The Regularized Total Least Squares Problem: Theoretical Properties and Three Globally Convergent Algorithms

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Total Least Squares (TLS) is a method for treating an overdetermined system of linear equations $Ax \approx b$, where both the matrix A and the vector b are contaminated by noise. In practical situations, the linear system is often ill-conditioned. For example, this happens when the system is obtained via discretization of ill-posed problems such as integral equations of the first kind (see e.g., [7] and references therein). In these cases the TLS solution can be physically meaningless and thus regularization is essential for stabilizing the solution.

Regularization of the TLS solution was addressed by several approaches such as truncation methods [6, 8] and Tikhonov regularization [1]. In this talk we will consider a third approach in which a quadratic constraint is introduced. It is well known [7, 11] that the quadratically constrained total least squares problem can be formulated as a problem of minimizing a ratio of two quadratic function subject to a quadratic constraint:

$$(RTLS) \quad \min_{x \in R^n} \left\{ \frac{\|Ax - b\|^2}{\|x\|^2 + 1} : \|Lx\|^2 \leq \rho \right\},$$

where $A \in R^{m \times n}, b \in R^m, \rho > 0$ and $L \in R^{k \times n} (k \leq n)$ is a matrix that defines a (semi)norm on the solution. The RTLS problem was extensively studied in recent years [2, 3, 7, 10, 11]. A key difficulty with this problem is its nonconvexity. As a result, several methods [7, 10] devised to solve it are not guaranteed to converge to a global optimum but rather to a point satisfying first order necessary optimality conditions.

We will present three globally and efficiently convergent algorithms, based on the algorithms proposed in [2, 3, 11], for solving the more general problem of minimizing a ratio of (possibly indefinite) quadratic functions subject to a quadratic constraint:

$$(RQ) \quad \min_{x} \left\{ f(x) \equiv \frac{f_1(x)}{f_2(x)} : \|Lx\|^2 \leq \rho \right\},$$

where

$$f_i(x) = x^T A_i x - 2b_i^T x + c_i, \quad i = 1, 2,$$

$A_1, A_2 \in R^{n \times n}$ are symmetric matrices, $b_1, b_2 \in R^n$, $c_1, c_2 \in R$. We do not assume that A_1 and A_2 are positive semidefinite (as in the case of the RTLS problem). The only assumption made is that the problem is well defined. Surprisingly, at least with respect to the methodologies and techniques presented in the talk, there is no real advantage in dealing with the specific instance of the RTLS problem.

The procedure devised in [2] relies on the following key observation due to [5] for fractional programs:
Observation: given $\alpha \in R$, the following two statements are equivalent:
1. $\min_x \{f_1(x)/f_2(x) : \|Lx\|^2 \leq \rho\} \leq \alpha$.
2. $\min_x \{f_1(x) - \alpha f_2(x) : \|Lx\|^2 \leq \rho\} \leq 0$.

Based on the latter observation, we develop an efficient algorithm for finding the global optimal solution by converting the original problem into a sequence of simple optimization problems of the form

$$(GTRS) \quad \min_x \left\{ x^T A x + 2b^T x + c : \|Lx\|^2 \le \rho \right\}$$

parameterized by a single parameter α. The optimal solution corresponds to a particular value of α, which can be found by a simple one-dimensional search. Problem (GTRS) is also known in the literature as the generalized trust region subproblem and, similarly to problem (RQ), is a nonconvex problem. Using the hidden convexity result of [4] we are able to convert the GTRS problem into a simple *convex* optimization problem that can be solved by finding the root of a one-dimensional secular equation. Overall, the algorithm finds an ε-optimal solution after solving $O(\log \varepsilon^{-1})$ GTRS problems. Practically, the numerical experiments in [2] show that a high-accuracy optimal solution is typically obtained after only few iterations.

The method devised in [11] was developed to solve the specific case of the RTLS problem. The starting point is the observation that x^* is an optimal solution of problem (RQ) if and only if

$$x^* \in \operatorname{argmin}_{y \in R^n} \{ f_2(y)(f(y) - f(x^*)) \ : \ \|Ly\|^2 \le \rho \},$$

(here $f_2(y) = \|y\|^2 + 1, f(y) = \|Ay - b\|^2/(\|y\|^2 + 1)$) which naturally leads to consider the following fixed point iterations:

$$x_{k+1} \in \operatorname{argmin}_{y \in R^n} \{ f_2(y)(f(y) - f(x_k)) : \|Ly\|^2 \le \rho \}.$$

The latter scheme, similarly to the one used in [2], also involves the solution of a GTRS problem at each iteration. A different method for solving the GTRS problem is discussed in [11]. Specifically, the GTRS is converted into an equivalent quadratic eigenvalue problem (QEP) for which efficient solvers are known to exist. The numerical results presented in [11] indicate that, similarly to the method proposed in [2], the method converges at a very fast rate and requires the solution of very few (up to 5) GTRS problems. The numerical results reported in [11] also indicate that the method produces a *global solution*. This fact was also validated empirically by comparing the two procedures in [2]. However, a proof of convergence to a global optimal solution of the RTLS was not given in [11].

The aforementioned results suggest that the problem (RQ) of minimizing a quadratically constrained ratio of two quadratic functions seems to share some kind of hidden convexity property, namely, it can be shown to be equivalent to some (tractable) convex optimization reformulation. In [3] we show that this is indeed the case. We obtain a simple condition in terms of the problem's data under which the attainment of the minimum in problem (RQ) is warranted. This condition allows us to derive an appropriate nonconvex reformulation of (RQ), and to apply an extension of the so-called S-Lemma for three quadratic homogeneous forms [9]. By so doing, we prove that problem (RQ) can be recast as a semidefinite programming problem for which efficient solution algorithms are known to exist (e.g., interior point methods). Based on the latter formulation, we propose a *third* globally and efficiently convergent algorithm for solving the RQ problem. Another byproduct of the aforementioned results is a superlinear convergence result for the iterative scheme suggested in [11], and which is extended for the *more general* class of problems (RQ). Moreover, it is shown that this algorithm produces an ε-global optimal solution in no more than $O(\sqrt{\log \varepsilon^{-1}})$ main loop iterations. This result also provides a theoretical justification to the successful computational results reported in the context of (RTLS) in [11] and [3].
The talk is partially based on joint works with Aharon Ben-Tal and Marc Teboulle.

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Amir Beck was born in Israel in 1975. He received the B.Sc. degree in pure mathematics (*Cum Laude*) in 1991, the M.sc. degree in operations research (*Suma Cum laude*) and the Ph.D. degree in operations research – all from Tel Aviv University (TAU), Tel Aviv, Israel. From 2003 to 2005 he was a Postdoctoral Fellow at the Minerva Optimization Center, Technion, Haifa, Israel.

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