}^{n}\lambda_i(y_i - \eta_i^2) \tag{29}$$

where a_{ij} is the element of row i and column j of A, c_i^t is the i-th row of A_n and η_i are the slack variables. Differentation with respect to y_i and $\eta_i, i = 1, \ldots, n$ results in the following necessary conditions:

$$\begin{pmatrix} A_n^t A_n & -I_n & -A_n^t a_n \end{pmatrix} \begin{pmatrix} y \\ l \\ 1 \end{pmatrix} = 0 \tag{30}$$

$$l^t y = 0 \tag{31}$$

$$l \geq 0 \tag{32}$$

$$y \geq 0 \tag{33}$$

where $l^t = (\ \lambda_1\ , \ldots,\ \lambda_n\ )$. Obviously, the set of equations (30)-(33) is a **GLCP** (In fact, it is a 'classical' **LCP**). If $l = 0$, it reduces to (1). If one of the components of l is nonzero, the corresponding component of y must be zero because of the complementarity conditions (31)-(33). Hence, if the unconstrained **LLS** solution is not nonnegative, the net effect of imposing nonnegativity constraints on the solution vector will be the rejection of a complete channel of data (a column of A).

3 Total linear least squares with nonnegativity constraints

The *total linear least squares problem with nonnegativity constraints* has the Lagrangean function:

$$L(B, x) = \sum_{i=1}^{m}\sum_{j=1}^{n}(a_{ij} - b_{ij})^2 - \lambda(x^t x - 1) - \sum_{i=1}^{m}\lambda_i b_i^t x - \sum_{i=m+1}^{m+n}\lambda_i(x_{i-m} - \xi_i^2) \tag{34}$$

where $\xi_i, i = 1, \ldots, n$ are the slack variables. Differentiation of the Lagrangean with respect to $b_{ij}, x_j, \xi_j,\ \ i = 1, \ldots, m,\ \ j = 1, \ldots, n$ results in

$$b_{ij} = a_{ij} + \lambda_i x_j \qquad i = 1, \ldots, m \ \ j = 1, \ldots, n \tag{35}$$

$$x_j\lambda = -\sum_{i=1}^{m} \lambda_i b_{ij} - \lambda_{j+m} \qquad j = 1, \ldots, n \tag{36}$$

$$\xi_i\lambda_i = 0 \qquad i = m+1, \ldots, m+n \tag{37}$$

Call $l^t = (\ \lambda_1\ \ldots\ \lambda_m\ )$ and $p^t = (\ \lambda_{m+1}\ \ldots\ \lambda_{m+n}\ )$. Then, together with equations (13)-(14), we find as the KKT-conditions:

$$B = A + lx^t \tag{38}$$

$$x\lambda = -B^t l - p \tag{39}$$

$$Bx = 0 \tag{40}$$

$$p^t x = 0 \tag{41}$$

$$x^t x = 1 \tag{42}$$

$$x \geq 0 \tag{43}$$

$$p \geq 0 \tag{44}$$

Observe that the matrix B is again a rank one modification of A. It is also straightforward to show that $\lambda = 0$ from (39), (40), (41) and (42). Eliminating B and l, we find the following equations:

$$A^t Ax - x\rho - p = 0 \tag{45}$$

with $\rho = x^t A^t Ax \geq 0$ and

$$p^t x = 0 \tag{46}$$

$$x^t x = 1 \tag{47}$$

$$x \geq 0 \tag{48}$$

$$p \geq 0 \tag{49}$$

This can be recast in the form of a *complementarity problem* as

$$(\ A^t A \quad -I_n \quad -I_n\ ) \begin{pmatrix} x \\ x\rho \\ p \end{pmatrix} = 0 \tag{50}$$

subject to the constraints (46)-(49). Observe that the solutions are *parametric* in the sense that the first and the second subvector in the solution should be related to each other by a nonnegative constant of proportionality ρ. This parameter ρ fullfills the role of the smallest eigenvalue of $A^t A$ in the solution of the **TLLS** problem without nonnegativity constraints. Because of this special structure, we propose to call the set of equations (46)-(50) a *parametric generalized linear complementarity problem.*

It is an easy exercise to demonstrate that the equations of the *parametric* **GLCP** (46)-(50) coincide precisely with the Karush-Kuhn-Tucker conditions for the following minimization problem:

$$minimize_{\ over\ all\ x\ \in\ \Re^n}\ x^t A^t Ax \tag{51}$$

subject to

$$x^t x = 1 \tag{52}$$

$$x \geq 0 \tag{53}$$

If we replace in (51) *minimization* by *maximization*, it suffices to require that the vector of Lagrange multipliers p be nonpositive. Hence, the corresponding parametric **GLCP** becomes:

$$\begin{pmatrix} A^tA & -I_n & I_n \end{pmatrix} \begin{pmatrix} x \\ x\rho \\ -p \end{pmatrix} = 0 \tag{54}$$

$$p^t x = 0 \tag{55}$$

$$x^t x = 1 \tag{56}$$

$$x \geq 0 \tag{57}$$

$$p \leq 0 \tag{58}$$

The oriented energy surface referred to in section 2, is a smooth surface. It is differentiable everywhere, except at the extremal points which occur at the right singular vectors of the matrix A [7]. If all components of one of the right singular vectors of A can be chosen nonnegative, this singular vector will necessarily be a stationary point of the optimization problem (51)-(53). Because of the smoothness of the energy surface, other stationary points will necessarily occur at the boundaries of the positive orthant, i.e. for nonnegative vectors x that have one or more zero components. Hence, stationary points of minimal and maximal oriented energy in nonnegative directions occur at nonnegative eigenvectors of A^tA and on the boundary planes of the positive orthant. This observation leads to a combinatorial solution scheme for the minimization (46)-(50) and the maximization problem (54)-(58) in the following section.

4 A combinatorial solution scheme

For 2 nonnegative n-vectors p and n, there are 2^n different complementarity patterns such that (46) is satisfied. For instance, 2 nonnegative but mutually orthogonal vectors x and p with 3 components may have the following zero-nonzero patterns:

x	0	0	0	0	.	.	.	.
	0	0	.	.	0	0	.	.
	0	.	0	.	0	.	0	.
p	.	.	.	.	0	0	0	0
	.	.	0	0	.	.	0	0
	.	0	.	0	.	0	.	0

where a '.' denotes any nonnegative scalar. Observe that, if $p = 0$, the solution to the *constrained complementarity problem* (45)-(49) reduces to an eigenvalue problem. This implies that, if the matrix A^tA has a nonnegative eigenvector, this is necessarily a stationary point of the minimization problem (51)-(53).
Consider the case where x is of the form $x^t = (\ 0 \quad x_2^t\ )$ and p has the complementary form $p^t = (\ p_1^t \quad 0\ )$ where p_1 is an $r \times 1$ nonnegative vector. Partition A in four blocks as:

$$A^tA = \begin{array}{c} \\ r \\ n-r \end{array} \begin{array}{c} \begin{array}{cc} r & n-r \end{array} \\ \begin{pmatrix} A_{11} & A_{12} \\ A_{12}^t & A_{22} \end{pmatrix} \end{array} \tag{59}$$

Then, equation (45) reduces to:

$$A_{12}x_2 = p_1 \qquad p_1 \geq 0 \tag{60}$$

$$A_{22}x_2 = x_2\rho \qquad x_2^tx_2 = 1 \qquad x_2 \geq 0 \qquad \rho \geq 0 \tag{61}$$

Hence, for this particular complementarity pattern, x_2 must be a nonnegative eigenvector of A_{22} while simultaneously, $A_{12}x_2$ must be nonnegative. Obviously, a similar claim can be deduced for all 2^n complementarity patterns, except for the one where $x = 0$, which violates the norm constraint $x^tx = 1$. Hence, the **TLLS** problem with nonnegativity constraints can be solved as follows: First, verify whether the eigenvector of A^tA, corresponding to the smallest eigenvalue, is nonnegative (or nonpositive). If so, the problem is solved. If not, find the solutions to (60)-(61) for all 2^n complemetarity patterns of x and p and pick the one that corresponds to the smallest scalar ρ.

Let us conclude this section with some observations:

- It follows directly from the eigenvalue interlacing property [11, pp.103] that the smallest eigenvalue of a principal submatrix is always larger than the smallest one of the complete matrix. If we have found a solution to the constrained eigenvalue problem (60)-(61) with r zeros at some specific positions, where ρ is the smallest eigenvalue of A_{22}, we have found the *optimal* solution *among the solutions with zeros at these r positions* . This does **not** mean that there is no better solution with r zeros in other positions!

- The *unconstrained* **TLLS** solution may provide a good indication of the position of the zero components in the optimal solution of the problem with nonnegativity constraints. Indeed, under fairly general conditions (for instance, if m/n is large, see [5] for details), the **TLLS** solution is an unbiased estimate of the linear relations between the columns of the matrix A, in the case that all data are noisy. Hence, one might expect that in the **TLLS** solution, components that correspond to zeros in the original, noiseless, problem, will be small in absolute value. One might for instance try out the solution to the constrained eigenvalue problem (60)-(61) with zero components at positions where the *unconstrained* **TLLS** solution is negative. As will be illustrated in section 7, this heuristic idea provides a good solution in most cases (if the signal-to-noise ratio is not too bad!).

- If one finds that in the constraint eigenvalue problem $A_{12}x_2 \leq 0$ instead of $A_{12}x_2 \geq 0$, the corresponding solution vector $(\ 0 \quad x_2^t \ )$ is a stationary point of the problem of *maximizing* $x^t A^t A x$ subject to $x \geq 0$.

5 Solution via a GLCP algorithm

The set of vectors satisfying the Karush-Kuhn-Tucker conditions is nothing else than the solution of the **GLCP** problem (46)-(50) with an additional constraint on the solution vector which must be of the special form (50). Instead of the combinatorial approach described in the previous section, we might also first solve the **GLCP** (46)-(50) with the algorithm described in [9]. The solution set is a collection of polyhedral cones. The vertices that generate one such a polyhedral cone, must be crosscomplementary. If the optimal solution is not a vertex of one of the polyhedral solution cones, it will be a nonnegative combination of these vertices. Such a nonnegative combination will have a certain number of zeros and the vector of Lagrange multipliers will have the complementary zero pattern. For each of the possibilities, we can again solve the constrained eigenvalue problem (60)-(61). Hence we have established the following solution scheme:

- Solve the **GLCP**

$$(\ A^t A \quad -I_n \quad -I_n \ ) \begin{pmatrix} q_1 \\ q_2 \\ q_3 \end{pmatrix} = 0 \tag{62}$$

$$q_1^t q_3 = 0 \tag{63}$$

$$q_2^t q_3 = 0 \tag{64}$$

$$q_1, q_2, q_3 \geq 0 \tag{65}$$

$$\tag{66}$$

  and determine the polyhedral solution cones generated by crosscomplementary vertices.

- Generate for each polyhedral solution cone all possible zero-nonzero patterns for nonnegative linear combinations of the vertices of that cone. Determine whether the constrained eigenvalue problem (60)-(61) has a solution.

- Of all solutions of the constrained eigenvalue problem, pick the ones with minimal ρ.

The **GSVD** may have a large number of solutions that may be grouped in polyhedral solutions cones. However, even if all complementary and cross-complementary solutions are known, the constrained eigenvalue problem (60)-(61) still needs to be solved for each of the zero-nonzero combinations of all polyhedral cones. Therefore in most cases, it is more straightforward to use the combinatorial solution scheme of the previous section rather than first solving the **GLCP**, especially as the number of variables n is large. This will be further illustrated numerically in section 7.

6 Total linear least squares with an inequality constraint

Let's now analyse the **TLLS** problem with the nonnegativity constraint (2) replaced by an inequality constraint of the form (3). Recall that the main reason for requiring $x^t x = 1$ was to enforce the rank deficiency of the approximating matrix B. In section 2, we have shown that the solution to the **TLLS** problem does not change when instead of $x^t x = 1$ we fix one of the components, say the n-th one, as $x_n = 1$. If the vector a in (3) is nonnegative ($\neq 0$), the quadratic constraint $x^t x = 1$ is no longer needed to ensure the rank deficiency of B, because x cannot be trivially equal to zero. In that case, the **TLLS** problem becomes a quadratic programming problem (which is equivalent to a **GLCP**). If however a would be strictly negative, $x = 0$ would satisfy (3) and we would also have $Bx = 0$. Hence, in this case, the quadratic constraint $x^t x = 1$ or a constraint on a component is needed to avoid a trivial solution.
Here, we shall assume that we have two constraints, one of the form $x^t x = 1$ and another of the form $x \geq a$, $a \neq 0$. It is assumed throughout that these 2 constraints are non-conflicting. Then the Lagrangean is given by:

$$L(B,x) = \sum_{i=1}^{m}\sum_{j=1}^{n}(a_{ij} - b_{ij})^2 - \lambda(x^t x - 1) - \sum_{i=1}^{m}\lambda_i b_i^t x - \sum_{i=m+1}^{m+n}\lambda_i(x_{i-m} - \xi_i^2 - a_i^2) \qquad (67)$$

The KKT-conditions are:

$$\begin{aligned} B &= A + lx^t && (68)\\ B^t l &= -x\lambda - p && (69)\\ p^t(x-a) &= 0 && (70)\\ Bx &= 0 && (71)\\ x^t x &= 1 && (72)\\ x &\geq a && (73)\\ p &\geq 0 && (74) \end{aligned}$$

where $p^t = (\ \lambda_{m+1}\ \ \lambda_{m+2}\ \ \lambda_{m+n}\ )$ is the vector of Lagrange multipliers associated with the inequality constraint. Again the modification of A into B is of rank 1 and we are interested in the modification for which the norm of l is minimal.
As in the previous sections, we can again eliminate B and l. Observe that here the Lagrange multiplier λ is not zero!

$$-A^t Ax + x(\rho^2 + \lambda) + p = 0 \qquad (75)$$

with

$$\begin{aligned} p^t(x-a) &= 0 && (76)\\ x^t x &= 1 && (77)\\ x &\geq a && (78)\\ p &\geq 0 && (79) \end{aligned}$$

and

$$\rho^2 = x^t A^t A x \tag{80}$$

Observe that the vectors $x - a$ and p are complementary. If $p = 0$, then (75) reduces to an eigenvalue problem. Suppose p is not identically zero but only some of its components, say the last $n - r$ ones. Then:

$$p = \begin{pmatrix} p_1 \\ 0 \end{pmatrix} \qquad x - a = \begin{pmatrix} x_1 - a_1 \\ x_2 - a_2 \end{pmatrix} = \begin{pmatrix} 0 \\ x_2 - a_2 \end{pmatrix} \tag{81}$$

Partition $A^t A$ as in (59). Then (75) can be rewritten as:

$$A_{11} a_1 + A_{12} x_2 = a_1(\rho^2 + \lambda) + p_1 \qquad p_1 \geq 0 \tag{82}$$

$$A_{12}^t a_1 + A_{22} x_2 = x_2(\rho^2 + \lambda) \qquad x_2 \geq a_2 \tag{83}$$

Observe that

$$x^t x = x_1^t x_1 + x_2^t x_2 = a_1^t a_1 + x_2^t x_2 = 1 \tag{84}$$

so that

$$x_2^t x_2 = 1 - a_1^t a_1 = \alpha^2 \quad (say) \tag{85}$$

Call

$$\gamma = \rho^2 + \lambda \tag{86}$$

Interestingly enough, the problem (83)-(85) is equivalent to a quadratic eigenvalue problem and can be solved as such. This was first observed in [10, Theorem 5.1]:

Lemma 2
The vectors z and the scalars λ satisfying

$$Cz = z\lambda + b \tag{87}$$

$$z^t z = \zeta^2 \tag{88}$$

where $C \in \Re^{n \times n}$ symmetric, $b \in \Re^n$ and $\zeta \in \Re$ are given, are solutions to the quadratic eigenvalue problem

$$(C - \lambda I_n)^2 y = \frac{1}{\zeta^2} b b^t y \tag{89}$$

For a detailed proof of this Lemma, we refer to [10], which also contains some interesting numerical experiments with several methods to solve (87)-(88). Here we present only the idea behind Lemma 2.
Assume that λ is not an eigenvalue of C (this case should be treated separately but causes no special complications), then

$$z = (C - \lambda I_n)^{-1} b \tag{90}$$

and from (88)

$$b^t (C - \lambda I_n)^{-2} b = \zeta^2 \tag{91}$$

Call $y = (C - \lambda I_n)^{-2} b$. Then

$$b^t y = \zeta^2 \tag{92}$$

Now we find from (90) that

$$(C - \lambda I_n)^2 y = b \tag{93}$$

and by multiplying this equation with $b^t y / \zeta^2 = 1$, we find precisely (89). This quadratic eigenvalue problem can easily be converted to an ordinary eigenvalue problem by the standard substitution

$$y^0 = y \qquad y^1 = y\lambda \tag{94}$$

Equation (89) then becomes:

$$\begin{pmatrix} 0 & I_n \\ \frac{bb^t}{\zeta^2} - C^2 & 2C \end{pmatrix} \begin{pmatrix} y^0 \\ y^1 \end{pmatrix} = \begin{pmatrix} y^0 \\ y^1 \end{pmatrix} \lambda \tag{95}$$

which is an ordinary $2n \times 2n$ eigenvalue problem. The eigenvectors have to be normalized such that (92) is satisfied.
Using these results, the quadratic eigenvalue problem represented by (83) can be converted to an ordinary eigenvalue problem:

$$\begin{pmatrix} 0 & I_{n-r} \\ \frac{1}{\alpha^2} A_{12}^t a_1 a_1^t A_{12} - A_{22}^2 & 2A_{22} \end{pmatrix} \begin{pmatrix} u^0 \\ u^1 \end{pmatrix} = \begin{pmatrix} u^0 \\ u^1 \end{pmatrix} \gamma \tag{96}$$

with

$$u^0 = -(A_{22} - \gamma I_{n-r})^{-1} x_2 \qquad u^1 = u^0 \gamma \tag{97}$$

which should be normalized such that

$$a_1^t A_{12} u = \alpha^2 \tag{98}$$

Hence, the stationary points for the Lagrangean (67) can be found as follows:

- Verify if the unconstrained **TLLS** solution satisfies all constraints. If so, this is the optimal solution, if not, proceed.
- For all nontrivial complementary patterns of $x - a$ and p, solve a problem as in (83) subject to (85). The solution requires an eigenvalue decomposition of the form (96). Normalize the eigenvectors such that (98) is satisfied and verify whether $x_2 \geq a$. If not, proceed with another complementary pattern.
- Compute the vector p_1 from (82). If it is nonnegative, we have a stationary vector.
- The solution x to the **TLLS** problem with the inequality constraint $x \geq a$ and the quadratic constraint $x^t x = 1$, corresponds to the one in which $x^t A^t A x$ is minimal.

Let's conclude this section with the following remarks and observations:

- Again as in section 5, one may convert (75)-(79) to a **GLCP** as follows: Define $y = x - a \geq 0$. Then (75) becomes

$$A^t Ay + A^t Aa - y(\rho^2 + \lambda) - a(\rho^2 + \lambda) - p = 0 \tag{99}$$

and (76) becomes

$$p^t y = 0 \tag{100}$$

Hence, we could first solve the **GLCP**

$$\begin{pmatrix} A^t A & -I_n & -I_n & -a & A^t Aa \end{pmatrix} \begin{pmatrix} q_1 \\ q_2 \\ q_3 \\ q_4 \\ 1 \end{pmatrix} = 0 \tag{101}$$

with the complementarity conditions:

$$q_1^t q_2 = 0 \qquad q_2^t q_3 = 0 \tag{102}$$

The solution set consists of a collection of polyhedrons (instead of polyhedral cones, because of the fact that the last component of each solution vector should be 1) and for each cone, one can see by inspection the zero-nonzero patterns that may occur. It is only for these zero-nonzero patterns that the quadratic eigenvalue problem (82)-(84) need to be solved. There is however a complication in the sense that we are not able to prove that $\rho^2 + \lambda \geq 0$. Hence, in principle, one needs to solve 2 **GLCP**s, one for $\rho^2 + \lambda \geq 0$ and the second one for $\rho^2 + \lambda \leq 0$.

- It is surprising how the solution of the **TLLS** problem with *nonnegativity* constraints, differs from the one of the **TLLS** problem with *inequality* constraints. In the **LLS** problem, there is no difference at all as can be seen from our derivation in section 2 (see also [1]).

- It is easy to derive that the set of equations (75)-(79) coincides with the KKT-conditions for the following quadratic programming problem with quadratic and linear constraints:

$$min_{\ over\ \ x \in \Re^n}\ x^t A^t Ax \tag{103}$$

subject to

$$x^t x = 1 \tag{104}$$

$$x \geq a \tag{105}$$

where $a \in \Re^n$.

- The solution scheme described in this section may easily be extended to inequality constraints of the form

$$a \leq x \leq b \tag{106}$$

where $a, b \in \Re^n$. Let p be the vector of Lagrange multipliers associated with $x \geq a$ and q the one associated with $x \leq b$. Then the KKT-conditions for the **TLLS** solution with a norm constraint $x^t x = 1$ and the constraints (106) are:

$$\begin{aligned} A^t A x &= x\gamma + p - q && (107)\\ p^t(x-a) &= 0 && (108)\\ q^t(b-x) &= 0 && (109)\\ p, q &\geq 0 && (110) \end{aligned}$$

where $\gamma = \rho^2 + \lambda$, λ being the Lagrange multiplier associated with $x^t x = 1$ and $\rho = x^t A^t A x$. These equations can be solved via a double combinatorial solution scheme: One for all the complementary patterns between p and $x - a$ and one for all possible complementary patterns between q and $x - b$. We shall however not pursue this extension.

7 Numerical examples

In this section, we present some numerical examples. The **GLCP** algorithm of [9] has been encoded in MATLAB and PASCAL [2]. The combinatorial solution schemes of sections 4 and 6 have been implemented in MATLAB as well.

Example 1:

Our first example concerns the maximization and minimization of $x^t A^t A x$ subject to $x^t x = 1$ and $x \geq 0$ where

$$A^t A = \begin{pmatrix} 89 & -32 & 26 \\ -32 & 151 & 27 \\ 26 & 27 & 139 \end{pmatrix}$$

The eigenvalues are $\lambda(A^t A) = \{174, 145, 60\}$. It can be verified numerically that none of the eigenvectors of $A^t A$ belongs to the positive orthant. In particular, the unconstrained **TLLS** solution is:

$$x_{TLLS} = \begin{pmatrix} 8.1650e-01 \\ 4.0825e-01 \\ -4.0825e-01 \end{pmatrix} \tag{111}$$

Let's find the solutions to the Karush-Kuhn-Tucker conditions for the *maximization* of $x^t A^t A x$ subject to $x^t x = 1$ and $x \geq 0$. The corresponding **GLCP** is:

$$\begin{pmatrix} A^t A & -I_3 & I_3 \end{pmatrix} q = 0 \qquad q \geq 0 \tag{112}$$

[2] The source codes can be obtained upon simple request.

where $q^t = (\ q_1^t \ \ q_2^t \ \ q_3^t\ )$ and the complementarity conditions are $q_1^t q_3 = 0$, $q_2^t q_3 = 0$. Here are the solution vertices:

	1	**2**	**3**	**4**	**5**	**6**	**7**
	1	32	13439	0	0	27	0
x	0	89	2848	26	0	0	1
	0	0	0	32	1	32	0
	89	0	1104935	0	26	3235	0
$x\rho$	0	12415	0	4790	27	0	151
	26	3235	426310	5150	139	5150	27
	0	0	0	0	0	0	32
$-p$	32	0	0	0	0	0	0
	0	0	0	0	0	0	0

There are 3 polyhedral solution cones, generated by the sets of vertices $\{\mathbf{1},\mathbf{6}\}$, $\{\mathbf{2},\mathbf{3},\mathbf{4},\mathbf{5},\mathbf{6}\}$, $\{\mathbf{4},\mathbf{7}\}$. Except for the pairs **1-6** and **4-7**, all pairs of crosscomplementary vectors have a vector of Lagrange multipliers which is zero. Hence, the corresponding solution vector x would be determined by nonnegative eigenvectors of $A^tAx = x\lambda$. Since there are none, these pairs are not relevant. For the pair **1-6**, we have $x_2 = 0$. Solving the resulting 2×2 constrained eigenvalue problem gives:

$$x = \begin{pmatrix} 3.9172e-01 \\ 0 \\ 9.2008e-01 \end{pmatrix} \qquad \lambda = 1.5007e+02 \qquad -p = \begin{pmatrix} 0 \\ 1.2307e+01 \\ 0 \end{pmatrix} \tag{113}$$

The vector x is indeed a nonnegative combination of the cross-complementary vertices **1-6**. For the pair **4 - 7** we have $x_1 = 0$:

$$x = \begin{pmatrix} 0 \\ 7.8004e-01 \\ 6.2573e-01 \end{pmatrix} \qquad \lambda = 1.7266e+02 \qquad -p = \begin{pmatrix} 8.6924e+00 \\ 0 \\ 0 \end{pmatrix} \tag{114}$$

Hence, the solution to the maximization problem is given by (114). Observe that the maximum is quite close to the maximal eigenvalue of A^tA.
For the minimization of x^tA^tAx subject to $x \geq 0$ and $x^tx = 1$, one has to solve:

$$(\ A^tA \quad -I_3 \quad -I_3\ )q = 0 \qquad q \geq 0$$

with complementarity conditions $q_1^t q_3 = 0, q_2^t q_3 = 0$. The solution vertices are

	1	2	3	4	5	6	7	8	9	10
	32	32	13439	13439	0	0	0	0	0	27
x	89	89	2848	2848	26	0	0	0	0	0
	0	0	0	0	32	1	1	1	1	32
	0	0	1104935	1104935	0	0	0	26	26	3235
$x\rho$	12415	12415	0	0	4790	0	27	0	27	0
	0	3235	0	426310	5150	139	139	139	139	5150
	0	0	0	0	0	26	26	0	0	0
p	0	0	0	0	0	27	0	27	0	0
	3235	0	426310	0	0	0	0	0	0	0

There are 4 polyhedral solution cones, generated by the vertex sets $\{\mathbf{1},\mathbf{3}\}$, $\{\mathbf{2},\mathbf{4},\mathbf{5},\mathbf{9},\mathbf{10}\}$, $\{\mathbf{5},\mathbf{7}\}$ and $\{\mathbf{8},\mathbf{10}\}$. In the solution cone $\{\mathbf{2},\mathbf{4},\mathbf{5},\mathbf{9},\mathbf{10}\}$, all vectors of Lagrange multipliers are 0. But there are no nonnegative eigenvectors. Hence, these solutions must not be taken into account. For the pair **1 - 3**, we find that $x_3 = 0$. Solving the constrained eigenvalue problem results in:

$$x = \begin{pmatrix} 9.2081e-01 \\ 3.9000e-01 \\ 0 \end{pmatrix} \qquad \lambda = 7.5447e+01 \qquad p = \begin{pmatrix} 0 \\ 0 \\ 3.4471e+01 \end{pmatrix} \tag{115}$$

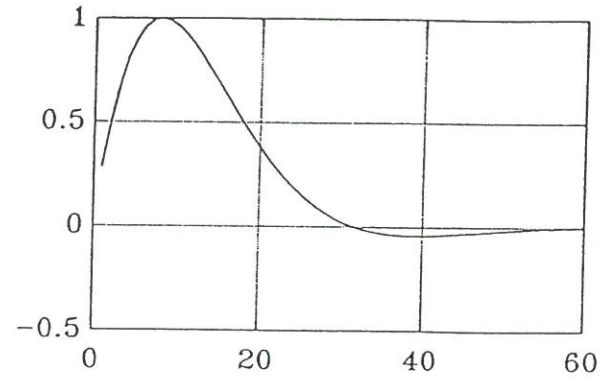
For the pair **5 - 7**, $x_1 = 0$ and the solution is given in (114). For the pair **8 - 10** , $x_2 = 0$ and the solution is given in (113). Hence, the solution of our minimization problem is given by (115).

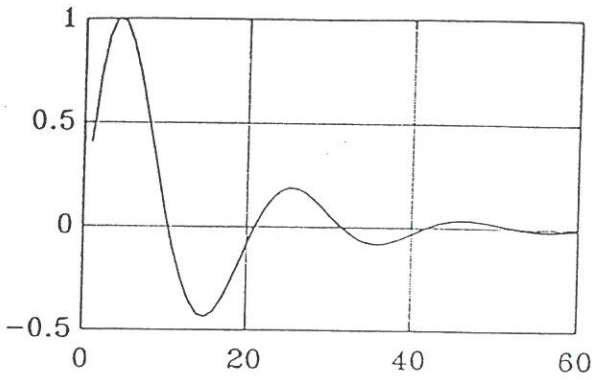
Example 2:

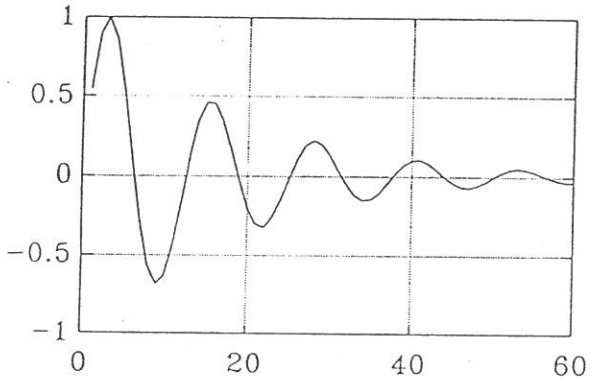
Consider the 5 spectra in figure 2. They are power spectra obtained from FFT on 128 points $k = 1, 2, \ldots, 128$ of the signals $a_i(k) = \alpha_i * sin(f_i * k) * exp(d_i * k)$ where

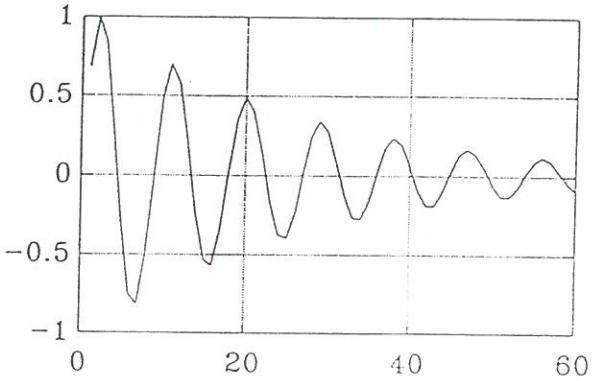
	f_i	d_i
1	0.1	0.10
2	0.3	0.08
3	0.5	0.06
4	0.7	0.04
5	0.9	0.02

The scalars $\alpha_i, i = 1, 2, 3, 4, 5$ are such that the maximum of each power spectrum is one. The signals in the time domain can be found in figure 1.
These spectra are stored as the columns of a 64×5 matrix B. An exact observation vector b was formed as $b = By$ where $y^t = (\ 1\ 0\ 2\ 0\ 3\ )$. Then the matrix A is constructed as $A = (\ B \quad -b\ )$. Normally distributed zero mean noise with standarddeviation 0.1 was added to all columns of A. The problem of determining the relative contribution of each of the spectra in the vector b is now one of solving a **TLLS** problem with nonnegativity









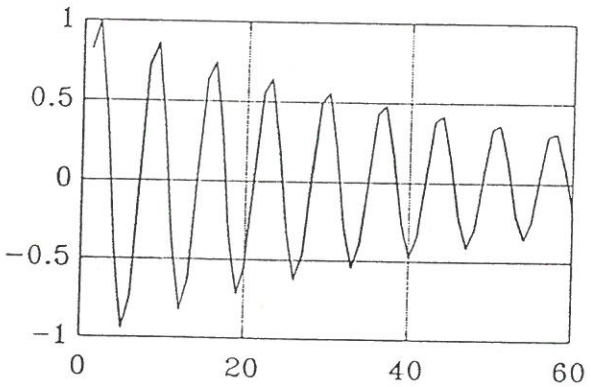


Figure 1: Five time domain signals with different frequency and damping

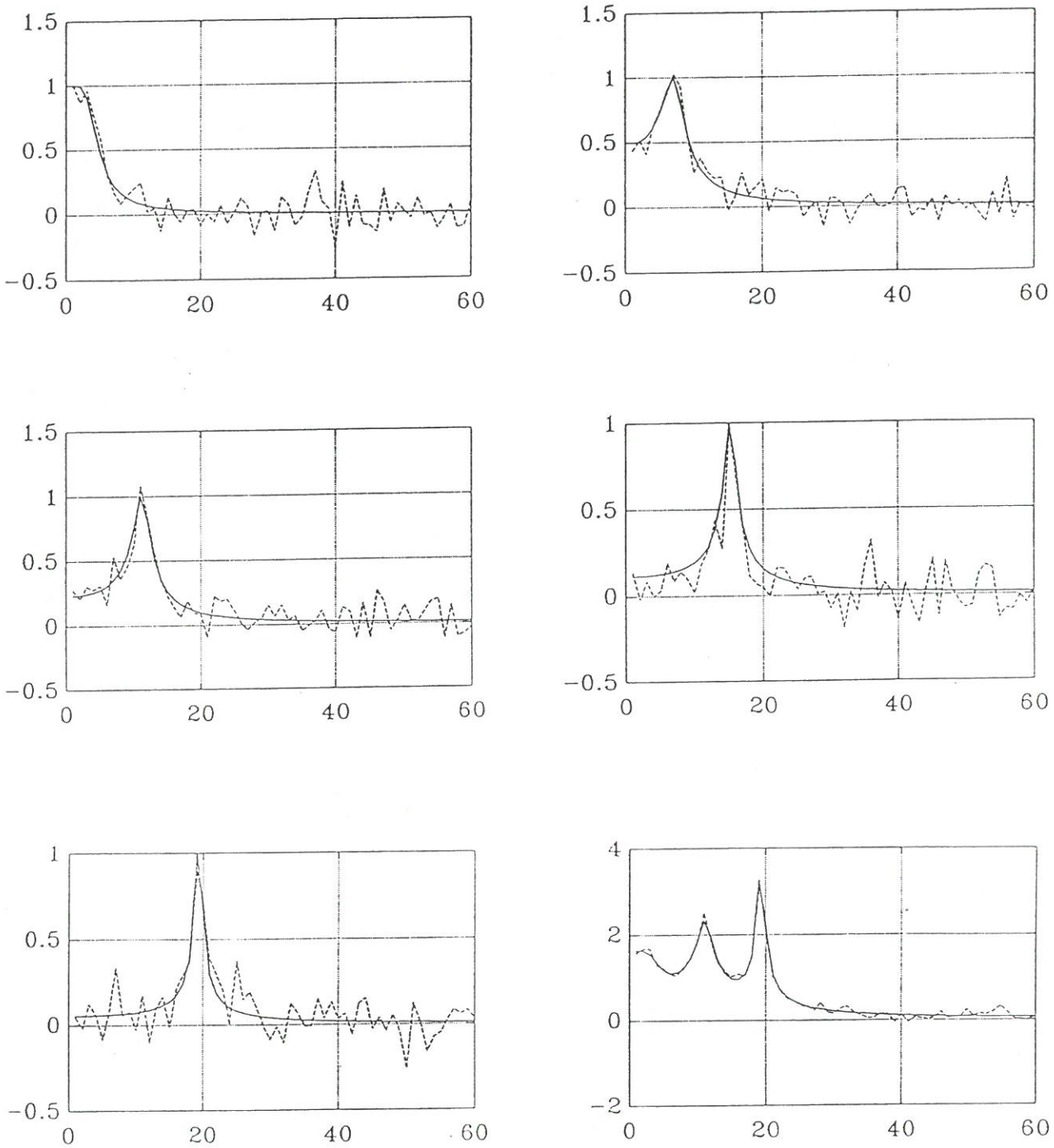


Figure 2: Fig.2a-2e: Five exact (full line) and noisy spectra ($- -$) of the signals in figure 1. Fig.2f: Vector b exact (full line) and noisy ($- -$), which consists of a nonnegative linear combination of these five spectra.

constraints.

The *unconstrained* **TLLS** solution can be computed as (we have normalized the last component to 1):

$$x_{TLLS} = \begin{pmatrix} 8.9474e-01 \\ -2.4725e-01 \\ 2.3224e+00 \\ 1.0582e-01 \\ 2.9620e+00 \\ 1.0000e+00 \end{pmatrix}$$

Hence, we may conjecture that an optimal solution will have a zero component at the second position. The corresponding smallest eigenvalue of A^tA (which is also the unconstrained minimum) is equal to $6.0495e-01$. Using the combinatorial approach of section 4, we have indeed found one solution to the constrained eigenvalue problem (60)-(61). It has its second component equal to zero (the results have been normalized so that the last component of x is 1):

$$x = \begin{pmatrix} 7.8314e-01 \\ 0.0000e+00 \\ 2.1898e+00 \\ 1.1609e-01 \\ 2.8962e+00 \\ 1.0000e+00 \end{pmatrix} \qquad p = \begin{pmatrix} 0.0000e+00 \\ 4.0281e-01 \\ 0.0000e+00 \\ 0.0000e+00 \\ 0.0000e+00 \\ 0.0000e+00 \end{pmatrix} \qquad \rho = 6.1143e-01$$

Observe also that the 4-th component of x is relatively small where in the exact solution it was 0. The **GLCP** problem (62)-(65) has 50 solution vertices but we did not detect all possible cross-complementary polyhedral solution cones.
Observe that, while the *unconstrained* **TLLS** solution violates the nonnegativity constraint, its components are relatively well estimated and the solution *with* a nonnegativity constraint does not seem to differ significantly from the unconstrained one. The explanation might be found in the statistical results on the **TLLS** problem. For this example, the signal-to-noise is quite good and the number of measurements is sufficiently high. Hence, the asymptotic theory of [5] applies and the *unconstrained* **TLLS** already provides a reasonable estimate (which is statistically unbiased).

Example 3

Consider again the matrix A^tA of example 1. Assume that we want a solution x of unit norm, satisfying:

$$x \geq a = \begin{pmatrix} 0.92 \\ 0.39 \\ 0.03 \end{pmatrix}$$

Using the combinatorial approach of section 6, where for each complementarity pattern we solve a quadratic eigenvalue problem, we find that there is one solution which corresponds to a minimum ($p \geq 0$) and one solution corresponding to a maximum ($p \leq 0$):

	minimum	maximum
x	$9.2033e-01$	$9.2000e-01$
	$3.9000e-01$	$3.9000e-01$
	$3.0000e-02$	$3.8730e-02$
p	$0.0000e+00$	$-8.7581e+02$
	$4.9759e-01$	$-3.7062e+02$
	$3.6340e+01$	$0.0000e+00$
$\gamma = \rho^2 + \lambda$	$7.6287e+01$	$1.0285e+03$
$\rho^2 = x^t A^t A x$	$7.7571e+01$	$7.8210e+01$

Assume that we want a solution x of unit norm, satisfying:

$$x \geq a = \begin{pmatrix} 0.83 \\ 0.41 \\ -0.35 \end{pmatrix}$$

Observe that elements of the vector a are close to the elements of the unconstrained TLLS solution (111). Using the combinatorial approach of section 6, we find that there is one solution which corresponds to a minimum ($p \geq 0$) and one solution corresponding to a maximum ($p \leq 0$):

	minimum	maximum
x	$8.4162e-01$	$8.3000e-01$
	$4.1132e-01$	$4.1000e-01$
	$-3.5000e-01$	$3.7815e-01$
p	$0.0000e+00$	$-1.1645e+02$
	$0.0000e+00$	$-4.6830e+01$
	$6.2295e+00$	$0.0000e+00$
$\gamma = \rho^2 + \lambda$	$2.2534e+02$	$6.2548e+01$
$\rho^2 = x^t A^t A x$	$1.0949e+02$	$6.0368e+01$

As expected, the optimum value of $\rho^2 = x^t A^t A x$ is close to the unconstrained optimum, which is 60.

8 Conclusions

In this paper, a numerical approach has been proposed for the solution of the Karush-Kuhn-Tucker conditions that arise from total linear least squares with nonnegativity constraints. An algorithm to solve a generalized linear complementarity problem can be used as a pre-processor. For the final solution, a certain constrained eigenvalue problem is to be solved.

We have also analysed total linear least squares problems with *inequality* constraints of the form $x \geq a$ where $a \neq 0$. The solution scheme is in this case more complicated than that for simple nonnegativity constraints. The constrained eigenvalue problem now becomes a constrained *quadratic* eigenvalue problem. The difference in complexity is surprising because for the **LLS** case, there is no fundamental difference between nonnegativity and inequality constraints [1]. We have illustrated our approach with several numerical examples.
Some further questions of interest might be the inclusion of weighting matrices in the total least squares problem. These could be available from a priori statistical information on the accuracy of the measurements. The derivation of reliable and fast algorithms for real large scale applications is certainly another point of interest.

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