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.

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

\[
\hat{x}_{\text{tls}} = \arg \min_{x, \hat{A}, \hat{b}} \| [A \ b] - [\hat{A} \ \hat{b}] \|_F \\
\text{subject to } \hat{A}x = \hat{b}
\]

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

\[
A = \bar{A} + \tilde{A}, \quad b = \bar{b} + \tilde{b}, \quad \bar{A}x = \bar{b},
\]

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

\[
\text{vec}([\tilde{A} \ \tilde{b}]) = 0 \quad \text{and} \quad \text{cov} \left( \text{vec} \left( [\tilde{A} \ \tilde{b}] \right) \right) = \sigma^2 I.
\]

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

\[
\| \Delta D \|_{V^{-1}} := \sqrt{\text{vec}^T(\Delta D) V^{-1} \text{vec}(\Delta D)}
\]
i.e.,

$$\min_{x, \hat{A}, \hat{b}} \| [A \ b] - [\hat{A} \ \hat{b}] \|_{V^{-1}} \quad \text{subject to} \quad \hat{A}x = \hat{b}. \quad (4)$$

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\textsuperscript{12,13} and the maximum likelihood principal component analysis problem.\textsuperscript{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 $V^{-1} = V_1^{-1} \otimes V_2^{-1}$, 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.\textsuperscript{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 $X_{\text{ext}}$ with $\hat{A}$ fixed to the value obtained on the previous iteration step:

   $$\min_{X_{\text{ext}}} \| [A \ b] - \hat{A}X_{\text{ext}} \|_{V^{-1}}, \quad (5)$$

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

   $$\min_{\hat{A}} \| [A \ b] - \hat{A}X_{\text{ext}} \|_{V^{-1}}. \quad (6)$$

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

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

where

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

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 $X_{\text{ext}}$ is the expectation step and the problem of computing $X_{\text{ext}}$, 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):

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

where

$$d := \text{vec}([A \ b]) \quad \text{and} \quad X_{\text{ext}} := [I_n \ x] \otimes I_m.$$
REFS 21–24 AS QUADRATICALLY CONSTRAINED RTLS PROBLEM STATED IN
HAVE BEEN CONSIDERED. A FIRST FORMULATION IS THE
OF CONSTRAINTS CAN BE ENVISAGED). SEVERAL FORMULATIONS
OR A DISCRETE DIFFERENCE OPERATOR, AND
QUADRATIC PENALTY TERM VALUE.

2-NORM OF THE SOLUTION VECTOR
IS FORCING AN UPPER BOUND ON A WEIGHTED
(RTLS) FUNCTION25:

FUNCTION25: BASED ON PENALTIES/CONSTRAINTS, AND METHODS BASED ON
TRUNCATION. 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 ENVSAGED). SEVERAL FORMULATIONS
HAVE BEEN CONSIDERED. A FIRST FORMULATION IS THE
QUADRATICALLY CONSTRAINED RTLS PROBLEM STATED IN
REFS 21–24 AS

\[ \min_{x,A,b} \| [A \ b] - \begin{bmatrix} \hat{A} \\ \hat{b} \end{bmatrix} \|_F^2 \]
SUBJECT TO \( \hat{A}x = \hat{b} \), \( \| Lx \|_2^2 \leq \delta^2 \),

(9)
OR, EQUIVALENTLY,

\[ \min_x \frac{\| Ax - b \|_2^2}{1 + \| x \|_2^2} \quad \text{SUBJECT TO } \| Lx \|_2^2 \leq \delta^2, \]

(10)
WHERE L IS A P BY N MATRIX, USUALLY THE IDENTITY MATRIX
OR A DISCRETE DIFFERENCE OPERATOR, AND \( \delta \) IS A GIVEN SCALAR
VALUE.

A SECOND FORMULATION ADDS A TIKHONOV-LIKE QUADRATIC PENALTY TERM \( \| Lx \|_2^2 \) TO THE TLS OBJECTIVE FUNCTION25:

\[ \min_x \frac{\| Ax - b \|_2^2}{1 + \| x \|_2^2} + \lambda \| Lx \|_2^2. \]

(11)
FOR \( \delta^2 \) SMALL ENOUGH (I.E., \( \delta^2 < \| Lx_{TLS} \|_2^2 \) WHERE \( x_{TLS} \) IS THE TLS SOLUTION), THERE EXISTS A VALUE OF THE PARAMETER \( \lambda > 0 \) SUCH THAT THE SOLUTION OF EQUATION (10) COINCIDES WITH THE SOLUTION OF EQUATION (11). A SUITABLE CONDITION FOR ATTAINABILITY OF THE MINIMA IN EQUATION (10) OR (11) IS:

\[ \sigma_{\min}([A \ N \ b]) < \sigma_{\min}(A) \]
WHERE THE COLUMNS OF N FORM A BASIS FOR THE NULLSPACE OF \( L^T \).

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 RECasted 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, RENAUT 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:

\[ \min_{\alpha} G(\alpha), \text{ WHERE } G(\alpha) := \min_{\| x \|_2^2 = \alpha^{-1}} \left\{ \frac{\| Ax - b \|_2^2}{\alpha} + \lambda \| Lx \|_2^2 \right\}. \]

(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 \( Ax = b_k \), 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],

\[ x_{TTLS,k} = -V_k^k (V_k^k)^T \| V_k^k \|_2^2, \]

WHERE WE PARTITION V AS (WITH L = N – K + 1):

\[ V = \begin{bmatrix} V_{11}^k & V_{12}^k \\ V_{21}^k & V_{22}^k \end{bmatrix} \]

(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 Strakoš. The idea is to find orthogonal $P$ and $Q$ such that

$$
P^\top \begin{bmatrix} b & A \end{bmatrix} Q = \begin{bmatrix} b_1 & A_{11} & 0 \\ 0 & 0 & A_{22} \end{bmatrix}.
$$

(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 $Ax \approx b$. 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 $AX \approx B$. 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 $AX \approx B$ problem. 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, approximate factorization and greatest common divisor computation in computer algebra, and image deblurring. The WTLS problem has applications in chemometrics and machine learning.

**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.

**Applications of TTLS:** TTLS has successfully been applied to biomedical inverse problems such as the reconstruction of epicardial potentials from body surface potentials and imaging by ultrasound inverse scattering. 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.

**ACKNOWLEDGEMENTS**

Diana Sima is postdoctoral fellow of FWO (Fund for Scientific Research-Flanders). Research supported by Research Council KUL: GOA MaNet, CoE EF/05/006 Optimization in Engineering (OPTEC), Belgian Federal Science Policy Office IUAP P6/04 (DYSCO), and PinView (Personal Information Navigator adapting through VIEWing), an EU FP7 funded Collaborative Project 216529.

**REFERENCES**


**FURTHER READING**

