Faculty of Mechatronics and
Interdisciplinary Engineering Studies
Technical University of Liberec, Liberec

Institute of Computer Science
Academy of Sciences of the Czech Republic, Prague

The Total Least Squares Problem and Reduction of Data in $AX \approx B$

Martin Plešinger

Report of the PhD Thesis, March 2008

Report of the PhD Thesis
The Total Least Squares Problem and Reduction of Data in $A\,X \approx B$

Author:	Martin Plešinger (`martin.plesinger@tul.cz`, `mata@cs.cas.cz`)
Supervisor:	Zdeněk Strakoš (`strakos@cs.cas.cz`)
Study programme:	P2612 Electrotechnics and informatics
Field of study:	3901V025 Science engineering
Departments:	Faculty of Mechatronics and Interdisciplinary Engineering, Institute of Novel Technologies and Applied Informatics, Technical University of Liberec, Studentská 2, 461 17 Liberec 1, Czech Republic
and	Institute of Computer Science, Department of Computational Methods, Academy of Sciences of the Czech Republic, Pod Vodárenskou věží 2, 182 07 Prague 8, Czech Republic

Typeset by $\mathcal{AMS}$–LaTeX.

Abstract

The presented thesis focuses on the solution of an orthogonally invariant linear approximation problem with multiple right-hand sides $AX \approx B$ through the *total least squares (TLS)* concept. With contribution of the early works of Golub and Reinsch (1970), Golub (1973), and van der Sluis (1975), the TLS theory for a problem with a single right-hand side was developed by Golub and Van Loan (1980). Then it was further extended by the so called *nongeneric solution* approach of Van Huffel and Vandewalle (1991), and finally revised by the *core problem theory* of Paige and Strakoš (2002, 2006). For a problem with multiple right-hand sides, a generalization of the TLS concept including a nongeneric solution was presented by Van Huffel and Vandewalle (1991).

Paige and Strakoš proved that for a problem with a single right-hand side, i.e., $Ax \approx b$, there is a reduction based on the singular value decomposition (SVD) of A which determines a *core problem* $A_{11}\, x_1 \approx b_1$, with all necessary and sufficient information for solving the original problem. The core problem always has the unique TLS solution, and, using the transformation to the original variables, it gives the solution of the original approximation problem identical to the minimum 2-norm solutions of all TLS formulations given by Van Huffel and Vandewalle. Moreover, the core problem can be efficiently computed using the (partial) upper bidiagonalization of the matrix $[\, b \,|\, A \,]$. Hnětynková, Plešinger and Strakoš (2006, 2007) derived, using the well known properties of Jacobi matrices, the core problem formulation from the relationship between the Golub-Kahan bidiagonalization and the Lanczos tridiagonalization.

This thesis extends the classical analysis by Van Huffel and Vandewalle. It starts with an investigation of the necessary and sufficient conditions for the existence of the TLS solution. It is shown that the TLS solution is in some cases different from the output returned by the *TLS algorithm* by Van Huffel (1988), see also Van Huffel, Vandewalle (1991). The second goal of the presented thesis is an extension of the core problem theory concept to problems with multiple right-hand sides. Here the SVD-based reduction is related to the band generalization of the Golub-Kahan bidiagonalization algorithm, which was for this purpose for the first time considered by Björck (2005) and Sima (2006). We prove that the reduction results in a minimally dimensioned subproblem $A_{11}\, X_1 \approx B_1$, containing all necessary and sufficient information for solving the original problem. Unlike in the single right-hand side case, the core problem in the multiple right-hand side case may not have a TLS solution.

Keywords: linear approximation problem, multiple right-hand sides, total least squares, orthogonal transformation, data reduction, Golub-Kahan bidiagonalization algorithm, Jacobi matrices, core problem.

Abstrakt

Předkládaná disertační práce se zabývá řešením lineárních aproximačních úloh s vícenásobnou pravou stranou $A\,X \approx B$ metodou *úplných nejmenších čtverců (TLS z anglického total least squares)*. Analýza TLS problému pro úlohu s jednou pravou stranou byla, v návaznosti na dřívější práce Goluba a Reinsche (1970), Goluba (1973) a van der Sluise (1975), publikována v článku Goluba a Van Loana (1980). Tato analýza byla později rozšířena o koncept *negenerického řešení*, který zavádějí Van Huffel a Vandewalle (1991). Zcela nový vhled do teorie přináší myšlenka *core problému* Paige a Strakoše (2002, 2006). Zobecněním TLS problému na úlohy s více pravými stranami, včetně konceptu negenerického řešení, se jako první zabývali Van Huffel a Vandewalle (1991).

Paige a Strakoš dokázali za přirozeného předpokladu ortogonální invariance, tedy nezávislosti řešení na volbě souřadného systému, že pro libovolný problém s jednou pravou stranou $A\,x \approx b$ existuje transformace zkonstruovaná pomocí singulárního rozkladu matice A, která redukuje původní problém na tak zvaný *core problém* $A_{11}\,x_1 \approx b_1$, obsahující nutnou a postačující informaci k řešení původního problému. Dále ukázali, že core problém má vždy nezávisle na původních datech řešení ve smyslu TLS a toto řešení je jednoznačné. Navíc TLS řešení core problému transformované zpět do proměnných původního problému je identické s příslušným (klasickým nebo negenerickým) v normě minimálním řešením původního problému. Redukce na core problém může být provedena velmi jednoduše transformací matice $[\,b\,|A\,]$ na horní bidiagonální tvar. Hnětynková, Plešinger a Strakoš (2006, 2007) odvodili vlastnosti core problému alternativně pomocí vlastností Jakobiho matic a užitím vztahu mezi Golubovou-Kahanovou bidiagonalizací a Lanczosovou tridiagonalizací.

Předkládaná práce rozšiřuje klasické výsledky Van Huffelové a Vandewalleho pro úlohy s násobnou pravou stranou. Zabývá se analýzou nutných a postačujících podmínek existence TLS řešení. Práce ukazuje, že v některých zvláštních případech může mít TLS problém řešení, které je však různé od výsledku spočteného tak zvaným *TLS algoritmem*, viz Van Huffel (1988), případně Van Huffel, Vandewalle (1991). Dále se práce zabývá rozšířením myšlenky core problému na úlohy s vícenásobnou pravou stranou. Zobecňuje redukci dat založenou na singulárním rozkladu a zabývá se jejím vztahem k pásovému zobecnění Golubova-Kahanova bidiagonalizačního algoritmu, které bylo pro tento účel prvně doporučeno Björckem (2005) a Simou (2006). Ukážeme, že pro libovolné $A\,X \approx B$ existuje transformace, která původni problém redukuje na podproblém $A_{11}\,X_1 \approx B_1$ minimální dimenze, obsahující nutnou a postačující informaci k řešení původního problému. Ukážeme však, že na rozdíl od úloh s jednou pravou stranou core problém pro úlohy s více pravými stranami obecně nemusí mít TLS řešení.

Klíčová slova: lineární aproximační problém, vícenásobná pravá strana, úplný problém nejmenších čtverců, ortogonální transformace, redukce dat, Golubova-Kahanova bidiagonalizace, Jakobiho matice, core problém.

Contents

Chapter 1

Introduction

We are interested in the linear approximation problem

$$A\,x \,\approx\, b\,, \qquad A \in \mathbb{R}^{m\times n}\,, \quad x \in \mathbb{R}^{n}\,, \quad b \in \mathbb{R}^{m}\,, \tag{1.1}$$

and its more general form

$$A\,X \,\approx\, B\,, \qquad A \in \mathbb{R}^{m\times n}\,, \quad X \in \mathbb{R}^{n\times d}\,, \quad B \in \mathbb{R}^{m\times d}\,. \tag{1.2}$$

Such linear approximation problems arise in a broad class of scientific and technical areas, for example in medical image deblurring (tomography), bioelectrical inversion problems, geophysics (seismology, radar or sonar imaging), astronomical observations. This thesis mainly focuses on the total least squares (TLS) formulation of (1.1), (1.2) that leads to a procedure that has been independently developed in various literature. It has been known by various names, for example, it is known as the *errors-in-variables modeling* in the statistical literature, see [23, 24, 25].

There exist a lot of approaches that are closely related to the TLS concept. For example, an additional difficulty appears when the system (1.1), (1.2) is *ill-posed*, here the matrix A is ill conditioned and typically a small perturbation of right-hand side causes large changes in the estimated solution. The matrix A is often numerically rank deficient and it has small singular values, but without a well defined numerical rank (singular values decay gradually without noticeable gap). In such cases the least squares (LS), the TLS or similar techniques might give a solution that is absolutely meaningless, because it is dominated by errors present in the data and possibly also by computational (rounding) errors. The *regularization techniques* must be used in order to obtain a meaningful solution, see for example [9, 11].

Model reduction represents another important area of applications. Here the matrix A represents a model and the vector b or columns of the matrix B represent the observation vectors, e.g. measured data, that naturally contain errors. The idea is to approximate the high order system (1.1) or (1.2) by a lower order one while approximating well the behavior of the whole system. Truncation and projection techniques used to reduce the dimensions of the linear system may also be viewed as a type of regularization. Such methods are, for example the *truncated-least squares (T-LS)* also called the *truncated-singular value decomposition (T-SVD)*, the *truncated-total least squares (T-TLS)*, see [19], or Krylov subspace methods and Lanczos-type processes [4]. The system (1.2) can in such applications contain significantly more observations (columns of B) than is the dimension of range of A, or the number of columns of A, i.e. $d \gg n$; similar situation can occur in various statistical applications.

The systems (1.1), (1.2) can be compatible, i.e., $b \in \mathcal{R}(A)$, $\mathcal{R}(B) \subset \mathcal{R}(A)$, or incompatible, i.e., $b \notin \mathcal{R}(A)$, $\mathcal{R}(B) \not\subset \mathcal{R}(A)$. The compatible case is simpler because it reduces to finding a solution of the system of linear algebraic equations. Thus here the incompatible case is often considered. Another uninteresting case is excluded by the assumption $A^T b \neq 0$ or $A^T B \neq 0$. In this case it is meaningless to approximate b or columns of B by the columns of A and the systems (1.1), (1.2) have trivial solutions $x = 0$ or $X = 0$, respectively. In particular we assume a nonzero matrix A and a nonzero right-hand side vector b or matrix B. We assume for simplicity only the real case, an extension to the complex data being straightforward.

Since the incompatible problem does not have a solution in the classical meaning, the solution is obtained by solving a minimization (optimization) problem. It is senseful to assume orthogonally (unitarily) invariant minimization problems, i.e. problems such that their solutions do not depend on the particular choice of bases in $\mathbb{R}^m$, $\mathbb{R}^n$ and $\mathbb{R}^d$ in (1.1) or (1.2). In other words, when the original problem is transformed to another basis, this transformed problem is solved, and its solution is transformed back to the original basis, then this back-transformed solution is identical to the solution obtained directly from solving original problem.

1.1 TLS problem

Various orthogonally invariant minimization techniques can be used for solving the linear approximation problems. The thesis focuses on the *total least squares (TLS)* concept. In the TLS also called *orthogonal regression* the correction is allowed to compensate for errors in the system (data) matrix A as well as in the vector of observations b. Thus in TLS, E and g are sought to minimize the Frobenius norm in

$$\min_{x,E,g} \| \, [\; g \,\big|\, E \;] \, \|_F \qquad \text{subject to} \qquad (A+E)\,x \,=\, b+g\,, \tag{1.3}$$

i.e., $(b+g) \in \mathcal{R}(A+E)$. In this section the theory of solving the TLS problems with single right-hand sides is summarized. For better explanation and understanding of presented theory including detailed proofs we refer to [6, 23].

In the whole section we consider $A^T b \neq 0$, in particular $A \neq 0$, $b \neq 0$. First, it is worth to note that the TLS problem may not have a solution for a given data A, b, see, e.g., [6]. In such cases without the TLS solution, when we try to reach the greatest lower bound of the norm of the correction, the corresponding nonoptimal solution grows to infinity (in norm) and contains components with arbitrary values.

Golub and Van Loan give in [6] a sufficient condition for existence of a TLS solution. Consider an orthogonally invariant linear approximation problem (1.1). In order to simplify the notation assume that $m > n$ (add zero rows if necessary). Denote $\sigma'_j \equiv \sigma_j(A)$ the jth largest singular value of A, and u'_j and v'_j the corresponding left and right singular vectors, respectively, $j = 1, \ldots, n$. Further denote $\sigma_j \equiv \sigma_j([\, b \,|\, A \,])$ the jth largest singular value of $[\, b \,|\, A \,]$, and u_j and v_j the corresponding left and right singular vectors, respectively, $j = 1, \ldots, n+1$.

Let A be of full column rank (i.e. $\sigma'_n > 0$ and, subsequently, $\sigma_{n+1} = 0$ iff the system (1.1) is compatible) and let σ_{n+1} be simple. Define the *correction matrix* $[\, g \,|\, E \,] \equiv -\, u_{n+1}\, \sigma_{n+1}\, v_{n+1}^T$, $\|[\, g \,|\, E \,]\|_F = \|[\, g \,|\, E \,]\| = \sigma_{n+1}$. The *corrected matrix* $[\, b+g \,|\, A+E \,]$ represents, by Eckart-Young-Mirsky theorem (see [23, Theorem 2.3, p. 31]), the unique best rank n approximation of $[\, b \,|\, A \,]$ in the Frobenius norm (and also in the 2-norm). Since σ_{n+1} is simple, the correction as well as the corrected matrices are unique. The right singular vector v_{n+1} represents a basis of the null space of the corrected matrix, i.e. $[\, b+g \,|\, A+E \,]\, v_{n+1} = 0$.

If the first component of the vector v_{n+1} is nonzero, i.e. $\gamma \equiv e_1^T v_{n+1} \neq 0$, then scaling v_{n+1} such that the first component is equal to -1 gives

$$\left[\frac{-1}{x_{\mathrm{TLS}}}\right] \equiv -\frac{1}{\gamma} v_{n+1}, \qquad \text{and} \qquad \left[\; b+g \;\middle|\; A+E \;\right] \left[\frac{-1}{x_{\mathrm{TLS}}}\right] = 0 .$$

Because σ_{n+1} is simple, the corrected and the correction matrices are unique, thus the vector x_{TLS} represents the *unique TLS solution* of the problem (1.3). If the first component of the vector v_{n+1} is zero, i.e. $\gamma \equiv e_1^T v_{n+1} = 0$, then the TLS problem (1.3) does not have a solution, see also [6, 23].

Golub and Van Loan give in [6] a sufficient condition

$$\sigma'_n > \sigma_{n+1} , \tag{1.4}$$

for the existence of the TLS solution. See [6], see also [22], or [18, p. 203], [23, proof of Lemma 3.1, pp. 64–65]. The condition (1.4) ensures that the smallest singular value of the extended matrix $[\,b\,|\,A\,]$ is simple and the corresponding right singular vector has nonzero first component, and, subsequently, it ensures existence of the TLS solution. This condition is, however, intricate because it is only sufficient *but not necessary* for the existence of a TLS solution. (In fact, the condition (1.4) is necessary and sufficient for the existence of the *unique* TLS solution.) If $\sigma'_n = \sigma_{n+1}$, then it may happen either $\sigma_n > \sigma_{n+1}$ with $e_1^T v_{n+1} = 0$, which means that the TLS problem does not have a solution, or $\sigma_n = \sigma_{n+1}$. In this case a TLS solution still may exist or may not exist. Thus, now we focus on the case when the smallest singular value of $[\,b\,|\,A\,]$ is multiple, i.e. $\sigma_n = \sigma_{n+1}$.

Now, let A be of full column rank and let σ_{n+1} be multiple. In particular there is an integer p such that

$$\sigma_p > \sigma_{p+1} = \ldots = \sigma_{n+1} .$$

The case $p = n$ reduces to the previous case. If $p = 0$, i.e. $\sigma_1 = \ldots = \sigma_{n+1}$, then $[\,b\,|\,A\,]^T [\,b\,|\,A\,] = \sigma_1^2 I_{n+1}$, and thus the columns of $[\,b\,|\,A\,]$ are mutually orthogonal (and σ_p is nonexistent). In this case the TLS problem has a nonunique solution, and from the construction below it will be clear that the minimum 2-norm TLS solution is trivial, $x_{\mathrm{TLS}} = 0$. Therefore for simplification of notation we consider $0 < p < n$ in the further text.

Since σ_{n+1} is multiple, a minimal correction matrix reducing the rank of $[\,b\,|\,A\,]$ to n is no longer unique. For an arbitrary given matrix $Q \in \mathbb{R}^{(n-p+1)\times(n-p+1)}$, $Q^{-1} = Q^T$, denote $\tilde{v} \equiv [\,v_{p+1}, \ldots, v_{n+1}\,]\, Q\, e_{n-p+1}$, a unit vector from the right singular vector subspace associated with σ_{n+1}, and $\tilde{u} \equiv [\,u_{p+1}, \ldots, u_{n+1}\,]\, Q\, e_{n-p+1}$, the corresponding unit vector from the left singular vector subspace. The matrix $[\,g\,|\,E\,] \equiv -\tilde{u}\,\sigma_{n+1}\,\tilde{v}^T$, $\|[\,g\,|\,E\,]\|_F = \|[\,g\,|\,E\,]\| = \sigma_{n+1}$, represents, by Eckart-Young-Mirsky theorem, a minimal norm correction such that $[\,b+g\,|\,A+E\,]$ is a rank n approximation of $[\,b\,|\,A\,]$. Because Q is arbitrary, the correction as well as the corrected matrices are not unique.

Similarly to the previous section, if $e_1^T \tilde{v} \neq 0$, then $\tilde{v}$ can be used for the construction of a solution of the TLS problem (1.3), by scaling $\tilde{v}$ such that the first component is equal to -1. Consequently, if there exists a vector with nonzero first component in the subspace $\mathcal{R}\,([\,v_{p+1}, \ldots, v_{n+1}\,])$, i.e. if $e_1^T\,[\,v_{p+1}, \ldots, v_{n+1}\,] \neq 0$, then the TLS problem (1.3) has a solution, but, clearly, this solution is not unique. The goal is to find the *minimum 2-norm TLS solution*.

Denote $\tilde{v} = (\,\tilde{\gamma}\,,\, w^T\,)^T$; the norm of the solution constructed from $\tilde{v}$ is equal to $\tilde{\gamma}^{-1}\,\|w\|$, where $\|w\|^2 = \|\tilde{v}\|^2 - \tilde{\gamma}^2 = 1 - \tilde{\gamma}^2$. Thus the goal is to minimize $\tilde{\gamma}^{-1}\,(1-\tilde{\gamma}^2)^{1/2}$, i.e., to maximize $\tilde{\gamma}$. The minimum 2-norm TLS solution is obtained by choosing Q such that the first component of $\tilde{v}$ is maximal over all unit vectors in $\mathcal{R}([\, v_{p+1}\,, \ldots, \, v_{n+1}\,])$. Put $Q \equiv H$, the Householder reflection matrix such that $e_1^T\,[\, v_{p+1}\,, \ldots, \, v_{n+1}\,]\, H = [\, 0\,, \ldots, \, 0\,, \gamma\,]$, where $\gamma \equiv e_1^T\,[\, v_{p+1}\,, \ldots, \, v_{n+1}\,]$, and put $v \equiv [\, v_{p+1}\,, \ldots, \, v_{n+1}\,]\, H\, e_{n-p+1}$. Scaling v gives the minimum 2-norm TLS solution

$$\left[\frac{-1}{x_{\mathrm{TLS}}}\right] \equiv -\,\frac{1}{\gamma}\,\left[\; v_{p+1}\,, \ldots, \, v_{n+1}\;\right] H\, e_{n-p+1} = -\,\frac{1}{\gamma}\, v\,,$$

with $\|x_{\mathrm{TLS}}\| = \gamma^{-1}\,(1-\gamma^2)^{1/2}$. If all (unit) vectors in $\mathcal{R}([\, v_{p+1}\,, \ldots, \, v_{n+1}\,])$ have zero first components, i.e. if $e_1^T\,[\, v_{p+1}\,, \ldots, \, v_{n+1}\,] = 0$, then the TLS problem (1.3) does not have a solution, see also [6, 23].

Van Huffel and Vandewalle give in [23] an equivalence which generalizes the Golub, Van Loan condition (1.4) for the existence of a TLS solution. See [23, Corollary 3.4, p. 65].

As already mentioned, an unpleasant situation occurs when the right singular vector subspace associated with the smallest singular value σ_{n+1} of $[\, b \,|\, A\,]$ does not contain a vector with nonzero first component. This situation is provided by the fact that the correlation between columns of the matrix A is stronger than the correlation between the column space of A and the right-hand side b. In such case there is no right singular vector that can be used for construction of a solution.

The idea of the so called nongeneric concept is the following, see [23]: because the solution can not be constructed from a vector corresponding to the smallest singular value, we try to use another, bigger, singular value and the corresponding left and right singular vectors for construction of a correction matrix and a solution. But, such a solution does not solve the original TLS problem (1.3).

Recall that we still assume $A^T b \neq 0$ and $m > n$. Let $\sigma_t > \sigma_{n+1}$ be the smallest singular value of $[\, b \,|\, A\,]$ such that $e_1^T\, v_t \neq 0$, i.e. $e_1^T\,[\, v_{t+1}\,, \ldots, \, v_{n+1}\,] = 0$ (this case includes all incompatible problems with rank deficient A, as mentioned). Since $V \equiv [\, v_1\,, \ldots, \, v_{n+1}\,]$ is an orthogonal matrix, such a singular value always exists. Put $[\, g \,|\, E\,] \equiv u_t\, \sigma_t\, v_t^T$, $\|[\, g \,|\, E\,]\|_F = \|[\, g \,|\, E\,]\| = \sigma_t$. Similarly to the previous cases $[\, b+g \,|\, A+E\,]\, v_t = 0$ and thus scaling the vector v_t such that the first component is equal to -1 gives the solution of the corrected system. This solution is in [23] called *nongeneric solution.*

Obviously, if $\sigma_{t-1} = \sigma_t$ (with $t > 1$) or $\sigma_t = \sigma_{t+1}$ (with $t < n$), then the correction as well as the solution are not unique. In the case of nonuniqueness the goal is to find the *minimum 2-norm nongeneric solution.* In order to handle a possible nonuniqueness define an integer $\tilde{p}$ such that

$$\sigma_{\tilde{p}} > \sigma_{\tilde{p}+1} = \ldots = \sigma_t \geq \ldots \geq \sigma_p > \sigma_{p+1} = \ldots = \sigma_{n+1}\,.$$

If $\tilde{p} = 0$, then it can be shown that the right-hand side b is orthogonal to the column space of A, and from the construction below it will be clear that the minimum 2-norm nongeneric solution becomes trivial, $x_{\mathrm{NGN}} = 0$ (and $\sigma_{\tilde{p}}$ is nonexistent).

Similarly to the case with nonunique solution there exists a Householder reflection matrix such that $e_1^T\,[\, v_{p+1}\,, \ldots, \, v_{n+1}\,]\, H = [\, 0\,, \ldots, \, 0\,, \gamma\,]$, where $\gamma \equiv e_1^T\,[\, v_{p+1}\,, \ldots, \, v_{n+1}\,]$. Further put $u \equiv [\, u_{\tilde{p}+1}\,, \ldots, \, u_{n+1}\,]\, H\, e_{n-\tilde{p}+1}$, and $v \equiv [\, v_{\tilde{p}+1}\,, \ldots, \, v_{n+1}\,]\, H\, e_{n-\tilde{p}+1}$. The matrix $[\, g \,|\, E\,] \equiv -\, u\, \sigma_t\, v^T$ has Frobenius norm (and also the 2-norm) equal to σ_t. Scaling v such that the first component is equal to -1 gives the minimum 2-norm nongeneric solution

$$\left[\frac{-1}{x_{\mathrm{NGN}}}\right] \equiv -\,\frac{1}{\gamma}\,\left[\; v_{\tilde{p}+1}\,, \ldots, \, v_{n+1}\;\right] H\, e_{n-\tilde{p}+1} = -\,\frac{1}{\gamma}\, v\,,$$

see [23].

Now, we already described all the possibilities that can occur. It remains to justify the addition of zero rows in (1.1) in order to satisfy the condition $m > n$, and to show that the incompatible problem with rank deficient matrix A does not have a TLS solution. Both can be easily shown through the core problem concept.

1.2 Core problem theory of Paige and Strakoš

Assuming $A^T b \neq 0$ and that the approximation problem (1.1) is orthogonally invariant, i.e. that the solution is independent on a particular choice of bases in $\mathbb{R}^m$ and $\mathbb{R}^n$, it easy to see that there exists an orthogonal transformation of the form

$$P^T \left[\, b \mid A \,\right] \left[\begin{array}{c|c} 1 & 0 \\ \hline 0 & Q \end{array}\right] = P^T \left[\, b \mid A\,Q \,\right] = \left[\begin{array}{c||c|c} b_1 & A_{11} & 0 \\ \hline 0 & 0 & A_{22} \end{array}\right], \qquad (1.5)$$

where $P^{-1} = P^T$, $Q^{-1} = Q^T$, and where A_{22} might have row and/or column dimensions equal to zero. In the nontrivial case (when A_{22} has at least one row and one column, even if $A_{22} = 0$) both the singular value decompositions (SVD) of $[\,b \,|\, A\,]$ and A can be easily got as a direct sum of the SVDs of the blocks $[\,b_1 \,|\, A_{11}\,]$ and A_{22}, and A_{11} and A_{22}, respectively. The original approximation problem $A\,x \approx b$ is in this way decomposed into two *independent* approximation subproblems,

$$A_{11}\,x_1 \approx b_1\,, \qquad A_{22}\,x_2 \approx 0\,, \qquad \text{where} \qquad x \equiv Q \left[\begin{array}{c} x_1 \\ \hline x_2 \end{array}\right].$$

The second subproblem $A_{22}\,x_2 \approx 0$ has a trivial solution $x_2 = 0$, and thus only the first subproblem $A_{11}\,x_1 \approx b_1$ needs to be solved, see [17]. Paige and Strakoš formulate the following definition.

Definition 1.1 (Core problem)**.** *The subproblem $A_{11}\,x_1 \approx b_1$ is a core problem within the approximation problem $A\,x \approx b$ if $[\,b_1 \,|\, A_{11}\,]$ is minimally dimensioned (and A_{22} maximally dimensioned) subject to (1.5).*

For any transformation (1.5) the subproblem $A_{11}\,x_1 \approx b_1$ contains all the sufficient information for solving the original problem. Since the core problem is the minimally dimensioned subproblem, i.e. the subproblem can not be reduced more, it must contain all the sufficient and only the necessary information for solving $A\,x \approx b$.

Understanding of the minimal dimensionality of $A_{11}\,x_1 \approx b_1$ can be gained by the following construction, which shows how to concentrate the relevant information into A_{11} and b_1, while moving the irrelevant and redundant information into A_{22}, see [17]. Let A have rank r and consider the SVD of $A = U'\,\Sigma'\,(V')^T$, $\Sigma' \equiv \mathrm{diag}\,(\,\Xi\,,\,0\,)$, $\Xi \equiv \mathrm{diag}\,(\,\sigma'_1\,,\,\ldots\,,\,\sigma'_r\,)$. Moreover assume only k of the nonzero singular values of A to be distinct. Consider $(U')^T b = [\,c_1^T\,,\,\ldots\,,\,c_k^T \,|\, c_{k+1}^T\,]^T$ the partitioning with respects to the multiplicities of the singular values of A.

The singular values are unique in any SVD representation. But their ordering, and sometimes some singular vectors, are not unique. In order to obtain the core problem, the matrix $(U')^T\,[\,b \,|\, A\,V'\,]$ will be transformed further, while maintaining the SVD of A. For c_j, choose an orthogonal matrix H_j (e.g. the Householder reflection matrix) such that $H_j\,c_j = e_1\,\delta_j$, where $\delta_j \equiv \|c_j\|$, for $j = 1\,,\,\ldots\,,\,k\,,\,k+1$. Then put $G \equiv \mathrm{diag}\,(\,H_1\,,\,\ldots\,,\,H_k\,,\,H_{k+1}\,)$, $H \equiv \mathrm{diag}\,(\,H_1\,,\,\ldots\,,\,H_k\,,\,I_{n-r}\,)$, and replace the matrix U' by $U'\,G$ and V' by $V'\,H$. This transformation will leave Σ' unchanged and therefore preserves the SVD of A. In this way the vector c is transformed into a vector having at most one nonzero component corresponding to each block of equal singular values of A, and therefore the original right-hand side vector b is transformed into a vector having at most $k+1$ nonzero entries. Clearly,

$\delta_j \neq 0$, $j = 1, \ldots, k$, if and only if the right-hand side b has nonzero projection onto the corresponding left singular vector subspace of A (i.e., $\delta_1 = \ldots = \delta_k = 0$ iff $b \perp \mathcal{R}$), and finally $\delta_{k+1} \neq 0$ iff $b \notin \mathcal{R}(A)$. Next permute the columns of $U' G$ and $V' H$ identically, in order to move the zero elements in the transformed c to the bottom of this vector, leaving d, the subvector of c with nonzero components only, at the top, while keeping Ξ diagonal. Finally if $\delta_{k+1} \neq 0$ move its row so that δ_{k+1} is immediately below d by a further permutation from the left to give, with obvious new notation and indexing,

$$(U' G \Pi_L)^T \left[\, b \,\middle|\, A (V' H \Pi_R) \,\right] = \left[\begin{array}{c||c|c} d & \Xi_1 & 0 \\ \delta_{k+1} & 0 & 0 \\ \hline 0 & 0 & \Xi_2 \end{array}\right] \tag{1.6}$$

the matrices Π_L, Π_R denote the permutations from the left and right, respectively, the vector d contains only the nonzero scalars $\delta_1, \ldots, \delta_k$, the matrix Ξ_1 is diagonal with simple and nonzero singular values; the row beginning with the scalar δ_{k+1} is nonexistent iff the problem (1.1) is compatible. The final partitioning in (1.6) corresponds to that in (1.5) with $P \equiv U' G \Pi_L$ and $Q \equiv V' H \Pi_R$. Denote $\bar{m}$, and $\bar{n} \equiv k$ the dimensions in (1.6) such that $A_{11} \in \mathbb{R}^{\bar{m}\times\bar{n}}$, $x_1 \in \mathbb{R}^{\bar{n}}$, and $b_1 \in \mathbb{R}^{\bar{m}}$; obviously $\bar{n} \leq \bar{m} \leq \bar{n}+1$.

It can be easily shown that the subproblem $A_{11} x_1 \approx b_1$ obtained by the transformation process (1.6) described above has indeed the desired minimality property, and thus it represents the core problem within $A x \approx b$, see also [17]. The core problem in the form given in (1.6) is called the *SVD form of the core problem.*

A decomposition of the form (1.5) can also be computed directly by choosing orthogonal matrices P and Q in order to reduce $[\, b \,|\, A \,]$ to a real upper bidiagonal matrix, see [17]. It can be done using for example Householder reflection matrices, see [7, §5.4.3, pp. 251–252]. The first zero element on the main diagonal or on the first superdiagonal determines the desired partitioning. The matrix A_{22} needs not be bidiagonalized. Alternatively the *partial* Golub-Kahan iterative bidiagonalization algorithm [5, 16] can be used. Putting $w_0 \equiv 0$ and the starting vector $s_1 \equiv b/\beta_1$, where $\beta_1 \equiv \|b\|$, the algorithm computes for $j = 1, 2, \ldots$

$$\begin{aligned} \alpha_j w_j &\equiv A^T s_j - w_{j-1} \beta_j , \\ \beta_{j+1} s_{j+1} &\equiv A w_j - s_j \alpha_j , \end{aligned} \tag{1.7}$$

where $\|w_j\| = 1$, $\alpha_j \geq 0$, and $\|s_{j+1}\| = 1$, $\beta_{j+1} \geq 0$, until $\alpha_j = 0$ or $\beta_{j+1} = 0$, or until the dimensions of A are exceeded, i.e. $j = \min\{m, n\}$. Consider $\alpha_j > 0$, $\beta_j > 0$, for $j = 1, \ldots, k$, and $\beta_{j+1} > 0$, and denote $S_j \equiv [s_1, \ldots, s_j]$, $W_j \equiv [w_1, \ldots, w_j]$,

$$L_j \equiv \begin{bmatrix} \alpha_1 & & & \\ \beta_2 & \alpha_2 & & \\ & \ddots & \ddots & \\ & & \beta_j & \alpha_j \end{bmatrix} \in \mathbb{R}^{j\times j} \qquad \text{and} \qquad L_{j+} \equiv \begin{bmatrix} L_j \\ \beta_{j+1} e_j^T \end{bmatrix} \in \mathbb{R}^{(j+1)\times j} .$$

The Golub-Kahan bidiagonalization (1.7) of the matrix A with $s_1 \equiv b/\|b\|$ yields one of the following two situations: if $\alpha_j > 0$, $\beta_j > 0$, $j = 1, \ldots, \tilde{n}$, and $\beta_{\tilde{n}+1} = 0$ or $\tilde{n} = m$, then $S_{\tilde{n}}^T A W_{\tilde{n}} = L_{\tilde{n}}$; or if $\alpha_j > 0$, $\beta_j > 0$, $j = 1, \ldots, \tilde{n}$, $\beta_{\tilde{n}+1} > 0$, and $\alpha_{\tilde{n}+1} = 0$ or $\tilde{n} = n$, then $S_{\tilde{n}+1}^T A W_{\tilde{n}} = L_{\tilde{n}+}$. In both cases, the matrices $S_{\tilde{n}}$ or $S_{\tilde{n}+1}$, and $W_{\tilde{n}}$ represent the first $\tilde{n}$ or $\tilde{n}+1$ columns of the matrix P, and the first $\tilde{n}$ columns of the matrix Q in (1.5), respectively. The Golub-Kahan algorithm (1.7) yields the core problem, i.e., $\tilde{n} \equiv \bar{n}$, such a core problem is called the *banded (bidiagonal) form of the core problem.*

A subproblem representing the core problem has several properties. We summarize the most important of them:

(G1) The matrix A_{11} is of full *column* rank equal to $\bar{n}$.

(G2) The right-hand side b_1 is of full *column* rank (i.e., b_1 is nonzero).

(G3) The matrices $(U_j')^T b_1$ are of full *row* rank for all j, where U_j' denotes an orthonormal basis of the left singular vector subspace corresponding to the jth distinct singular value of A_{11}.

(G4) The matrix $[\, b_1 \,|\, A_{11} \,]$ is of full *row* rank.

(G5) The matrix A_{11} has no zero or multiple singular values, so any zero singular values or repeats that A has, must appear in A_{22}.

It is worth to note that there also exists an alternative definition of the core problem using properties (G1), (G3). This definition is used in the presented thesis for the first time, there is also showed the equivalence with the Paige and Strakoš definition used [17].

Further, the basic properties of a core problem can be derived from the relationship between the Lanczos tridiagonalization and the Golub-Kahan bidiagonalization, and from the properties of Jacobi matrices, see [13] by Hnětynková and Strakoš, [14] by Hnětynková, Strakoš and the author of the thesis, and [15] the doctoral thesis of Hnětynková.

The core problem plays an important role in the TLS formulation. Let $A\,x \approx b$ be a linear approximation problem and $\tilde{A}_{11}\,\tilde{x}_1 \approx \tilde{b}_1$ the core problem within $A\,x \approx b$ in the bidiagonal form. Because $\alpha_j > 0$ and $\beta_j > 0$ for $j = 1, \ldots, \bar{n}$, the matrix $\tilde{A}_{11}^T\,\tilde{A}_{11}$ is a Jacobi matrix, in both cases. Similarly $[\, \tilde{b}_1 \,|\, \tilde{A}_{11} \,]^T\,[\, \tilde{b}_1 \,|\, \tilde{A}_{11} \,]$ is a Jacobi matrix – thus, all its eigenvalues are simple, all its eigenvectors have nonzero first and last components. The matrix $[\, \tilde{b}_1 \,|\, \tilde{A}_{11} \,]^T\,[\, \tilde{b}_1 \,|\, \tilde{A}_{11} \,]$ contains $\tilde{A}_{11}^T\,\tilde{A}_{11}$ as a trailing principal submatrix, which is crucial in the forthcoming analysis.

From the properties of Jacobi matrices, it follows that the eigenvalues of the matrix $[\, \tilde{b}_1 \,|\, \tilde{A}_{11} \,]^T\,[\, \tilde{b}_1 \,|\, \tilde{A}_{11} \,]$ are *strictly interlaced* by the eigenvalues of $\tilde{A}_{11}^T\,\tilde{A}_{11}$. Because the singular values are independent on the given form of the core problem, we omit tildes in the further text; we obtain in the incompatible case, both matrices A_{11} and $[\, b_1 \,|\, A_{11} \,]$ have distinct and nonzero singular values and the singular values of A_{11} strictly interlace the singular values of $[\, b_1 \,|\, A_{11} \,]$,

$$\sigma_{\bar{n}}\,(A_{11}) \;>\; \sigma_{\bar{n}+1}\,(\,[\, b_1 \,|\, A_{11} \,]\,)\,. \tag{1.8}$$

Appending the right-hand side vector b_1 to the core problem matrix A_{11} decreases the smallest singular value. The core problem always satisfies the Golub, Van Loan condition (1.4) and thus it always has the unique TLS solution (i.e., the smallest singular value $\sigma_{\bar{n}+1}\,([\, b_1 \,|\, A_{11} \,])$ is simple and the corresponding right singular vector has nonzero first component).

It remains to compare the solution $x \equiv Q\,[\, x_1^T \,|\, 0 \,]^T$ obtained using the core problem transformation (1.5) to all the TLS formulation in [6, 23]. Let $A\,x \approx b$ be a general linear approximation problem and $A_{11}\,x_1 \approx b_1$ a core problem within $A\,x \approx b$ obtained by a transformation to the form (1.5). Denote for simplicity x_1 the unique TLS solution of this core problem. Now, the question is, what this solution represents in the original variables.

Assume $m > n$ (add zero rows if necessary), moreover we focus on the incompatible case, i.e. $b \notin \mathcal{R}\,(A)$. Consequently the matrix $[\, b_1 \,|\, A_{11} \,]$ is square and the matrix A_{22} is either square (iff $m = n + 1$), or is has more rows than columns. Denote $\sigma_{\min}\,(M)$ the smallest singular value of M for simplicity (for all $[\, b_1 \,|\, A_{11} \,]$, A_{11} and A_{22}, the index of the smallest singular value is equal to the number of their columns). Recall that the SVD of $[\,b\,|\,A\,]$ can be obtained as a direct sum of SVDs of $[\,b_1\,|\,A_{11}\,]$ and A_{22}, just by extending the singular vectors corresponding to the first block by zeros on the bottom and the singular vectors corresponding to the second block by zeros on the top.

There are three different possibilities:

Case A. If

$$\sigma_{\min}(A_{22}) > \sigma_{\min}([\,b_1\,|\,A_{11}\,]),$$

then, because $\sigma_{\min}(A_{11}) > \sigma_{\min}([\,b_1\,|\,A_{11}\,])$ by (1.8), the smallest singular value of $[\,b\,|\,A\,]$ is simple and $\sigma_n(A) > \sigma_{n+1}([\,b\,|\,A\,])$. Consequently the original problem $A\,x \approx b$ has by (1.4) the unique TLS solution. The TLS solution of the original problem is given by this right singular vector and obviously it is identical to the solution of the core problem transformed back to the original variables, i.e. $x_{\mathrm{TLS}} \equiv Q\,[\,x_1^T\,|\,0\,]^T$.

Case B. If

$$\sigma_{\min}(A_{22}) = \sigma_{\min}([\,b_1\,|\,A_{11}\,]),$$

then the smallest singular value of $[\,b\,|\,A\,]$ is multiple and it is equal to $\sigma_n(A)$. The Golub, Van Loan condition (1.4) is no more satisfied. From (1.8) it follows that *the multiplicity of the smallest singular value of A increase by appending the right-hand side b.* The original problem $A\,x \approx b$ has a TLS solution but it is not unique. The minimum norm TLS solution of the original problem is given by the right singular vector of $v_\ell = \mathrm{diag}(1, Q)\,\bar{v}_\ell$, i.e. it is identical to the solution of the core problem $[\,b_1\,|\,A_{11}\,]$ transformed back to the original variables, i.e. $x_{\mathrm{TLS}} \equiv Q\,[\,x_1^T\,|\,0\,]^T$.

Case C. If

$$\sigma_{\min}(A_{22}) < \sigma_{\min}([\,b_1\,|\,A_{11}\,]),$$

then the singular values $\sigma_n(A) \equiv \sigma_{n+1}([\,b\,|\,A\,]) \equiv \sigma_{\min}(A_{22})$ have the same multiplicities. All the right singular vectors corresponding to $\sigma_{n+1}([\,b\,|\,A\,])$ have zero first components. The original problem $A\,x \approx b$ does not have a TLS solution. The (minimum 2-norm) nongeneric solution of $A\,x \approx b$ is given by the solution of the core problem transformed back to the original variables, i.e. $x_{\mathrm{NGN}} \equiv Q\,[\,x_1^T\,|\,0\,]^T$.

Summarizing, for any approximation problem (1.1) the vector $x \equiv Q\,[\,x_1^T\,|\,0\,]^T$, where x_1 is the unique TLS solution of the core problem within $A\,x \approx b$, represents the corresponding minimum 2-norm solution given in [6, 23]. For the given $A\,x \approx b$ it is reasonable, and Paige and Strakoš in [17] also recommended, first to find a core problem $A_{11}\,x_1 \approx b_1$ using orthogonal transformations (or by Golub-Kahan iterative bidiagonalization), then solve the core problem $A_{11}\,x_1 \approx b_1$, put $x_2 = 0$, and define the solution of the original problem define as $x \equiv Q\,[\,x_1^T\,|\,0\,]^T$. The assumption $x_2 = 0$ here does not follow from a theory, it is a postulate: do not mix the useful (necessary and sufficient) information with the useless data contained in A_{22} in the solution of $A\,x \approx b$. Consequently the core problem theory is consistent with earlier work and it explains and clarifies the concept of nongeneric solution. The nongeneric concept becomes justified although the minimum 2-norm nongeneric solution does not solve the TLS problem (1.3).

Clearly, from the core problem concept,

$$\sigma_{\min}(A_{22}) \geq \sigma_{\min}([\,b_1\,|\,A_{11}\,]) \tag{1.9}$$

is the *necessary and sufficient condition for the existence of a TLS solution.* (If the matrix A_{22} is trivial, i.e. it has no columns, then the problem always has the unique TLS solution.)

1.3 Goals of the thesis

The thesis focuses on solution of an orthogonally invariant linear approximation problem with multiple right-hand sides $A\,X \approx B$ through the TLS concept. The main goal of the thesis is to generalize the analysis of the TLS concept given for problems with single right-hand sides in [6, 23, 17] and to build up a consistent theory which would cover the multiple right-hand sides case.

For a problem with multiple right-hand sides, a partial generalization of the TLS concept was presented by S. Van Huffel and J. Vandewalle in [23]. They cover some particular cases for which they define a TLS solution. They also present an algorithm which for any data gives an output, which is, however, not identified with a theoretically justified TLS theory. Therefore we attempt in Chapter 3, as the first goal of the presented thesis, to revise and complete, within our abilities, their analysis.

C. C. Paige and Z. Strakoš proved in [17] that for a problem with a single right-hand side $A\,x \approx b$ there is a reduction which determines a core problem $A_{11}\,x_1 \approx b_1$ within the original problem, with all necessary and sufficient information for solving the original problem. The core problem always has the unique TLS solution, and, using the transformation to the original variables, it gives the solution of the original approximation problem identical to the minimum 2-norm solutions of all TLS formulations given in [6, 23]. The core problem theory represents a new approach to understanding of the TLS concept. It makes the theory complete and transparent, and it also fundamentally changes a view to practical computations. The second goal of the presented thesis is therefore to extend the core problem theory, if possible, to problems with multiple right-hand sides. The reduction based on the SVD of A, motivated by the work of D. M. Sima and S. Van Huffel [20, 21], is given in Chapter 4. Another approach, based on a banded generalization of the Golub-Kahan bidiagonalization algorithm, is given in Chapter 5, motivated by the series of lectures [1, 2, 3] by Å. Björck, and also the work [17, 13, 14, 15] of C. C. Paige, Z. Strakoš, I. Hnětynková and partially of the author of this thesis.

Chapter 6 investigates the relationship between the SVD-based and the banded reduction approaches. An extension of the minimally dimensioned subproblem concept to the multiple right-hand side case has some difficulties. In particular, the minimally dimensioned reduced subproblem may not have a TLS solution.

Core problem computation in finite precision arithmetic must resolve a problem of relevant stopping criteria. Difficulties connected with revealing of core problem are illustrated on examples in Chapter 7. We do not address this question fully in the thesis, but present an example of the noise-revealing property of the Golub-Kahan bidiagonalization, which can be very useful in hybrid methods for solving ill-posed problems, see Chapter 8.

The thesis ends with conclusions, some open questions and directions for further research, in Chapter 9.

Chapter 2

Main results of the thesis

In this chapter we summarize the main results of the presented thesis related to the TLS problems with the multiple right-hand sides (1.2). These results are organized as follows: in Section 2.1 there are summarized results from Part II (Chapter 3) of the thesis; the results from Part III (Chapters 4, 5, and 6) are summarized in Section 2.2; and Section 2.3 contains results form Part IV (Chapters 7 and 8).

Some particular results related to the TLS problems with the single right-hand sides are already mentioned in Introduction. These are: the alternative definition of the core problem within the problem with single right-hand side based on the properties (G1), (G3), see Definition 1.3 in Section 1.4.3 in the thesis (there is shown the equivalence with the Paige and Strakoš definition used in [17]). The second result related to the problems with single right-hand sides is an alternative proof of core problem properties using the relationship between the Lanczos tridiagonalization and the Golub-Kahan bidiagonalization and using the properties of Jacobi matrices. See Section 1.4.4 in the thesis and see also [14].

2.1 Theoretical fundamentals of total least squares formulation in $A\,X \,\approx\, B$

In Chapter 3 we summarize results of Van Huffel and Vandewalle [23] for the problems with multiple right-hand sides. In [23] there are two basic problem cases (both simply extend the single right-hand side case) for which exists a TLS solution and a wide class of problems for which the solution does not exist (we denote it $\mathscr{S}$). In [23] there is an algorithm which is commonly used (or its variants) for solving TLS problems. It is well known that this algorithm computes either a TLS solution (if it is applied on the basic two cases mentioned above), or so called *nongeneric solution* when a problem belongs to the class $\mathscr{S}$. We give a theorem which guarantees existence of a TLS solution for the wider class of problems (including the two basic cases). Furthermore this theorem shows that the existence of a class of problems for which a TLS solution exists but the algorithm by Van Huffel, Vandewalle does not compute it. We briefly introduce the used notation and then we give the theorem and a basic classification of the TLS problems.

Consider an orthogonally invariant linear approximation problem (1.2). We assume $A^T B \neq 0$ and $m \geq n + d$ (add zero rows if necessary). Consider a SVD of $[\, B \,|\, A \,] = U \Sigma V^T$, $s \equiv \operatorname{rank}([\, B \,|\, A \,])$, where $\Sigma = \operatorname{diag}(\sigma_1, \ldots, \sigma_s, 0)$, and $\sigma_1 \geq \ldots \geq \sigma_s > \sigma_{s+1} = \ldots = \sigma_{n+d} \equiv 0$. In order to handle a possible multiplicity of σ_{n+1} we introduce the following notation

$$\sigma_{n-q} > \underbrace{\sigma_{n-q+1} = \ldots = \sigma_n}_{q} = \underbrace{\sigma_{n+1} = \ldots = \sigma_{n+e}}_{e} > \sigma_{n+e+1}\,, \tag{2.1}$$

where q singular values to the left and $e-1$ singular values to the right are equal to σ_{n+1}, and $q \geq 0$, $e \geq 1$. For convenience we denote $n-q \equiv p$. If $q = n$, then σ_p is nonexistent. Similarly, if $e = d$, then σ_{n+e+1} is nonexistent. It will be useful to consider the following partitioning:

$$V = \left[\begin{array}{c|c} V_{11}^{(q)} & V_{12}^{(q)} \\ \hline V_{21}^{(q)} & V_{22}^{(q)} \end{array}\right], \tag{2.2}$$

where $V_{11}^{(q)} \in \mathbb{R}^{d\times(n-q)}$, $V_{12}^{(q)} \in \mathbb{R}^{d\times(d+q)}$, $V_{21}^{(q)} \in \mathbb{R}^{n\times(n-q)}$, $V_{22}^{(q)} \in \mathbb{R}^{n\times(d+q)}$.

Theorem 2.1. *Let $[\,B\,|\,A\,] = U\,\Sigma\,V^T$ be the SVD with the partitioning given by (2.2). If $\operatorname{rank}(V_{12}^{(q)}) = d$, then consider an orthogonal matrix $\tilde{Q}$ such that*

$$\left[\begin{array}{c} V_{12}^{(q)} \\ \hline V_{22}^{(q)} \end{array}\right] \tilde{Q} = \left[\begin{array}{c|c} \Omega & \tilde{\Gamma} \\ \hline \tilde{Y} & \tilde{Z} \end{array}\right], \qquad \tilde{Q} = \left[\begin{array}{c|c} \tilde{Q}_1 & \tilde{Q}_2 \end{array}\right] \tag{2.3}$$

where $\tilde{Q}_1 \in \mathbb{R}^{(q+d)\times q}$, $\tilde{Q}_2 \in \mathbb{R}^{(q+d)\times d}$, and $\tilde{\Gamma} \in \mathbb{R}^{d\times d}$ is nonsingular, and define

$$\begin{aligned} \left[\begin{array}{c|c} G & E \end{array}\right] &\equiv -\left[\begin{array}{c|c} B & A \end{array}\right] \left[\begin{array}{c} \tilde{\Gamma} \\ \hline \tilde{Z} \end{array}\right] \left[\begin{array}{c} \tilde{\Gamma} \\ \hline \tilde{Z} \end{array}\right]^T \\ &= -\left[\, u_{p+1}\,, \ldots, u_{n+d} \,\right] \operatorname{diag}(\sigma_{p+1}\,, \ldots, \sigma_{n+d}) \\ &\qquad \tilde{Q}_2\,\tilde{Q}_2^T \left[\, v_{p+1}\,, \ldots, v_{n+d} \,\right]^T. \end{aligned} \tag{2.4}$$

Then the following two assertions are equivalent:

(i) *There exists an index k, $0 \leq k \leq e < d$, and an orthogonal matrix $\hat{Q}$ in the block diagonal form*

$$\hat{Q} = \left[\begin{array}{c|c} Q' & 0 \\ \hline 0 & I_{d-k} \end{array}\right] \in \mathbb{R}^{(q+d)\times(q+d)}, \qquad Q' \in \mathbb{R}^{(q+k)\times(q+k)}, \tag{2.5}$$

and using $\hat{Q}$ in (2.3), (2.4) instead of $\tilde{Q}$ gives the same $[\,G\,|\,E\,]$.

(ii) *The matrix $[\,G\,|\,E\,]$ satisfies*

$$\left\| \left[\begin{array}{c|c} G & E \end{array}\right] \right\|_F = \left(\sum_{j=n+1}^{n+d} \sigma_j^2 \right)^{1/2}. \tag{2.6}$$

The matrix $[\,G\,|\,E\,]$ represents a correction that makes the problem compatible and which has by (ii) minimal Frobenius norm. Then the matrix $X \equiv -\tilde{Z}\,\tilde{\Gamma}^{-1}$ represents a TLS solution.

Then Chapter 3 of the thesis analyzes when such $\hat{Q}$ exists We consider the further partitioning of the matrix $V_{12}^{(q)} = [\,W^{(q,e)}\,|\,V_{12}^{(-e)}\,]$, where $W^{(q,e)} \in \mathbb{R}^{d\times(q+e)}$, $V_{12}^{(-e)} \in \mathbb{R}^{d\times(d-e)}$. The complete classification is presented on Figure 2.1 on p. 16, it quickly recapitulates properties of problems and differences between problems in the individual classes.

2.2 Data reduction

In Chapters 4, 5, and 6 the thesis extends the core problem concept of Paige and Strakoš [17] to the problems with multiple right-hand sides. We show that for a general orthogonally invariant linear approximation problem (1.2) there exist orthogonal matrices P, Q, R which transform the *original data* $[\,B\,|\,A\,]$ into the block form

$$\begin{aligned} P^T \left[\; B \;\middle|\; A \;\right] \left[\begin{array}{c|c} R & 0 \\ \hline 0 & Q \end{array}\right] &= \left[\; P^T B\, R \;\middle|\; P^T A\, Q \;\right] \\ &\equiv \left[\begin{array}{c|c||c|c} B_1 & 0 & A_{11} & 0 \\ \hline 0 & 0 & 0 & A_{22} \end{array}\right] \end{aligned} \tag{2.7}$$

where B_1 and A_{11} are of minimal dimensions and all irrelevant and redundant information is thus moved into the block A_{22}.

Chapter 4 investigates a transformation of the form (2.7) based on the subsequent SVD decompositions of the right-hand side matrix B, then of the system matrix A, and finally SVDs of the blocks of the already transformed right-hand side. Note that in the single right-hand side it is sufficient to use only the SVD of A. In Chapter 4 there is also shown the existence of another transformation which uses LQ decomposition instead of the first SVD of B, SVD of A, and QR decompositions of the blocks of the transformed right-hand side, giving the same dimensions of the reduced problem. Thus it is sufficient to use only one SVD in the multiple right-hand side case, too. Any such transformation yields a subproblem $A_{11}\, X_1 \approx B_1$ having, in analogy to the single right-hand side case, the following properties:

(G1) The matrix $A_{11} \in \mathbb{R}^{\bar{m}\times\bar{n}}$ is of *full column rank* equal to $\bar{n} \le \bar{m}$.

(G2) The matrix $B_1 \in \mathbb{R}^{\bar{m}\times\bar{d}}$ is of *full column rank* equal to $\bar{d} \le \bar{m}$.

(G3) Let ς'_j be the singular value of A_{11} with the multiplicity r_j, let U'_j be the matrix with the corresponding orthonormal singular vectors as its columns. Then the matrices $(U'_j)^T B_1 \equiv D_j \in \mathbb{R}^{r_j\times\bar{d}}$ are of *full row rank* equal to $r_j \le \bar{d}$, for $j = 1, \ldots, k+1$.

(G4) The extended matrix $[\,B_1\,|\,A_{11}\,] \in \mathbb{R}^{\bar{m}\times(\bar{n}+\bar{d})}$ is of *full row rank* equal to $\bar{m} \equiv \bar{n} + r_{k+1} \le \bar{n} + \bar{d}$.

(G5) The matrix A_{11} does not have any zero singular value. Its singular values have multiplicities equal to at most $\bar{d}$.

Moreover, the reduction which uses the subsequent SVDs (not the LQ or QR decompositions) yields a subproblem having special properties:

(S1) The matrix $A_{11} \in \mathbb{R}^{\bar{m}\times\bar{n}}$ is diagonal with positive components sorted in nonincreasing sequence on the main diagonal.

(S2) The matrix $B_1 \in \mathbb{R}^{\bar{m}\times\bar{d}}$ has mutually orthogonal nonzero columns, sorted in a nonincreasing sequence with respect to their norms.

(S3) The matrices $(U'_j)^T B_1 \equiv D_j \in \mathbb{R}^{r_j\times\bar{d}}$ have mutually orthogonal nonzero rows sorted in a nonincreasing sequence with respect to their norms, for $j = 1, \ldots, k+1$.

Chapter 5 investigates a transformation of the form (2.7) based on banded generalization of the Golub-Kahan iterative bidiagonalization algorithm. This algorithm was proposed by Å. Björck [1, 2, 3], and D. M. Sima, S. Van Huffel [20, 21] for this purpose. This chapter starts with the description of the banded algorithm. Furthermore it summarizes some obvious properties of the obtained subproblem which has a structure illustrated by the following example:

$$
\left[\, \tilde{B}_1 \,\middle|\, \tilde{A}_{11} \,\right] = \left[\begin{array}{ccc||ccccccc}
\gamma_1 & \beta_{12} & \beta_{13} & \alpha_1 & & & & & & \\
 & \gamma_2 & \beta_{23} & \beta_{24} & \alpha_2 & & & & & \\
 & & \gamma_3 & \beta_{34} & \beta_{35} & \alpha_3 & & & & \\
 & & & \gamma_4 & \beta_{45} & \beta_{46} & \alpha_4 & & & \\
 & & & & & \gamma_5 & \beta_{57} & \alpha_5 & & \\
 & & & & & & \gamma_6 & \beta_{68} & & \\
 & & & & & & & \gamma_7 & \alpha_6 & \\
 & & & & & & & & \gamma_8 & \alpha_7
\end{array}\right],
$$

where $\alpha_i > 0$, $\gamma_j > 0$. These obvious properties are namely (G1), (G2), and (G4).

In order to show the other properties and motivated by the work [13, 14, 15] we define a wedge-shaped matrices – a class of symmetric banded matrices. In Chapter 5 there is proven that eigenvalues and eigenvectors of wedge-shaped matrices have some important properties which in some way generalize properties of Jacobi matrices. (See Sections 5.5.1, Eigenvalues of generalized Jacobi matrices; 5.6.1, Eigenvectors of generalized Jacobi matrices; 5.6.2, Eigenspaces of generalized Jacobi matrices.) We show that the matrices $[\tilde{B}_1 \,|\, \tilde{A}_{11}\,]^T\,[\tilde{B}_1 \,|\, \tilde{A}_{11}\,]$, $\tilde{A}_{11}^T\,\tilde{A}_{11}$, and $\tilde{A}_{11}\,\tilde{A}_{11}^T$ are wedge-shaped. This allows us to show that the banded subproblem has properties (G3) and (G5), too. Moreover we showed some further properties of the banded subproblem, for example that the matrix $[\,\tilde{B}_1 \,|\, \tilde{A}_{11}\,]$ has singular values with multiplicities equal to at most $\tilde{d} \equiv \mathrm{rank}\,(B)$.

In Chapter 6 of the thesis we show that the properties (G1)–(G3) guarantee minimality of the dimensions of the problem $A_{11}\,X_1 \approx B_1$ obtained by the SVD-based reduction as well as $\tilde{A}_{11}\,\tilde{X}_1 \approx \tilde{B}_1$ obtained by the banded algorithm. Thus both of these reduced problems represents the same subproblem which is the minimal subproblem of the original problem. We define the core problem within a problem with multiple right-hand sides analogously to Paige and Strakoš in [17].

Definition 2.1 (Core problem)**.** *The subproblem* $A_{11}\,X_1 \approx B_1$ *is a core problem within the approximation problem* $A\,X \approx B$ *if* $[\,B_1 \,|\, A_{11}\,]$ *is minimally dimensioned (and* A_{22} *maximally dimensioned) subject to (2.7).*

We further use the properties (G1)–(G3) for an alternative definition of a core problem in the multiple right-hand side case.

Definition 2.2 (Core problem)**.** *Any approximation problem* $A\,X \approx B$ *having properties (G1)–(G3) is called a core problem.*

Further the Chapter 6 investigates the question whether the core problem in the multiple right-hand side case has a TLS solution. We show on an example that the core problem with the multiple right-hand sides can contain two or more independent subproblems (also having properties (G1)–(G3)). The independence of such subproblems within a core problem can cause that the core problem does not have a TLS solution even if all its subproblems have TLS solutions. The question how to identify such composed core problem and how to decompose it is not resolved yet in the thesis.

2.3 Implementation, computations, and related issues

Chapters 7 and 8 focus on computation of a core problem in the single right-hand side case and applicability of the presented theory in hybrid methods.

The computation of a core problem (in the single right-hand side case) is always based on the partial Golub-Kahan iterative bidiagonalization algorithm. Chapter 7 summarizes the well known facts about the stable implementation of the bidiagonalization and on an example investigates a sensitivity of a computation. An artificially constructed problem contains a core problem with known dimensions, the matrix A_{22} (see (1.5)) is multiplied by a positive scalar γ. We observe the computed bidiagonal components depending on the value of γ. It can be observed that the core problem identification is more difficult with growing norm of $\gamma\, A_{22}$.

Chapter 8 investigates application of bidiagonalization in the hybrid methods for solving ill-posed problems $A\,x = b$ with the right-hand side polluted by a (white) noise, i.e. $b \equiv b^{\text{exact}} + b^{\text{noise}}$. The presented hybrid approach uses information about the noise level in the data revealed by the Golub-Kahan bidiagonalization. We analyze the left vectors from the bidiagonalization in the frequency domain. (Similar approach based on the analysis of residual vectors in frequency domain is discussed in [12, 10].)

We illustrate on an example `shaw(400)`, see [8], the noise propagation in the left vectors from the Golub-Kahan bidiagonalization, see Figure 2.2 on p. 17. We implement an experimental hybrid method based on this observation with inner TSVD regularization. This method gives satisfactory results on the considered example and we believe that a similar idea can be used in practical problems. In our further work we aim to focus on construction of an effective stopping criteria for hybrid methods based on the discrepancy principle.

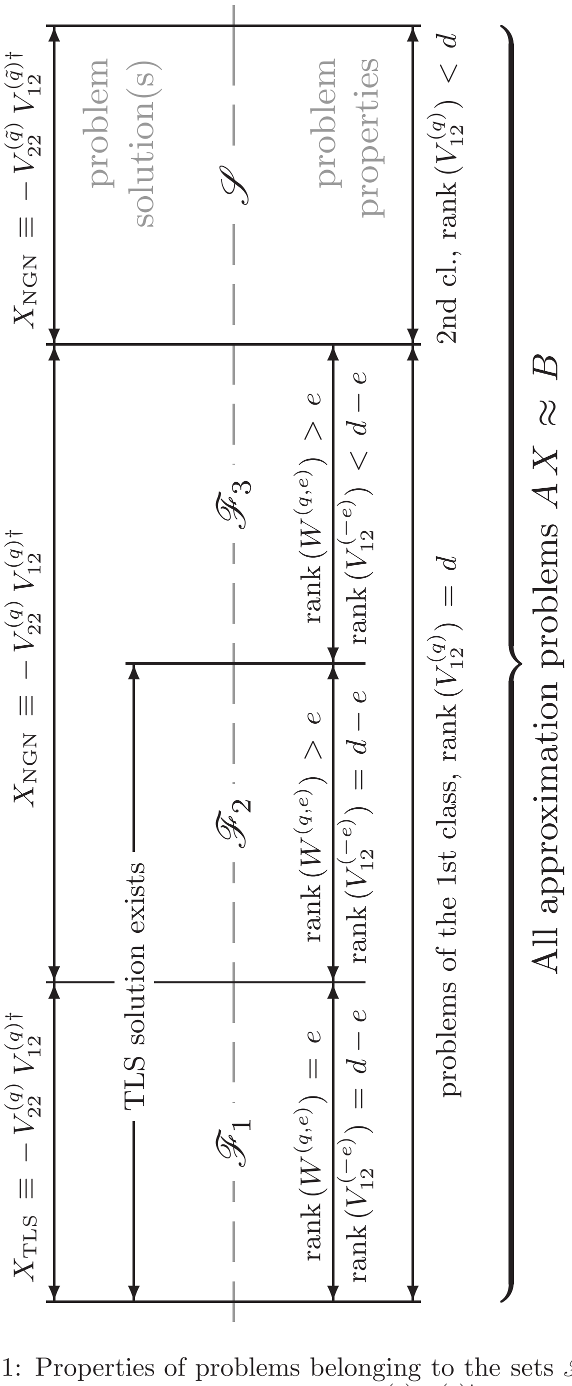

Figure 2.1: Properties of problems belonging to the sets $\mathscr{F}_1$, $\mathscr{F}_2$ and $\mathscr{F}_3$. Note that the matrix $X \equiv -V_{22}^{(q)}\, V_{12}^{(q)\dagger}$ represents the result computed by the algorithm by Van Huffel and Vandewalle.

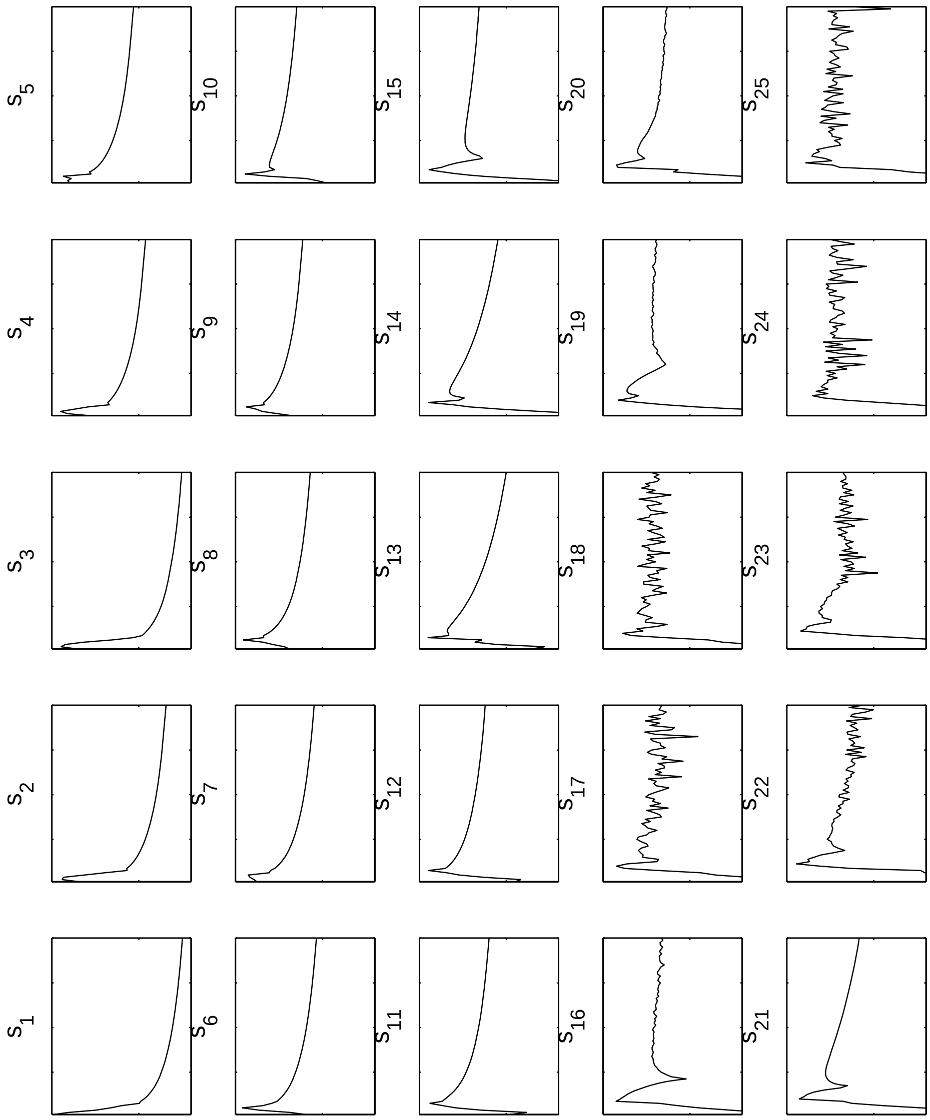

Figure 2.2: The first eighty Fourier coefficients of the left vectors from the Golub-Kahan bidiagonalization in the trigonometric basis; computed by `fft` MATLAB command. The noise level is maximal in the vector s_{18} then it is partially projected out in s_{19}. All graphs are in logarithmic scale with range 10^{-8}–10^{0}.

Chapter 3

Conclusions and open questions

In this chapter we summarize results presented in the thesis. We formulate some open questions and mention some possible directions for further work.

3.1 Conclusions

Part I (Chapter 1) of the thesis summarizes fundamentals of the total least squares theory in the single right-hand side case based on the work of Golub, Van Loan, Van Huffel, Vandewalle, Paige, Strakoš and others. Parts II and III of the presented thesis investigate an extension of the concept of the core reduction of Paige and Strakoš to a general unitary invariant linear algebraic approximation problem $A\,X \approx B$; we focus on the problems with *multiple right-hand sides*.

First, in Part II (Chapters 2, and 3), starting from the results of Van Huffel and Vandewalle, we investigate the fundamental question of the existence of the TLS solution, and present a basic classification of the TLS problems. It is shown that the formulation of the TLS problem with multiple right-hand sides is significantly more complicated than the single right-hand side TLS problem and the results of Chapter 3 reflect the difficulties which have been revealed in our work on the subject.

The data reduction in Part III (Chapters 4, 5, and 6), which aims at the minimally dimensioned core problem containing the necessary and sufficient information for solving the problem with the original data, starts with the SVD-based transformation, which extends the work of Paige and Strakoš. Another reduction, in the single right-hand side case described by Paige, Strakoš, Hnětynková and the author of this thesis is based on the banded generalization of the Golub-Kahan iterative bidiagonalization, as suggested by Å. Björck and D. M. Sima. Using some properties of the class of generalized Jacobi matrices we investigate further properties of the suggested banded form of the reduced problem.

We have presented the proof of minimality of the SVD-based form as well as the banded form, and proved their equivalence. This allows to define the core problem for problems with multiple right-hand sides. In particular, we relate the solvability of the reduced problem obtained via the core problem approach to the result of the classical TLS algorithm by S. Van Huffel applied directly on the original problem. We showed that the solution computed by the classical TLS algorithm of Van Huffel is not necessarily the TLS solution of the given approximation problem.

Contrary to the single right-hand side case, the core problem may not have the TLS solution. We describe so called *decomposable core problems* and show that there exists a whole class of decomposable core problems which do not have the

TLS solution. Because the core problems in the problems with single right-hand sides are non decomposable, its TLS solution always exists. We formulate, with some ambiguity, the following conjecture:

Conjecture 3.1. *Any non decomposable core problem has the unique TLS solution.*

In decomposable core problems that we have presented the difficulty is caused by the fact that the problem links together data from different *independent subproblems*. If Conjecture 3.1 is correct, then the decomposing of decomposable core problem reveals the hidden structure of independent subproblems which should be treated separately. Then the obtained solution naturally differs form the solution obtained by the classical TLS algorithm by Van Huffel and Vandewalle which considers all data in one problem.

If Conjecture 3.1 is not correct, then the TLS formulation for the problems with multiple right-hand sides lacks in some cases a consistently defined solution. We still do not know how to identify and decompose *all* decomposable problems. Therefore we were unable to prove or disprove Conjecture 3.1.

Part IV (Chapters 7, and 8) of this thesis presents on an example a possible hybrid method for solving ill-posed problems, this method uses the Golub-Kahan bidiagonalization and it is based on core problem ideas, concerning fundamental data decomposition while accumulating necessary and sufficient data in a partially constructed A_{11} block. It is shown that the Golub-Kahan iterative bidiagonalization can be used for revealing the level of noise present in the data. In the example we combine the outer regularization accomplished by the bidiagonalization (the Lanczos-type process), which projects the original problem onto a Krylov subspace of small dimensions, with inner TSVD regularization.

Numerical results are presented. Unfortunately, they are not yet compared with results obtained by other hybrid methods. We believe that the presented idea can be used in practical computations as a contribution towards building efficient and reliable stopping criteria of the outer iterative process.

3.2 Open questions and possible directions for further research

Now we shortly summarize some questions which are interesting in the context of the material presented in this thesis but which are out of the scope of the presented text. In Part II, one can ask about the relationship between the TLS solution and the solution computed by the algorithm by Van Huffel, Vandewalle, and about an interpretation of such a relationship in application areas such as computational statistics. Similarly, it is desirable to give a possible statistical interpretation of the decomposability of the (core) problem. We believe that the statistical point of view and its combination with the matrix computation point of view can help in getting further understanding.

We are well aware of many important questions related to practical implementations and computations. For example, one can expect that a suitable preprocessing of the matrix right-hand side B can improve the behavior of the banded generalization of the Golub-Kahan algorithm. Numerical behavior can be studied in relationship with the block Lanczos algorithm.

Numerical analysis and solution of ill-posed problems illustrated in Part IV produces in the context of the core problem approach many very interesting problems. The presented noise-revealing idea is certainly worth of further effort. Hybrid methods for large ill-posed problems represent a very hot topic in scientific computing.

3.3 List of publications and conference talks of the author of this thesis related to the subject

Some parts of this work was presented on several international and local conferences, and papers for international journals are in preparation.

Papers in journals

[J1] Iveta Hnětynková, Martin Plešinger, Zdeněk Strakoš: *Lanczos tridiagonalization, Golub-Kahan bidiagonalization and core problem*, PAMM, Proceedings in Appl. Math. and Mechanics 6 (2006), pp. 717–718.

Papers in preparation

[J2] Iveta Hnětynková, Martin Plešinger, Diana Maria Sima, Zdeněk Strakoš, Sabine Van Huffel: *Classification of TLS problems in $AX \approx B$ and the relationship to the work of Van Huffel and Vandewalle*, in preparation.

[J3] Iveta Hnětynková, Martin Plešinger, Zdeněk Strakoš: *Noise revealing via Golub-Kahan bidiagonalization with application in hybrid methods*, in preparation.

Proceedings contributions

[P1] Martin Plešinger, Zdeněk Strakoš: *Core reduction and least squares problems* (in Czech), Proceedings of X. PhD. Conference '05 (F. Hakl, Ed.), Praha, ICS AS CR & Matfyzpress (2005), pp. 102–108.
(`http://www.cs.cas.cz/hakl/doktorandsky-den/files/2005/dk05proc.pdf`)

[P2] Martin Plešinger, Zdeněk Strakoš: *Singular value decomposition – application in image deblurring* (in Czech), Seminar on Numerical Analysis '06, Praha, ICS AS CR (2006), pp. 78–81.

[P3] Martin Plešinger, Zdeněk Strakoš: *Some remarks on bidiagonalization and its implementation*, Proceedings of XI. PhD. Conference '06 (F. Hakl, Ed.), Praha, ICS AS CR & Matfyzpress (2006), pp. 104–114.
(`http://www.cs.cas.cz/hakl/doktorandsky-den/files/2006/dk06proc.pdf`)

[P4] Iveta Hnětynková, Martin Plešinger, Zdeněk Strakoš: *Golub-Kahan Iterative Bidiagonalization and Stopping Criteria in Ill-Posed Problems*, In: Seminar on Numerical Analysis '07 (R. Blaheta, J. Starý, Eds.), Ostrava, Institute of Geonics AS CR (2007), pp. 43–45.

[P5] Iveta Hnětynková, Martin Plešinger, Diana Maria Sima, Zdeněk Strakoš: *Total Least Squares Problem in Linear Algebraic Systems with Multiple Right-Hand Side*, In: Seminar on Numerical Analysis '07 (R. Blaheta, J. Starý, Eds.), Ostrava, Institute of Geonics AS CR (2007), pp. 81–84.

[P6] Martin Plešinger, Zdeněk Strakoš: *Total least squares formulation in problems with multiple right-hand sides* (in Czech), Proceedings of XII. PhD. Conference '07 (F. Hakl, Ed.), Praha, ICS AS CR & Matfyzpress (2007), pp. 70–74.

International conferences (talks and posters)

[I1] Iveta Hnětynková, Martin Plešinger, Zdeněk Strakoš: *Lanczos tridiagonalization and the core problem*, 77th Annual Meeting of the Gesell-

schaft für Angewandte Mathematik und Mechanik e.V., Technische Universität Berlin, Germany, March 27–31, 2006.

[I2] Iveta Hnětynková, Martin Plešinger, Zdeněk Strakoš: *Golub-Kahan bidiagonalization and stopping criteria in solving ill-posed problems*, Joint GAMM SIAM Conference on Applied Linear Algebra, Düsseldorf, Germany, July 24–27, 2006.

[I3] Poster: Iveta Hnětynková, Martin Plešinger, Zdeněk Strakoš: *On core problem formulation in linear approximation problems with multiple right-hand sides*, 4th International Workshop on Total Least Squares and Errors-in-Variables Modeling, Arenberg castle, Leuven, Belgium, August 21–23, 2006.

[I4] Iveta Hnětynková, Martin Plešinger, Zdeněk Strakoš: *Analysis of the TLS problem with multiple right-hand sides*, 22nd Biennial Conference on Numerical Analysis, University of Dundee, Scotland, UK, June 26–29, 2007.

[I5] Poster: Iveta Hnětynková, Martin Plešinger, Diana Maria Sima, Zdeněk Strakoš, Sabine Van Huffel: *On total least squares formulation in linear approximation problems with multiple right-hand sides*, Computational Methods with Appl., Harrachov, Czech Republic, August 19–25, 2007.

[I6] Iveta Hnětynková, Martin Plešinger, Diana Maria Sima, Zdeněk Strakoš, Sabine Van Huffel: *On total least squares problem with multiple right-hand sides*, IMA Conference on Numerical Linear Algebra and Optimisation, University of Birmingham, UK, September 13–15, 2007.

[I7] Iveta Hnětynková, Martin Plešinger, Zdeněk Strakoš: *On fundamentals of total least squares problems*, 13th Czech-French-German Conference on Optimization Heidelberg, Germany, September 17–21, 2007.

Local conferences (talks and posters)

[L1] Martin Plešinger: *Core reduction and least squares problems*, X. PhD. Conference, Hosty – Týn nad Vltavou, November 5–7, 2005.

[L2] Martin Plešinger, Zdeněk Strakoš: *Singular value decomposition – application in image deblurring*, SNA '06, Modelling and Simulation of Challenging Engineering Problems, Monínec – Sedlec-Prčice, January 16–20, 2006.

[L3] Martin Plešinger: *Two Topics from Theory of Linear Approximation Problems*[1], XI. PhD. Conference, Monínec – Sedlec-Prčice, September 18–20, 2006.

[L4] Iveta Hnětynková, Martin Plešinger, Zdeněk Strakoš: *Golub-Kahan Iterative Bidiagonalization and Stopping Criteria in Ill-Posed Problems*, Seminar on Numerical Analysis SNA '07, Ostrava, January 22–26, 2007.

[L5] Iveta Hnětynková, Martin Plešinger, Diana Maria Sima, Zdeněk Strakoš: *Total Least Squares Problem in Linear Algebraic Systems with Multiple Right-Hand Side*, Seminar on Numerical Analysis SNA '07, Ostrava, January 22–26, 2007.

[L6] Poster: Iveta Hnětynková, Martin Plešinger, Diana Maria Sima, Zdeněk Strakoš, Sabine Van Huffel: *On total least squares formulation in linear approximation problems with multiple right-hand sides*, Seminar on Numerical Analysis SNA '08, Liberec, January 28–February 1, 2008.

[1] This talk was awarded the price of Institute of Computer Science AS CR for the best lecture.

Seminar lectures

[S1] MARTIN PLEŠINGER: *Singular Value Decomposition, Application in Image Deblurring*, Faculty of Mechatronics Seminar, TU Liberec, December 14, 2005.

[S2] MARTIN PLEŠINGER: *Core reduction and least squares problems* $A\,x \approx b$, Faculty of Mechatronics Seminar, TU Liberec, December 21, 2005.

[S3] MARTIN PLEŠINGER: *Core problem, Golub-Kahan bidiagonalization, Lanczos tridiagonalization*, Depatrment of Modelling of Processes Seminar, FM, TU Liberec, April 13, 2006.

[S4] MARTIN PLEŠINGER: *Reduction of data in* $A\,X \approx B$ Seminar at Institute of Computer Science, AS CR, November 14, 2006.

[S5] MARTIN PLEŠINGER: *Solving total least squares problems with multiple right-hand sides* , Institute of Novel Technologies and Applied Informatics Seminar, FM, TU Liberec, February 27, 2007.

[S6] MARTIN PLEŠINGER: *Solving total least squares problems with multiple right-hand sides*, Seminar at Inst. of Computer Science, AS CR, March 13, 2007.

Bibliography

[1] ÅKE BJÖRCK: *Bidiagonal Decomposition and Least Squares*, Presentation, Canberra (2005).
(http://wwwmaths.anu.edu.au/events/sy2005/odatalks/canb05.pdf)

[2] ÅKE BJÖRCK: *A Band-Lanczos Generalization of Bidiagonal Decomposition*, Presentation, Conference in Honor of G. Dahlquist, Stockholm (2006).
(http://www.mai.liu.se/~akbjo/kth06.pdf)

[3] ÅKE BJÖRCK: *A band-Lanczos algorithm for least squares and total least squares problems*, book of abstracts of 4th Total Least Squares and Errors-in-Variables Modeling Workshop, Leuven, Katholieke Universiteit Leuven (2006), pp. 22–23.

[4] ROLAND W. FREUND: *Model reduction methods based on Krylov subspaces*, Acta Numerica, No. 12 (2003), pp. 267–319.

[5] GENE HOWARD GOLUB, WILLIAM KAHAN: *Calculating the singular values and pseudo-inverse of a matrix*, SIAM J. Numer. Anal., Ser. B, 2 (1965), pp. 205–224.

[6] GENE HOWARD GOLUB, CHARLES F. VAN LOAN: *An analysis of the total least squares problem*, Numer. Anal. 17 (1980), pp. 883–893.

[7] GENE HOWARD GOLUB, CHARLES F. VAN LOAN: *Matrix Computations, 3rd edition*, The Johns Hopkins University Press, Baltimore and London, 1996.

[8] PER CHRISTIAN HANSEN: *Regularization Tools – version 3.2 for MALTAB 6.0, a package for analysis and solution of discrete ill-posed problems.*
(http://www2.imm.dtu.dk/~pch/Regutools/index.html).

[9] PER CHRISTIAN HANSEN: *Rank-Deficient and Discrete Ill-Posed Problems, Numerical Aspects of Linear Inversion*, Philadelphia, SIAM Publications, 1998.

[10] PER CHRISTIAN HANSEN, TOKE KOLDBORG JENSEN: *Noise propagation in regularizing iterations for image deblurring*, in preparation.

[11] PER CHRISTIAN HANSEN, JAMES G. NAGY, DIANNE P. O'LEARY: *Deblurring Images: Matrices, Spectra, and Filtering*, Philadelphia, SIAM Publications, 2006.

[12] PER CHRISTIAN HANSEN, MISHA ELENA KILMER, RIKKE KJELDSEN: *Exploiting Residual Information in the Parameter Choice for Discrete Ill-Posed Problems*, BIT, Vol 46 (2006), pp. 41–59.

[13] IVETA HNĚTYNKOVÁ, ZDENĚK STRAKOŠ: *Lanczos tridiagonalization and core problems*, Linear Algebra Appl., Vol. 421 (2007), pp. 243–251.

[14] Iveta Hnětynková, Martin Plešinger, Zdeněk Strakoš: *Lanczos tridiagonalization, Golub-Kahan bidiagonalization and core problem*, PAMM, Proc. Appl. Math. Mech. 6 (2006), pp. 717–718.

[15] Iveta Hnětynková: *Krylov subspace approximations in linear algebraic problems*, Ph.D. thesis, Dept. of Numerical Mathematics, Facutly of Mathematics and Physics, Charles University, Prague, 2006.

[16] Christopher C. Paige: *Bidiagonalization of matrices and solution of linear equations*, SIAM J. Numer. Anal. 11 (1974), pp. 197–209.

[17] Christopher C. Paige, Zdeněk Strakoš: *Core problem in linear algebraic systems*, SIAM J. Matrix Anal. Appl. 27 (2006), pp. 861–875.

[18] Beresford Neill Parlett: *The Symmetric Eigenvalue Problem*, Philadelphia, SIAM Publications, 1998.

[19] Bhaskar D. Rao: *Unified treatment of LS, TLS and truncated SVD methods using a weighted TLS framework*, In: Recent Advances in Total Least Squares Techniques and Errors-in-Variables Modeling (S. Van Huffel, Ed.), Philadelphia, SIAM Publications (1997), pp. 11–20.

[20] Diana Maria Sima, Sabine Van Huffel: *Core problems in $AX \approx B$*, Technical Report, Dept. of Electrical Engineering, Katholieke Universiteit Leuven (2006).

[21] Diana Maria Sima: *Regularization techniques in model fitting and parameter estimation*, Ph.D. thesis, Dept. of Electrical Engineering, Katholieke Universiteit Leuven, 2006.

[22] R. C. Thompson: *Principal submatrices IX: Interlacing inequalities for singular values of submatrices*, Linear Algebra and Applications 5 (1972), pp. 1–12.

[23] Sabine Van Huffel, Joos Vandewalle: *The Total Least Squares Problem: Computational Aspects and Analysis*, Philadelphia, SIAM Publications, 1991.

[24] Sabine Van Huffel (Ed.): *Recent Advances in Total Least Squares Techniques and Errors-in-Variables Modeling*, Proceedings of the Second Int. Workshop on TLS and EIV, Philadelphia, SIAM Publications, 1997.

[25] Sabine Van Huffel, Philippe Lemmerling (Eds.): *Total Least Squares and Errors-in-Variables Modeling: Analysis, Algorithms and Applications*, Dordrecht, Kluwer Academic Publishers, 2002.