



Total least squares methods

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Recent advances in total least squares approaches for solving various errors-in-variables modeling problems are reviewed, with emphasis on the following generalizations:

1. the use of weighted norms as a measure of the data perturbation size, capturing prior knowledge about uncertainty in the data;
2. the addition of constraints on the perturbation to preserve the structure of the data matrix, motivated by structured data matrices occurring in signal and image processing, systems and control, and computer algebra;
3. the use of regularization in the problem formulation, aiming at stabilizing the solution by decreasing the effect because of intrinsic ill-conditioning of certain problems.

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For extensive reviews of the total least squares (TLS) approach and its applications, we refer the reader to the following

- *Overview papers*: Refs 1–4;
- *Proceedings and special issues*: Refs 5–8; and
- *Books*: Refs 9–10.

The focus of this paper is on computational algorithms for solving the generalized TLS problems. The reader is referred to the errors-in-variables literature for the statistical properties of the corresponding estimators, as well as for a wider range of applications.

WEIGHTED AND STRUCTURED TOTAL LEAST SQUARES PROBLEMS

The TLS solution

$$\begin{aligned} \hat{x}_{\text{tls}} &= \arg \min_{x, \hat{A}, \hat{b}} \left\| \begin{bmatrix} A & b \end{bmatrix} - \begin{bmatrix} \hat{A} & \hat{b} \end{bmatrix} \right\|_F \\ &\text{subject to } \hat{A}x = \hat{b} \end{aligned} \quad (1)$$

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of an overdetermined system of equations $Ax \approx b$ is appropriate when all elements of the data matrix $\begin{bmatrix} A & b \end{bmatrix}$ are noisy and the noise is zero mean, independent, and identically distributed. More precisely, (under regularity conditions) \hat{x}_{tls} is a consistent estimator for the true parameter value \bar{x} in the *errors-in-variables (EIV) model*

$$A = \bar{A} + \tilde{A}, \quad b = \bar{b} + \tilde{b}, \quad \bar{A}\bar{x} = \bar{b}, \quad (2)$$

where the vector of perturbations $\text{vec}(\begin{bmatrix} \tilde{A} & \tilde{b} \end{bmatrix})$ is zero mean and has covariance matrix that is equal to the identity up to a scaling factor, i.e.,

$$\begin{aligned} \mathbb{E} \left(\text{vec} \left(\begin{bmatrix} \tilde{A} & \tilde{b} \end{bmatrix} \right) \right) &= 0 \quad \text{and} \\ \text{cov} \left(\text{vec} \left(\begin{bmatrix} \tilde{A} & \tilde{b} \end{bmatrix} \right) \right) &= \sigma^2 I. \end{aligned} \quad (3)$$

The noise assumption (3) implies that all elements of the data matrix are measured with equal precision, an assumption that may not be satisfied in practice.

A natural generalization of the EIV model (Eq. (2,3)) is to allow the covariance matrix of the vectorized noise to be of the form $\sigma^2 V$, where V is a given positive definite matrix. The corresponding estimation problem is the TLS problem (1) with the Frobenius norm $\|\cdot\|_F$ replaced by the weighted matrix norm

$$\|\Delta D\|_{V^{-1}} := \sqrt{\text{vec}^\top(\Delta D) V^{-1} \text{vec}(\Delta D)}$$

i.e.,

$$\min_{x, \hat{A}, \hat{b}} \left\| \begin{bmatrix} A & b \end{bmatrix} - \begin{bmatrix} \hat{A} & \hat{b} \end{bmatrix} \right\|_{V^{-1}} \quad \text{subject to} \quad \hat{A}x = \hat{b}. \quad (4)$$

In [Ref 11, Section 4.3] this problem is called *weighted total least squares (WTLS)*. Closely related to the WTLS problem are the weighted low-rank approximation problem^{12,13} and the maximum likelihood principal component analysis problem.^{14,15}

As opposed to the weighted least squares problem, which is a trivial generalization of classical least squares, the WTLS problem does not have, in general, a closed form solution similar to the one of the TLS problem. The most general WTLS problem with analytic solution has a weight matrix of the form $V^{-1} = V_2^{-1} \otimes V_1^{-1}$, where \otimes is the Kronecker product, V_1 is $m \times m$, and V_2 is $(n + 1) \times (n + 1)$ (m is the number of equations and n is the number of unknowns in $Ax \approx b$). For general weight matrix, the problem can be solved by local optimization methods. However, there is no guarantee that a globally optimal solution will be found.

There are two main categories of local optimization methods for solving WTLS problems: alternating projections and variable projections.¹⁶ They are based on the observation that the constraint of the WTLS problem (4) is bilinear, which implies that the problem is linear in either x or \hat{A} and, therefore, can be solved globally and efficiently. Alternating projections is an iterative optimization algorithm that on each iteration step

1. solves a (linear) least squares problem in an $n \times (n + 1)$ extended parameter X_{ext} with \hat{A} fixed to the value obtained on the previous iteration step:

$$\min_{X_{\text{ext}}} \left\| \begin{bmatrix} A & b \end{bmatrix} - \hat{A}X_{\text{ext}} \right\|_{V^{-1}}, \quad (5)$$

2. solves a least squares problem in \hat{A} with X_{ext} fixed to the optimal value of Eq. (5)

$$\min_{\hat{A}} \left\| \begin{bmatrix} A & b \end{bmatrix} - \hat{A}X_{\text{ext}} \right\|_{V^{-1}}. \quad (6)$$

The parameter x is recovered from X_{ext} , as follows

$$x := X_{\text{ext},1}^{-1}x_{\text{ext},2},$$

$$\text{where } X_{\text{ext}} = \begin{bmatrix} \xrightarrow{n} & \xleftarrow{1} \\ X_{\text{ext},1} & x_{\text{ext},2} \end{bmatrix}. \quad (7)$$

In the statistical literature, the alternating projections algorithm is given the interpretation of *expectation maximization (EM)*. The problem of computing the optimal approximation \hat{A} given X_{ext} is the expectation step and the problem of computing X_{ext} , given \hat{A} is the maximization step of the EM procedure.

The variable projections method uses the closed-form solution of the expectation problem (6):

$$f(x) := \sqrt{d^T (V^{-1} - V^{-1}X_{\text{ext}}^T (X_{\text{ext}}V^{-1}X_{\text{ext}}^T)^{-1} X_{\text{ext}}V^{-1})d}, \quad (8)$$

where

$$d := \text{vec} \left(\begin{bmatrix} A & b \end{bmatrix} \right) \quad \text{and} \quad X_{\text{ext}} := \begin{bmatrix} I_n & x \end{bmatrix} \otimes I_m.$$

This is a projection of the rows of $\begin{bmatrix} A & b \end{bmatrix}$ on the subspace perpendicular to $\begin{bmatrix} x \\ -1 \end{bmatrix}$. The minimization over x is then an unconstrained nonlinear least squares problem $\min_x f(x)$, which can be solved by standard optimization methods, e.g., the Levenberg-Marquardt method.

Another generalization of the TLS problem (1) is to add constraints on the approximation matrix $\begin{bmatrix} \hat{A} & \hat{b} \end{bmatrix}$.¹⁷ Such constraints are needed in applications where the data matrix is structured and the approximation is required to have the same structure. For example, in signal processing the output y of a finite impulse response (FIR) system to an input u is given by multiplication of a Toeplitz matrix constructed from u by the vector of the impulse response samples. In an FIR system estimation problem, where both the input and the output are noisy, the approximation matrix is required to have Toeplitz structure for the result to have interpretation as a description of an FIR system.

Similar to the WTLS problems, in general, *structured total least squares (STLS)* problems¹¹ have no analytic solution in terms of the singular value decomposition (SVD) of the data matrix. Beck and Ben-Tal¹⁸ solved globally STLS problems with block-circulant structure by using the discrete Fourier transform and the solution of standard TLS problems. For other types of structure one has to resort to local optimization methods. In case of linearly structured problems, the constraint of the STLS optimization problem is bilinear, so that the alternating projections and variable projections methods, similar to the ones developed for the WTLS problem, can be used.

REGULARIZED AND TRUNCATED TOTAL LEAST SQUARES PROBLEMS

Linear approximation problems $Ax \approx b$ are considered ill-posed when small variations in the data A and b lead to large variations in the computed solution x . In the context of ordinary least squares, methods such as ridge regression, Tikhonov regularization¹⁹ or truncated SVD²⁰ are often employed to stabilize the computations. In recent years, several regularization formulations have also been explored in the context of the TLS problem. We distinguish between methods based on penalties/constraints, and methods based on truncation.

The basic idea of *regularized total least squares (RTLS)* is forcing an upper bound on a weighted 2-norm of the solution vector x (although other types of constraints can be envisaged). Several formulations have been considered. A first formulation is the quadratically constrained RTLS problem stated in Refs 21–24 as

$$\min_{x, \hat{A}, \hat{b}} \| [A \ b] - [\hat{A} \ \hat{b}] \|_F^2$$

$$\text{subject to } \hat{A}x = \hat{b}, \|Lx\|_2^2 \leq \delta^2, \quad (9)$$

or, equivalently,

$$\min_x \frac{\|Ax - b\|_2^2}{1 + \|x\|_2^2} \quad \text{subject to } \|Lx\|_2^2 \leq \delta^2, \quad (10)$$

where L is a p by n matrix, usually the identity matrix or a discrete difference operator, and δ is a given scalar value.

A second formulation adds a Tikhonov-like quadratic penalty term $\|Lx\|_2^2$ to the TLS objective function²⁵:

$$\min_x \frac{\|Ax - b\|_2^2}{1 + \|x\|_2^2} + \lambda \|Lx\|_2^2. \quad (11)$$

For δ^2 small enough (i.e., $\delta^2 < \|Lx^{\text{TLS}}\|_2^2$ where \hat{x}^{TLS} is the TLS solution), there exists a value of the parameter $\lambda > 0$ such that the solution of Eq. (10) coincides with the solution of Eq. (11). A sufficient condition for attainability of the minima in Eq. (10) or (11) is: $\sigma_{\min}([A \ N \ b]) < \sigma_{\min}(AN)$, where the columns of N form a basis for the nullspace of $L^T L$.^{22,24,25}

As opposed to classical regularization methods in the context of ordinary least squares, these formulations do not have closed-form solutions. Although local optimization methods are used in practice, the analysis in Refs 24,25 suggests that both formulations can be recast in a global optimization framework,

namely into scalar minimization problems, where each function evaluation requires the solution of a quadratically constrained linear least squares problem.²⁶

The constrained formulation (10) has been solved via a sequence of quadratic eigenvalue problems by Ref 22. Combining this approach with the nonlinear Arnoldi method and reusing information from all previous quadratic eigenvalue problems, a more efficient method for large RTLS problems has been proposed in Ref 27. Further, Renault and Guo²³ suggested an iterative method based on a sequence of linear eigenvalue problems, which has also been accelerated by solving the linear eigenproblems by the nonlinear Arnoldi method and by a modified root finding method based on rational interpolation.²⁸

For the quadratic penalty formulation (11), a complete analysis has been presented in Ref 25. A simple reformulation into a scalar minimization makes the problem more tractable:

$$\min_{\alpha} \mathcal{G}(\alpha), \text{ where } \mathcal{G}(\alpha) := \min_{\|x\|_2^2 = \alpha - 1} \left\{ \frac{\|Ax - b\|_2^2}{\alpha} + \lambda \|Lx\|_2^2 \right\}. \quad (12)$$

In Ref 29 another related formulation called dual RTLS is proposed. It minimizes the norm $\|Lx\|_2^2$ subject to compatibility of the corrected system, as well as to upper bounds on $\|A - \hat{A}\|_F$ and $\|b - \hat{b}\|_2$.

Truncation methods are another class of methods for regularizing linear ill-posed problems in the presence of measurement errors. In essence, they aim at limiting the contribution of noise or rounding errors by cutting off a certain number of terms in an SVD expansion. The *truncated total least squares* (TTLS) solution with truncation level k is the minimum 2-norm solution of $A_k x = b_k$, where $[A_k \ b_k]$ is the best rank- k approximation of $[A \ b]$. More precisely, if $U \Sigma V^T$ is the SVD of $[A \ b]$,

$$x^{\text{TTLS},k} = -V_{12}^k (V_{22}^k)^{\dagger} = -V_{12}^k (V_{22}^k)^T / \|V_{22}^k\|^2, \quad (13)$$

where we partition V as (with $l = n - k + 1$):

$$V = \begin{matrix} \xleftrightarrow{k} & \xleftrightarrow{l} \\ \begin{bmatrix} V_{11}^k & V_{12}^k \\ V_{21}^k & V_{22}^k \end{bmatrix} & \begin{matrix} \updownarrow n \\ \updownarrow 1 \end{matrix} \end{matrix} \quad (14)$$

The regularizing properties of truncated total least squares and a filter factor expansion of the TTLS solution have been described in Ref 30. Sima and Van Huffel³¹ showed that the filter factors associated with the TTLS solution provide more information for

choosing the truncation level compared with truncated SVD, where the filter factors are simply zeros and ones.

APPLICATIONS AND CURRENT TRENDS

Core problem: The concept of core problem in linear algebraic systems has been developed by Paige and Strakoš³². The idea is to find orthogonal P and Q such that

$$P^T [b \quad A Q] = \left[\begin{array}{c|c|c} b_1 & A_{11} & 0 \\ \hline 0 & 0 & A_{22} \end{array} \right]. \quad (15)$$

The block A_{11} is of full column rank, has simple singular values and b_1 has nonzero projections onto the left singular vectors of A_{11} . These properties guarantee that the subproblem $A_{11} x_1 \approx b_1$ has minimal dimensions and contains all necessary and sufficient information for solving the original problem $A x \approx b$. All irrelevant and redundant information is contained in A_{22} .

Low-rank approximation: TLS problems aim at approximate solutions of overdetermined linear systems of equations $A X \approx B$. Typical application of TLS methods, however, are problems for data approximation by linear models. Such problems are mathematically equivalent to low-rank approximation, which in turn is *not* equivalent to the $A X \approx B$ problem.⁴ This suggests that from a data modeling point of view, a low-rank approximation is a better framework than the solution of an overdetermined

linear system of equations. This viewpoint of the TLS data modeling approach is presented in Ref 3.

Application of STLS in system identification and model reduction is described in Refs 10,33,34. Further applications of STLS include the shape from moments problem,³⁵ approximate factorization and greatest common divisor computation in computer algebra,³⁶ and image deblurring.^{37,38} The WTLS problem has applications in chemometrics^{14,15} and machine learning.³⁹

Applications of RTLS: RTLS formulations, including weighted and structured generalizations, have been used in various ill-posed problems. A notorious inverse problem—blind deconvolution of one- or two-dimensional data—has received special attention. Restoring one-dimensional signals from noisy measurements of both the point-spread function and the observed data has been addressed by Refs 40,41 as a regularized structured TLS problem. A two-dimensional generalization has been used for image restoration in Ref 42. Interesting structured regularized problem formulations and efficient algorithms for image deblurring are analyzed in Refs 37,38,43–48. RTLS has also been used in image reconstruction of electrical capacitance tomography.⁴⁹

Applications of TTLS: TTLS has successfully been applied to biomedical inverse problems such as the reconstruction of epicardial potentials from body surface potentials⁵⁰ and imaging by ultrasound inverse scattering.⁵¹ TTLS is also used as an alternative to ridge regression in the estimation step of the regularized EM algorithm for the analysis of incomplete climate data.⁵²

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