The Total Least Squares Problem with Multiple Right-Hand Sides

$AX \approx B$

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Outline

Motivation

I. TLS with single right-hand side

- I.1 Full column rank case
- I.2 An example of rank deficient case
- I.3 Core problem reduction

II. TLS with multiple right-hand sides

- II.1 Problem formulation
- II.2 Analysis by Van Huffel & Vandewalle
- II.3 Complete classification
- II.4 Core problem—SVD-based reduction
- II.5 Generalized Golub-Kahan algorithm
- II.6 TLS solution of a core problem

Summary

Motivation (single right-hand side case)

Consider a simple problem

$$Ax \approx b, \qquad A = [t_1, t_2, \ldots, t_m]^T, \quad x = v, \quad b = [\ell_1, \ell_2, \ldots, \ell_m]^T$$

where ℓ_j are distances *measured* in m times t_j and v is an *unknown* (constant) velocity.

Since the measured distances (and also times) contain *errors*, the problem is not compatible

$$b \notin \mathcal{R}(A),$$

and does not have a solution in the classical sense.

The goal to approximate v using some minimization technique, e.g. *(ordinary) least squares*.

Ordinary Least Squares

Let $Ax \approx b$, where $A \in \mathbb{R}^{m \times n}$, $x \in \mathbb{R}^n$, $b \in \mathbb{R}^m$, then

$$x_{\mathsf{LS}} \equiv \arg\min_{x \in \mathbb{R}^n} \|b - Ax\|$$

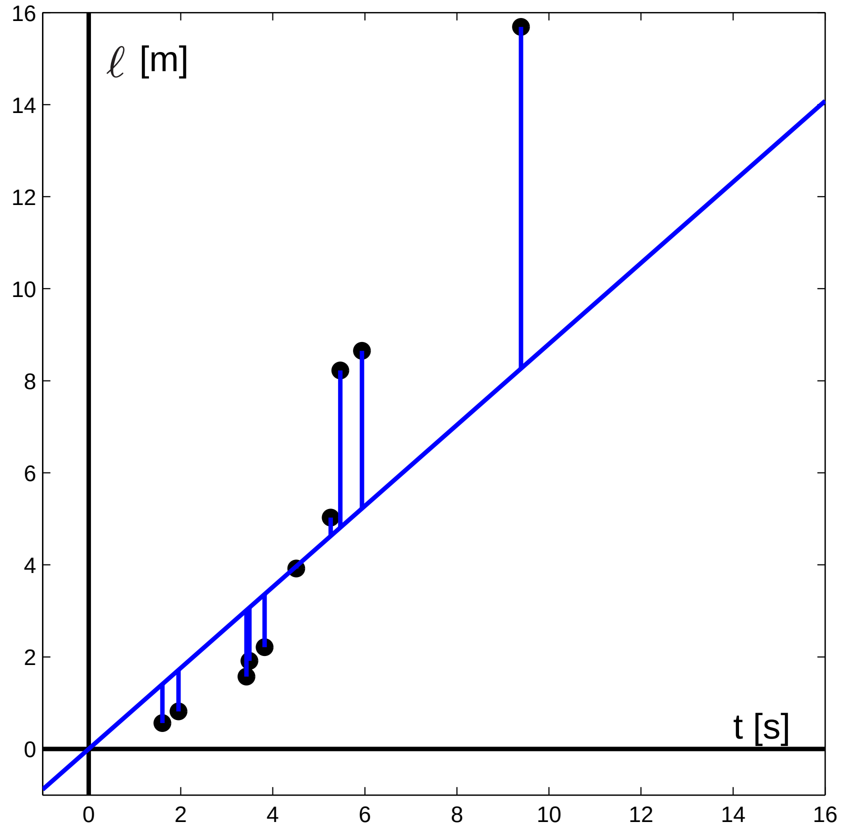
the vector minimizing the residual, is called the *least squares (LS) solution*. Alternatively,

$$\min_{g \in \mathbb{R}^m} \|g\| \quad \text{s.t.} \quad Ax = b + g, \quad (\text{or } \; b + g \in \mathcal{R}(A)).$$

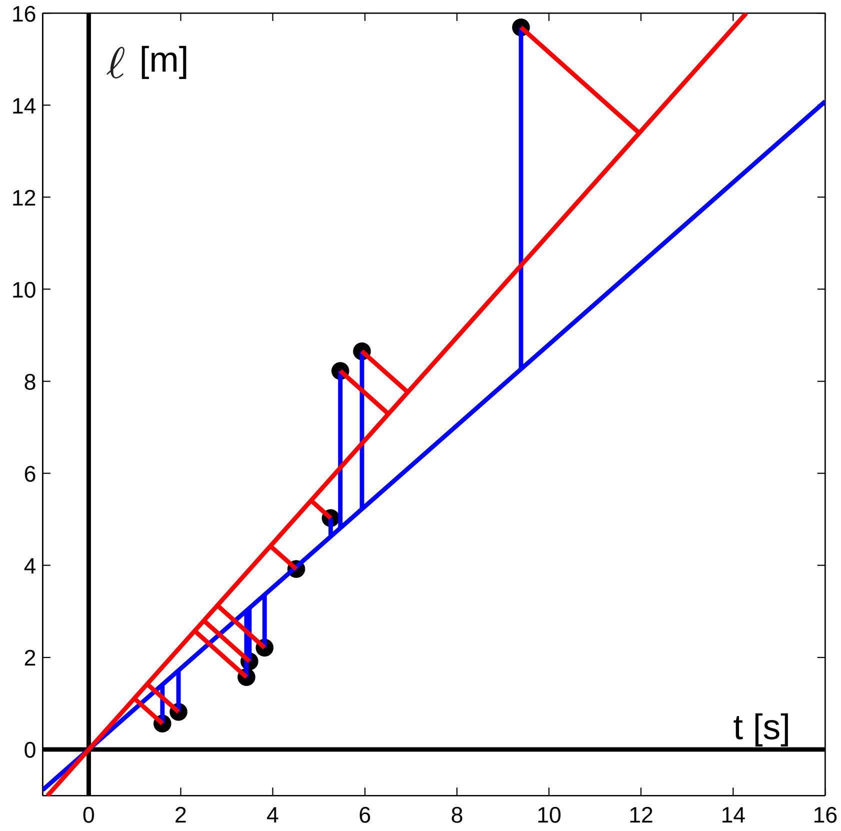
If the LS solution is not unique, then the *minimal* one is considered,

$$x_{\mathsf{LS}} = A^{\dagger} b.$$

LS leads to minimization of sum of squares of “vertical” distances:



The errors may be in both ℓ_js as well as in t_js, let us try, e.g.:



Different Least Squares Approaches

Except of the *ordinary least squares (LS, OLS)* also called *linear regression*,

$$\min_{g\in\mathbb{R}^m} \|g\| \quad \text{s.t.} \quad Ax = b + g, \quad (\text{or } \; b + g \in \mathcal{R}(A)),$$

one can use the *data least squares (DLS)*,

$$\min_{E\in\mathbb{R}^{m\times n}} \|E\|_F \quad \text{s.t.} \quad (A + E)x = b, \quad (\text{or } \; b \in \mathcal{R}(A + E)),$$

or the *total least squares (TLS)* also called *orthogonal regression*, or *errors-in-variables (EIV) modeling*,

$$\min_{g\in\mathbb{R}^m,\, E\in\mathbb{R}^{m\times n}} \|[g, E]\|_F \quad \text{s.t.} \quad (A + E)x = b + g, \quad (\text{or } \; b{+}g \in \mathcal{R}(A{+}E)).$$

Scaling

All three approaches can be unified using the *scaled TLS (ScTLS)*

$$\min_{g\in\mathbb{R}^m,\, E\in\mathbb{R}^{m\times n}} \|[g\gamma, E]\|_F \quad \text{s.t.} \quad (A+E)x = b+g,$$

where $\gamma \in (0,\infty)$. The ScTLS problem:

with	$\gamma = 1$	leads to TLS,
for	$\gamma \longrightarrow 0$	tends to ordinary LS,
for	$\gamma \longrightarrow \infty$	tends to DLS.

See [Paige, Strakoš, 2002a, 2002b].

Scaling of individual columns of A by $S = \text{diag}(s_1, \ldots, s_n)$, $s_i > 0$, and weighting of individual rows by $W = \text{diag}(w_1, \ldots, w_m)$, $w_j > 0$, is also possible. Instead of $Ax \approx b$ we solve $(WAS)y \approx Wb$ with $x = Sy$; see [Golub, Van Loan, 1980].

I. TLS problem (Single right-hand side case)

I.1 Full column rank case

Consider a linear approximation problem

$$A\,x \approx b\,, \qquad \text{or equivalently} \qquad \left[\, b \,\middle|\, A \,\right] \begin{bmatrix} -1 \\ x \end{bmatrix} \approx 0\,,$$

where $A \in \mathbb{R}^{m\times n}$, $b \in \mathbb{R}^{m}$, $A^T b \neq 0$, $b \notin \mathcal{R}(A)$, $\text{rank}(A) = n$, thus $m \geq n+1$.

Total least square (TLS) problem:

$$\min_{e\,,G} \left\| \left[\, e \,\middle|\, G \,\right] \right\|_F \qquad \text{subject to} \qquad (\,A + G\,)\,x = b + e\,.$$

(If there is more than one solution we look for the minimal one.)

Thus we look for a correction $[\, g \,|\, E \,]$ matrix such that

$$[\, b + g \,|\, A + E \,]$$

is:

1) rank deficient, and
2) its null-space contains vector with nonzero first component,

$$\left[\; b + g \;\middle|\; A + E \;\right] \begin{bmatrix} -1 \\ x \end{bmatrix} = 0\,.$$

The *minimal rank-reducing correction* can be obtained by the singular value decomposition (SVD) of the matrix $[\, b \,|\, A \,]$.

The minimal rank reducing correction

Consider the singular value decomposition (SVD),

$$[\, b \,|\, A \,] \;=\; U \,\Sigma\, V^T \;=\; \sum_{j=1}^{n+1} u_j \sigma_j v_j^T \,.$$

Then

$$[\, g \,|\, E \,] \;=\; -\, u_{n+1}\, \sigma_{n+1}\, v_{n+1}^T, \qquad \|[\, g \,|\, E \,]\|_F = \sigma_{n+1}$$

is the minimal rank reducing correction. Since $V^T = V^{-1}$

$$[\, b + g \,|\, A + E \,]\, v_{n+1} \;=\; 0 \,.$$

Denote $v_{n+1} = [\, \nu \,, w^T \,]^T$. If $\nu \neq 0$, then

$$[\, b + g \,|\, A + E \,] \begin{bmatrix} -1 \\ -\frac{1}{\nu}\, w \end{bmatrix} = 0 \,, \qquad \text{and} \qquad x_{\mathsf{TLS}} \;=\; -\frac{1}{\nu}\, w \,.$$

Uniqueness

If $\sigma_n = \sigma_{n+1}$, then the smallest singular value is not unique.

Let $q+1$ be the multiplicity of σ_{n+1}, i.e., $q \geq 0$ and

$$\sigma_{n-q} > \sigma_{n-q+1} = \ldots = \sigma_{n+1} \, .$$

Consider the partitioning

$$V \equiv \begin{bmatrix} \overbrace{\begin{matrix} V_{11}^{(q)} \\ V_{21}^{(q)} \end{matrix}}^{n-q} & \overbrace{\begin{matrix} V_{12}^{(q)} \\ V_{22}^{(q)} \end{matrix}}^{q+1} \end{bmatrix} \begin{matrix} \} \, 1 \\ \} \, n \end{matrix} \, .$$

If $\quad \sigma_1 = \sigma_{n+1} \, , \quad$ then $\quad \sigma_{n-q} \, , \; V_{11}^{(q)} \, , \; V_{21}^{(q)} \quad$ are nonexistent.

Classical results

If $V_{12}^{(q)} \neq 0$ with $q = 0$, then
the TLS problem has the *unique (basic) solution*.

If $V_{12}^{(q)} \neq 0$ with $q > n$, then
the TLS problem has infinitely many solutions, the goal is to find the *minimum norm solution*.

If $V_{12}^{(q)} = 0$, then
the TLS problem *does not have a solution* (but the TLS concept can be extended to the so called *nongeneric solution*; the *classical TLS algorithm*)

See [Golub, Van Loan, 1980], [Van Huffel, Vandewalle, 1991].
Recall that here $V_{12}^{(q)} \in \mathbb{R}^{1\times(q+1)}$.

I.2 An example of rank deficient case

Consider the incompatible problem with rank deficient system matrix

$$\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \xi_1 \\ \xi_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}.$$

With the correction

$$\left[\, g \,\middle|\, E \,\right] = \left[\begin{array}{c|cc} 0 & 0 & 0 \\ 0 & 0 & \varepsilon \end{array}\right], \qquad \varepsilon \neq 0$$

the problem becomes compatible

$$\begin{bmatrix} 1 & 0 \\ 0 & \varepsilon \end{bmatrix} \begin{bmatrix} \xi_1 \\ \xi_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}.$$

Obviously $\| \, [\, g \,|\, E \,] \, \|_F = \varepsilon$, thus there is no minimal correction!

The problem with rank deficient system matrix *does not have a solution*; see [Van Huffel, Vandewalle, 1991].

I.3 Core problem reduction

Consider the TLS formulation

$$\min \|[g|E]\|_F \qquad \text{s.t.} \qquad (A+E)x = b+g$$

and an orthogonal transformation

$$\widetilde{A}\widetilde{x} \equiv (P^T A Q)(Q^T x) \approx (P^T b) \equiv \widetilde{b},$$

where $P^T = P^{-1}$, $Q^T = Q^{-1}$.

Because

$$\|[g|E]\|_F = \left\| P^T [g|E] \begin{bmatrix} 1 & 0 \\ 0 & Q \end{bmatrix} \right\|_F = \|[P^T g | P^T E Q]\|_F \equiv \|[\widetilde{g}|\widetilde{E}]\|_F$$

the TLS formulation is orthogonally invariant.

Let P, Q, be orthogonal matrices such that

$$P^T \left[\, b \,|\, A \,\right] \begin{bmatrix} 1 & 0 \\ 0 & Q \end{bmatrix} = P^T \left[\, b \,|\, A\,Q \,\right] = \underbrace{\begin{bmatrix} b_1 \\ \hline 0 \end{bmatrix}}_{\widetilde{b}} \!\!\!\! \begin{array}{c} \| \\ \| \end{array} \!\!\!\! \underbrace{\begin{array}{c|c} A_{11} & 0 \\ \hline 0 & A_{22} \end{array}}_{\widetilde{A}} .$$

The original problem is decomposed into independent subproblems

$$A_{11}\, x_1 \approx b_1, \qquad \text{and} \qquad A_{22}\, x_2 \approx 0\,,$$

where the second has a solution $x_2 = 0$, and

$$x = Q\,\widetilde{x} = Q \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = Q \begin{bmatrix} x_1 \\ 0 \end{bmatrix}.$$

The solution of the original problem is fully determined by the solution of the first subproblem.

Theorem (Core problem)

For any A, b, $A^T b \neq 0$, $b \notin \mathcal{R}(A)$ there exist orthogonal matrices P, Q, such that

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

and:

(P1) A_{11} is of full *column* rank.

(P2) A_{11} has simple singular values, and b_1 has *nonzero* projections onto all (one-dimensional) left singular vector subspaces of A_{11},

- $[b_1|A_{11}]$ is of full *row* rank.
- The subproblem $A_{11}x_1 \approx b_1$ called *core problem* has minimal dimensions.
- The subproblem $A_{11}x_1 \approx b_1$ *has the unique TLS solution*.

Let x_1 be the unique TLS solution of $A_{11}x_1 \approx b_1$.

If the original problem *has* a TLS solution ($V_{12}^{(q)} \neq 0$), then the vector

$$x \equiv Q \begin{bmatrix} x_1 \\ 0 \end{bmatrix} \tag{1}$$

is identical to the *minimum norm solution* (which is uniqe for $q = 0$).

If the original problem *does not have* a TLS solution ($V_{12}^{(q)} = 0$), then (1) is identical to the (minimum norm) nongeneric solution (introduced in [Van Huffel, Vandewalle, 1991]).

See [Paige, Strakoš, 2006] (also [Hnětynková, Strakoš, 2007], or [Hnětynková, P., Sima, Strakoš, Van Huffel, 2011]).

Construction of the core problem

The core problem can be obtained in three steps:

Step 1: Decomposition of the system matrix A

Step 2: Transformation of the modified right-hand side

Step 3: Final permutation

Step 1: Decomposition of the system matrix A

Consider the singular value decomposition (SVD) of A

$$A = U' \Sigma' V'^T ,$$

$$\Sigma = \text{diag}\,(\varsigma_1' I_{m_1} , \varsigma_2' I_{m_2} , \ldots , \varsigma_k' I_{m_k} , 0) \in \mathbb{R}^{m \times n} ,$$

where $\varsigma_1' > \varsigma_2' > \ldots > \varsigma_k' > 0$.

The original problem is transformed to

$$\left[\, b \,|\, A \,\right] \quad \longrightarrow \quad U'^T \left[\, b \,|\, A V' \,\right] = \left[\, \widetilde{b} \,|\, \Sigma \,\right] ,$$

where $\widetilde{b} \equiv U'^T b$.

Step 2: Transformation of the right-hand side b

Split $\widetilde{b}$ horizontally with respect to the multiplicities of the singular values of A,

$$\left[\,\widetilde{b}\,\middle|\,\Sigma\,\right] = \left[\begin{array}{c||c|c|c|c||c} \widetilde{b}_1 & \varsigma_1'\,I_{m_1} & & & & 0 \\ \hline \widetilde{b}_2 & & \varsigma_2'\,I_{m_2} & & & 0 \\ \hline \vdots & & & \ddots & & \vdots \\ \hline \widetilde{b}_k & & & & \varsigma_k'\,I_{m_k} & 0 \\ \hline\hline \widetilde{b}_{k+1} & 0 & 0 & \cdots & 0 & 0 \end{array}\right].$$

There exist Householder transformation matrices H_j such that

$$H_j^T\,\widetilde{b}_j = \begin{bmatrix} \|\,\widetilde{b}_j\,\|_2 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \in \mathbb{R}^{m_j}, \qquad j = 1,\ldots,k+1,$$

where $m_{k+1} \equiv m - \mathrm{rank}(\,A\,)$.

Denote

$$
\begin{aligned}
S_L &\equiv \text{diag}\,(\, H_1\,,\, H_2\,,\,\ldots\,,\, H_k\,,\, H_{k+1}\,) \in \mathbb{R}^{m\times m}\,,\\
S_R &\equiv \text{diag}\,(\, H_1\,,\, H_2\,,\,\ldots\,,\, H_k\,,\, I_{n-r}\,) \in \mathbb{R}^{n\times n}\,,
\end{aligned}
$$

and thrasnform the problem to

$$
\left[\, \widetilde{b} \,\middle|\, \Sigma \,\right] \qquad \longrightarrow \qquad S_L^T \left[\, \widetilde{b} \,\middle|\, \Sigma\, S_R \,\right] = \left[\, S_L^T\, \widetilde{b} \,\middle|\, \Sigma \,\right].
$$

$S_L^T \widetilde{b}$ has at most one nonzero entry corresponding to each ς_j', e.g.,

$$
\left[\, S_L^T\, \widetilde{b} \,\middle|\, \Sigma \,\right] =
\left[\begin{array}{c||c|ccc||c|ccc}
\|\, \widetilde{b}_1 \,\|_2 & \varsigma_1' & & & & & & & \\
\hline
0 & & \varsigma_1' & & & & & & \\
\vdots & & & \ddots & & & & & \\
0 & & & & \varsigma_1' & & & & \\
\hline\hline
\|\, \widetilde{b}_2 \,\|_2 & & & & & \varsigma_2' & & & \\
\hline
0 & & & & & & \varsigma_2' & & \\
\vdots & & & & & & & \ddots & \\
0 & & & & & & & & \varsigma_2'
\end{array}\right].
$$

Step 3: Final permutation

The nonzero elements in $(\, S_L^T \widetilde{b} \,)$ are permuted up such that

$$\left[\, S_L^T \widetilde{b} \,\middle|\, \Sigma \,\right] \quad \longrightarrow \quad \Pi_L^T \left[\, S_L^T \widetilde{b} \,\middle|\, \Sigma\, \Pi_R \,\right] =$$

$$= \left[\begin{array}{c|c}
\begin{array}{c||c|c|c}
\|\,\widetilde{b}_1\,\|_2 & \varsigma_1' & & \\ \hline
\vdots & & \ddots & \\ \hline
\|\,\widetilde{b}_k\,\|_2 & & & \varsigma_k' \\ \hline\hline
\|\,\widetilde{b}_{k+1}\,\|_2 & 0 & \cdots & 0
\end{array} & 0 \\ \hline
0 & \begin{array}{c|c|c||c}
\varsigma_1'\, I_{(m_1-1)} & & & 0 \\ \hline
 & \ddots & & \vdots \\ \hline
 & & \varsigma_k'\, I_{(m_k-1)} & 0 \\ \hline\hline
0 & \cdots & 0 & 0
\end{array}
\end{array}\right] \equiv$$

$$\equiv \left[\begin{array}{c||c|c}
b_1 & A_{11} & 0 \\ \hline
0 & 0 & A_{22}
\end{array}\right],$$

where the red block contains only ς_j' for which $\widetilde{b}_j \neq 0$.

Summarizing,

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

where $\quad P \equiv U' \, S_L \, \Pi_L \,,\;\; Q \equiv V' \, S_R \, \Pi_R \,.$

Matrices

$U'\,,\,V'$	arise from SVD of A	(in Step 1),
$S_L\,,\,S_R$	arise from the partitioning of $\widetilde{b} = U'^T\,b$	(in Step 2),
$\Pi_L\,,\,\Pi_R$	are permutation matrices	(in Step 3).

Computation (?) of the core problem

Golub-Kahan (GK) iterative bidiagonalization algorithm:

For the given A, b,

$$z_1 \equiv b/\beta_1 \,, \qquad \beta_1 \equiv \|b\| \,,$$

$$\begin{aligned} \alpha_1 \, w_1 &\equiv A^T z_1 \,, \\ \beta_2 \, z_2 &\equiv A w_1 - \alpha_1 \, z_1 \,, \\ &\vdots \\ \alpha_\ell \, w_\ell &\equiv A^T z_\ell - \beta_\ell \, w_{\ell-1} \,, \\ \beta_{\ell+1} \, z_{\ell+1} &\equiv A w_\ell - \alpha_\ell \, z_\ell \,. \end{aligned}$$

with $\alpha_\ell > 0$, $\beta_\ell > 0$ choosen such that $\|z_\ell\| = \|w_\ell\| = 1$.

Denote $Z_k \equiv [z_1, \ldots, z_k]$, $W_k \equiv [w_1, \ldots, w_k]$,

$$L_k \equiv \begin{bmatrix} \alpha_1 & & & \\ \beta_2 & \alpha_2 & & \\ & \ddots & \ddots & \\ & & \beta_k & \alpha_k \end{bmatrix}, \qquad L_{k+} \equiv \begin{bmatrix} \alpha_1 & & & \\ \beta_2 & \alpha_2 & & \\ & \ddots & \ddots & \\ & & \beta_k & \alpha_k \\ & & & \beta_{k+1} \end{bmatrix} = \begin{bmatrix} L_k \\ \beta_{k+1} e_k^T \end{bmatrix}.$$

Then the GK algorithm can be written in a matrix form

$$A^T Z_k = W_k L_k^T,$$
$$A W_k = Z_{k+1} L_{k+},$$

and $Z_k^T Z_k = W_k^T W_k = I_k$.

Since the original problem is incompatible $b \notin \mathcal{R}(A)$, the first the GK breaks down while computing some α_t entry, which separates the core problem

$$[Z_t, Z_t^\perp]^T [b|A] \begin{bmatrix} 1 & 0 \\ 0 & [W_t, W_t^\perp] \end{bmatrix} = \left[\begin{array}{c||ccccc|c} \beta_1 & \alpha_1 & & & & & 0 \\ & \beta_2 & \alpha_2 & & & & 0 \\ & & \ddots & \ddots & & & \vdots \\ & & & \beta_{t-1} & \alpha_{t-1} & & 0 \\ & & & & \beta_t & & 0 \\ \hline 0 & 0 & \cdots & 0 & 0 & & \widehat{A}_{22} \end{array}\right]$$

$$= \left[\begin{array}{c||c|c} \widehat{b}_1 & \widehat{A}_{11} & 0 \\ \hline 0 & 0 & \widehat{A}_{22} \end{array}\right].$$

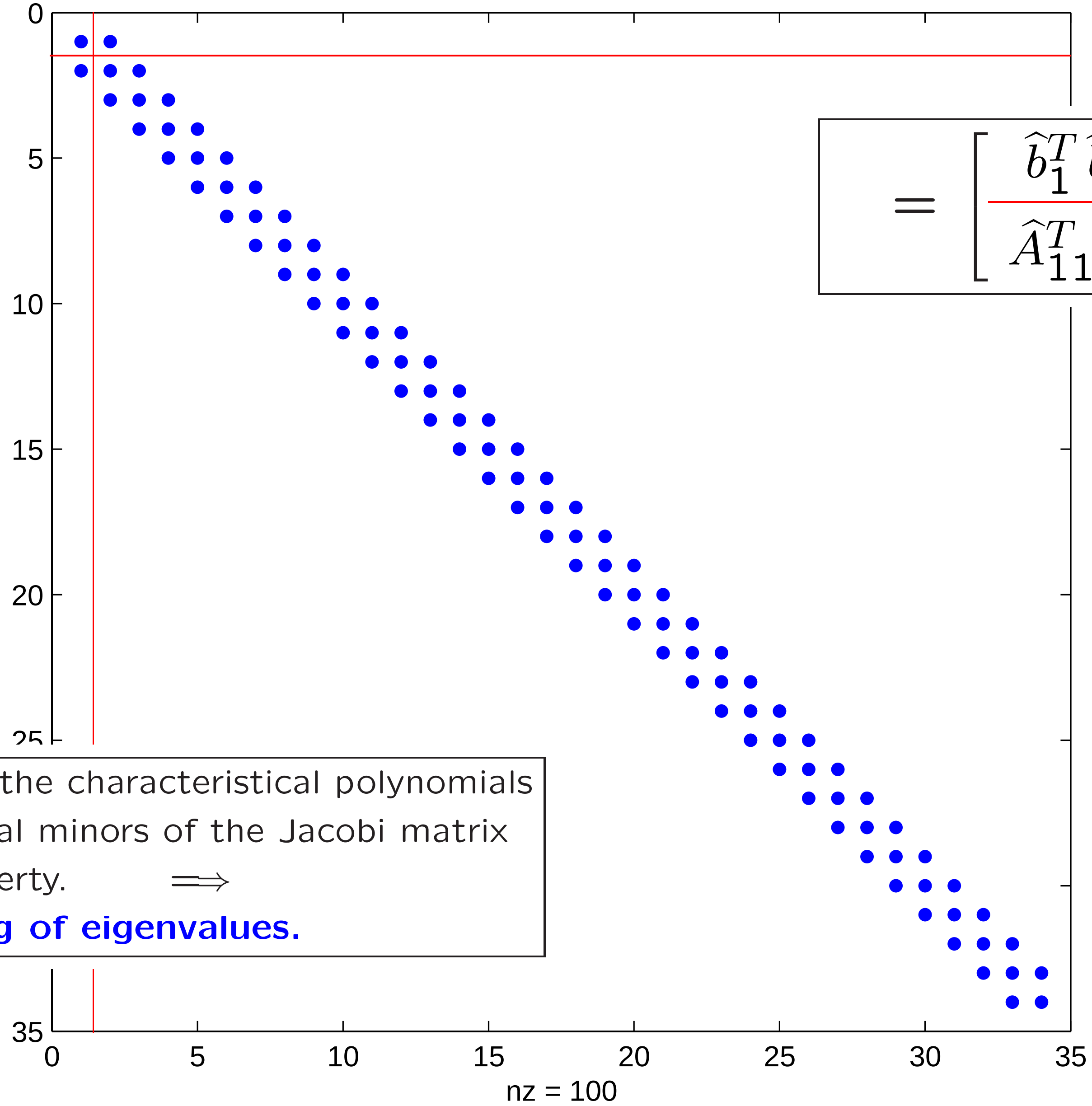
Some of the properties of core problem are obvious (full column rank of $\widehat{A}_{11}$, full row rank of $[\widehat{b}_1|\widehat{A}_{11}]$).

The rest of the properties, including the existence of the *unique TLS solution* can be show exploiting the relationship between eigenvalues of tridiagonal Jacobi tridiagonal

$$\left[\, \widehat{b}_1 \,\middle|\, \widehat{A}_{11} \,\right]^T \left[\, \widehat{b}_1 \,\middle|\, \widehat{A}_{11} \,\right] \qquad \text{and it submatrix} \qquad \widehat{A}_{11}^T \widehat{A}_{11}.$$

See, [Paige, Strakoš, 2006], [Hnětynková, Strakoš, 2007].

tridiagonal Jacobi matrix $[\,\widehat{b}_1 \,|\, \widehat{A}_{11}\,]^T\,[\,\widehat{b}_1 \,|\, \widehat{A}_{11}\,] =$

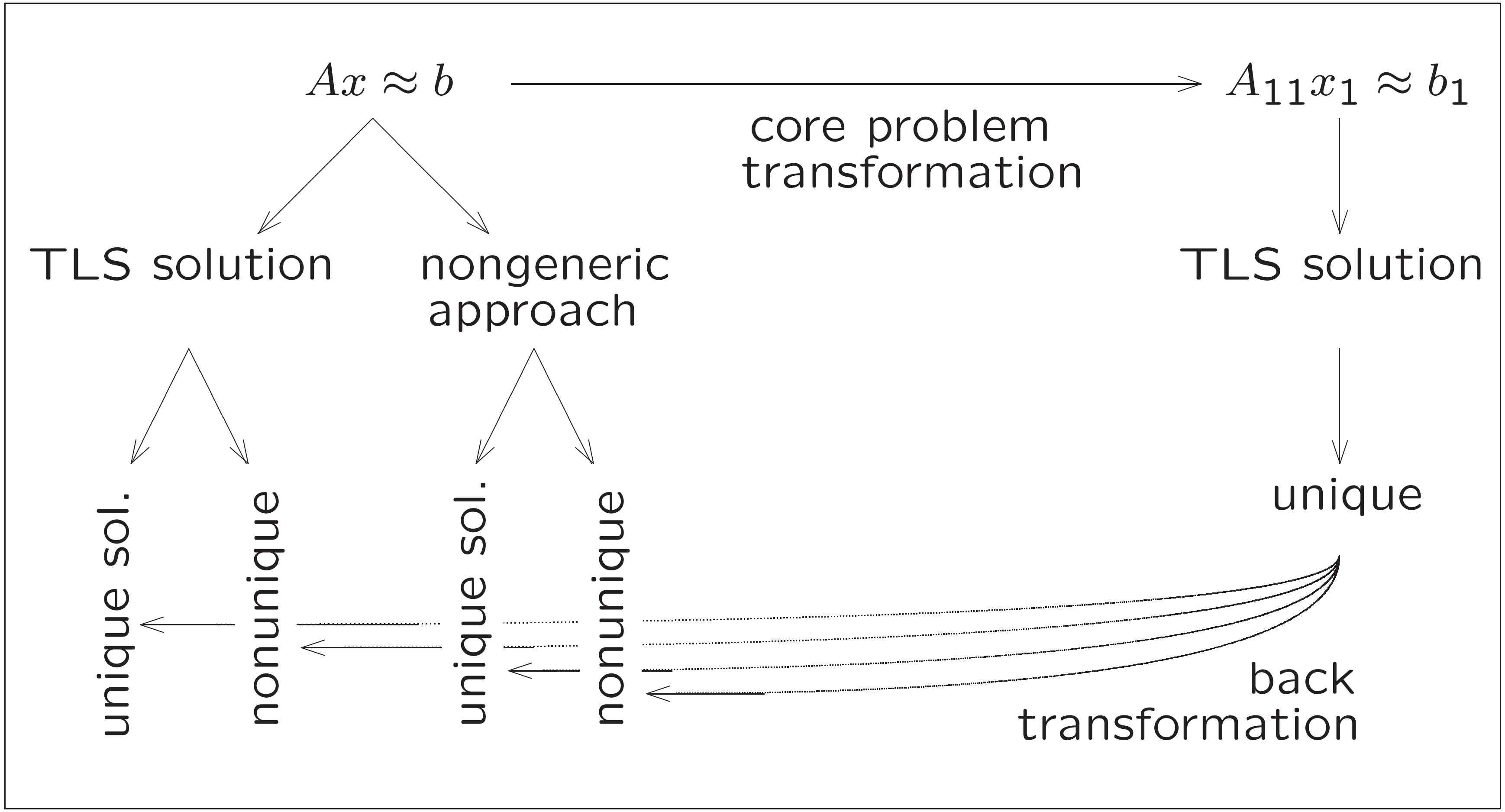


$$= \left[\begin{array}{c|c} \widehat{b}_1^T\,\widehat{b}_1 & \widehat{b}_1^T\,\widehat{A}_{11} \\ \hline \widehat{A}_{11}^T\,\widehat{b}_1 & \widehat{A}_{11}^T\,\widehat{A}_{11} \end{array}\right]$$

The sequence of the characteristical polynomials of leading principal minors of the Jacobi matrix has Sturm's property. $\Longrightarrow$

Strict interlacing of eigenvalues.

Conclusion to the single RHS case



II. Multiple right-hand sides

II.1 Problem formulation

Consider an orthogonally invariant linear approximation problem

$$A\,X \approx B\,, \qquad \text{or equivalently} \qquad \left[\,B\,|\,A\,\right]\left[\frac{-I_d}{X}\right] \approx 0\,,$$

where $A \in \mathbb{R}^{m\times n}\,,\quad B \in \mathbb{R}^{m\times d}\,,\quad A^T B \neq 0\,,\quad m \geq n+d\,.$

Total least square (TLS) problem:

$$\min_{E\,,G} \left\| \left[\,E\,|\,G\,\right] \right\|_F \qquad \text{subject to} \qquad (\,A + G\,)\,X = B + E\,.$$

Consider the SVD,

$$[\, B \,|\, A \,] \;=\; U \, \Sigma \, V^T \,, \qquad \Sigma \;\equiv\; \text{diag}\,(\, \sigma_j \,)\,,$$

$$\sigma_{n-q} \;>\; \sigma_{n-q+1} \;=\; \ldots \;=\; \sigma_{n+1} \;=\; \ldots \;=\; \sigma_{n+e} \;>\; \sigma_{n+e+1}\,,$$

with the partitioning

$$V \;\equiv\; \left[\begin{array}{c|c|c} \overbrace{V_{11}^{(q)}}^{n-q} & \overbrace{V_{12}^{(q,e)}}^{q+e} & \overbrace{V_{13}^{(e)}}^{d-e} \\ \hline V_{21}^{(q)} & V_{22}^{(q,e)} & V_{23}^{(e)} \end{array} \right] \begin{array}{l} \} \, d \\ \} \, n \end{array} \;.$$

If $\sigma_1 \;=\; \sigma_{n+1}\,,$ then $\sigma_{n-q}\,,\; V_{11}^{(q)}\,,\; V_{21}^{(q)}$ are nonexistent.

If $\sigma_{n+1} \;=\; \sigma_{n+d}\,,$ then $\sigma_{n+e+1}\,,\; V_{13}^{(e)}\,,\; V_{23}^{(e)}$ are nonexistent.

II.2 Analysis by Van Huffel & Vandewalle

Classical analysis gives:

If rank $([V_{12}^{(q,e)} \,|\, V_{13}^{(e)}]) = d$ and $q = 0$, then
the TLS problem has the unique (basic) solution.

If rank $([V_{12}^{(q,e)} \,|\, V_{13}^{(e)}]) = d$ and $e = d$, then
the TLS problem has infinitely many solutions, the goal is to find the minimum norm solution.

If rank $([V_{12}^{(q,e)} \,|\, V_{13}^{(e)}]) < d$, then
the TLS problem does not have a solution, but the TLS concept can be extended to the so called nongeneric solution.

See [Van Huffel, Vandewalle, 1991].

Trouble:

The case $[\,V_{12}^{(q,e)}\,|\,V_{13}^{(e)}\,]$ is of full row rank, $q > 0$, and $e < d$, is not analyzed in [Van Huffel, Vandewalle, 1991], a solution is not defined.

The TLS algorithm, by Van Huffel, however gives as an output

$$\mathtt{X} := -[\,V_{22}^{(q,e)}\,|\,V_{23}^{(e)}\,]\,[\,V_{12}^{(q,e)}\,|\,V_{13}^{(e)}\,]^{\dagger}$$

for any problem $A\,X \approx B$ with full row rank $[\,V_{12}^{(q,e)}\,|\,V_{13}^{(e)}\,]$.

See also the truncated-TLS (T-TLS) approach.

II.3 Complete classification

The block $V_{12}^{(q,e)}$ corresponds to the singular value σ_{n+1}, while the block $V_{13}^{(e)}$ corresponds to singular values $\sigma_j < \sigma_{n+1}$.

We propose to look at individual ranks of the matrices $V_{12}^{(q,e)}$, $V_{13}^{(e)}$.

Let $[\, V_{12}^{(q,e)} \,|\, V_{13}^{(e)} \,]$ be full row rank (equal to d).

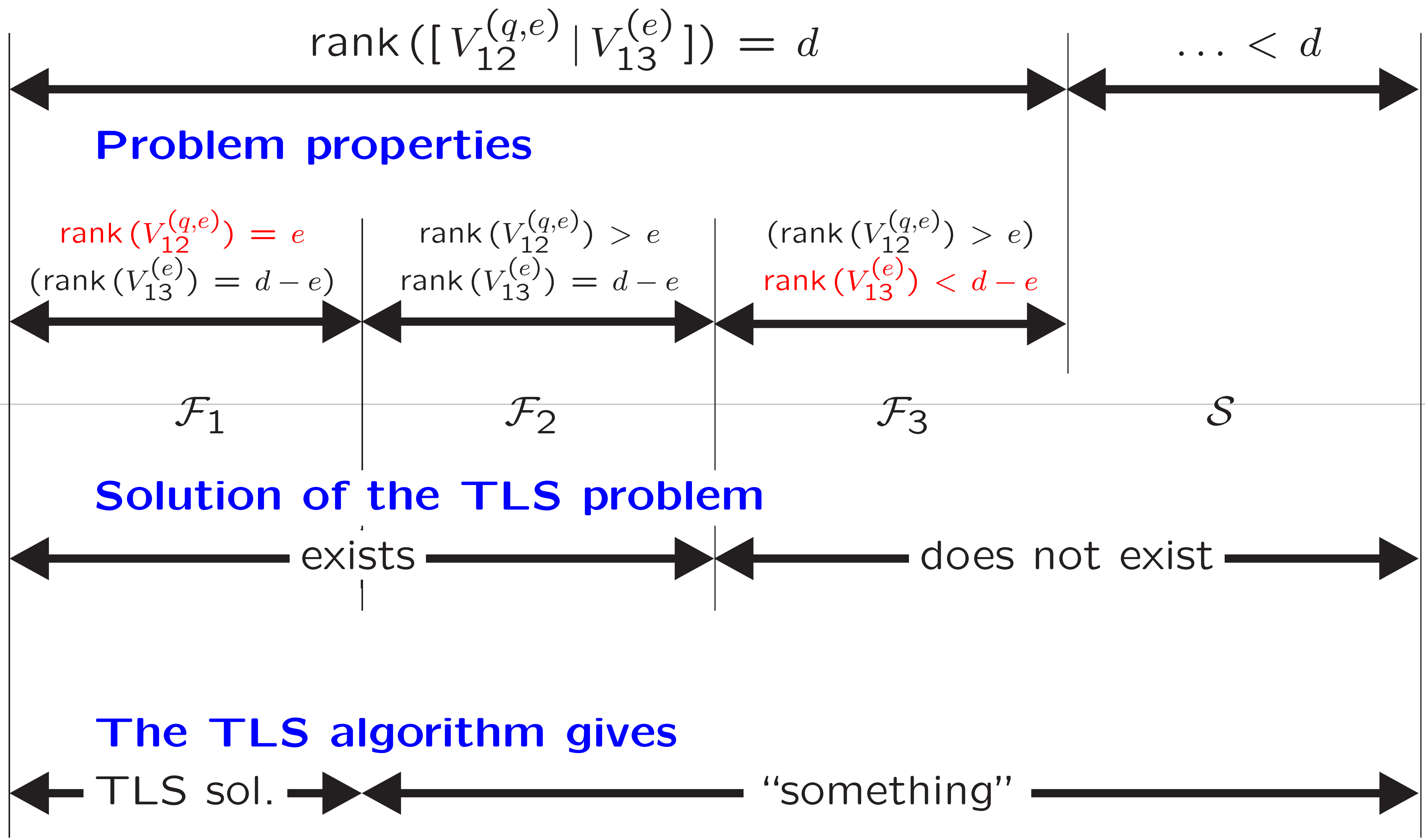
If rank $(V_{12}^{(q,e)}) = e$, then rank $(V_{13}^{(e)}) = d - e$ (maximal),
the TLS problem has a solution (possibly nonunique),
the TLS algorithm computes the minimal norm solution.

Including the cases $q = 0$ and $e = d$ (and also $d = 1$).

If rank $(V_{12}^{(q,e)}) > e$ and rank $(V_{13}^{(e)}) = d - e$, then
the TLS problem has a solution (possibly nonunique),
such solution can not computed by the TLS algorithm.

If rank $(V_{13}^{(e)}) < d - e$, then rank $(V_{12}^{(q,e)}) > e$ and
the TLS problem does not have a solution.

See [Hnětynková, P., Sima, Strakoš, Van Huffel, 2011].



See [Hnětynková, P., Sima, Strakoš, Van Huffel, 2011].

An example of $\mathcal{F}_2$ problem

Let

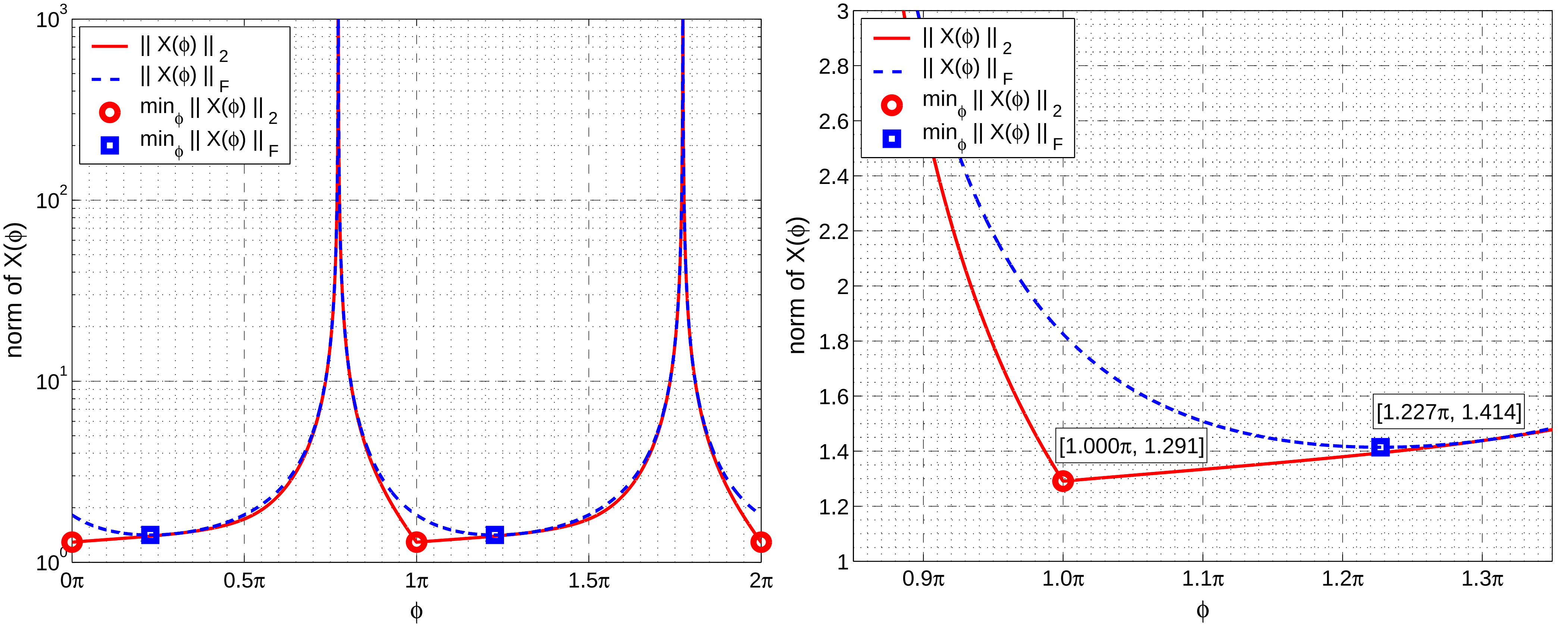
$$\left[\, B \,|\, A \,\right] \equiv U \left[\begin{array}{c|cc|c} 3 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 1 \end{array}\right] \left(\frac{1}{4} \left[\begin{array}{c|cc|c} -1 & -3 & \sqrt{3} & \sqrt{3} \\ 3 & -1 & \sqrt{3} & -\sqrt{3} \\ \hline \sqrt{3} & \sqrt{3} & 1 & 3 \\ \sqrt{3} & -\sqrt{3} & -3 & 1 \end{array}\right] \right)^T,$$

where $A \in \mathbb{R}^{4\times 2}$, $B \in \mathbb{R}^{4\times 2}$ (it is easy to verify that $A^T B \neq 0$). Here $q = 1$, $e = 1$,

$$V_{12}^{(q,e)} = \frac{1}{4}\begin{bmatrix} -3 & \sqrt{3} \\ -1 & \sqrt{3} \end{bmatrix}, \qquad V_{13}^{(e)} = \frac{1}{4}\begin{bmatrix} \sqrt{3} \\ -\sqrt{3} \end{bmatrix},$$

have rank two and one, respectively.

$\mathcal{F}_2$ problem and the minimum norm solution



II.4 Core problem—SVD-based reduction

For a given A, B, there exist orthogonal matrices P, Q, R, such that

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

where A_{22} may be nonexistent. The reduced problem

$$A_{11}\, X_1 \approx B_1 \qquad \text{satisfies:}$$

(P1) Matrices A_{11}, B_1 are of full *column* rank,

(P2) Matrices $U_{A,j}^T B_1$, where $U_{A,j}$ denotes a basis of the jth left Singular vector subspace of A_{11}, are of full *row* rank.

- Matrix $[B_1|A_{11}]$ is of full *row* rank.
- The subproblem called *core problem* has minimal dimensions.

Construction of the core problem

The core problem can be obtained in four subsequent steps:

Step 0: Preprocessing of the right-hand side B

Step 1: Decomposition of the system matrix A

Step 2: Transformation of the modified right-hand side

Step 3: Final permutation

Manuscript(s) [Hnětynková, P., Strakoš, 2012-3?].

Step 0: Preprocessing of the right-hand side B

Consider SVD of B,

$$B = U_B \Sigma_B V_B^T .$$

Define

$$\left[\, C \,\middle|\, 0 \,\right] \equiv U_B \Sigma_B , \quad \text{where} \quad C \in \mathbb{R}^{m \times s}, \quad s \equiv \text{rank}\,(B) .$$

Multiplication by $\text{diag}\,(V_B, I_n)$ and omitting zero columns in gives

$$\left[\, B \,\middle|\, A \,\right] \quad \longrightarrow \quad \left[\, B V_B \,\middle|\, A \,\right] \quad \longrightarrow \quad \left[\, C \,\middle|\, A \,\right] .$$

The new problem has the right-hand side C with **mutually orthogonal and nonzero columns**.

Step 1: Decomposition of the system matrix A

Consider SVD of A

$$A = U' \Sigma' V'^T ,$$

$$\Sigma = \mathrm{diag}\,(\varsigma'_1 I_{m_1} , \varsigma'_2 I_{m_2} , \ldots , \varsigma'_k I_{m_k} , 0) \in \mathbb{R}^{m \times n} ,$$

where $\varsigma'_1 > \varsigma'_2 > \ldots > \varsigma'_k > 0$.

The original problem is transformed to

$$\left[\, C \, \middle| \, A \, \right] \qquad \longrightarrow \qquad U'^T \left[\, C \, \middle| \, A V' \, \right] = \left[\, \tilde{C} \, \middle| \, \Sigma' \, \right] ,$$

where $\tilde{C} \equiv U'^T C$.

Step 2: Transformation of the right-hand side C

Split $\widetilde{C}$ horizontally with respect to the multiplicities of the singular values of A,

$$\left[\, \widetilde{C} \,\middle|\, \Sigma' \,\right] = \left[\begin{array}{c||c|c|c||c} \widetilde{C}_1 & \varsigma_1' I_{m_1} & & & \\ \hline \vdots & & \ddots & & 0 \\ \hline \widetilde{C}_k & & & \varsigma_k' I_{m_k} & \\ \hline\hline \widetilde{C}_{k+1} & & 0 & & 0 \end{array}\right].$$

Compute SVD of $\widetilde{C}_j$ and define

$$\begin{bmatrix} D_j \\ 0 \end{bmatrix} \equiv U_j^T \widetilde{C}_j = \Sigma_j V_j^T, \qquad D_j \in \mathbb{R}^{r_j \times s}$$

where $r_j \equiv \text{rank}(\widetilde{C}_j) \le \min\{m_j, s\}$, for $j = 1, \ldots, k+1$,
D_j have **mutually orthogonal and nonzero rows**.

Denote

$$S_L \equiv \text{diag}\,(\,U_1\,,\,U_2\,,\,\ldots\,,\,U_k\,,\,U_{k+1}\,) \in \mathbb{R}^{m\times m}\,,$$
$$S_R \equiv \text{diag}\,(\,U_1\,,\,U_2\,,\,\ldots\,,\,U_k\,,\,I_{n-r}\,) \in \mathbb{R}^{n\times n}\,.$$

Then the problem is transformed to

$$\left[\,\widetilde{C}\,\middle|\,\Sigma_A\,\right] \qquad \longrightarrow \qquad S_L^T\left[\,\widetilde{C}\,\middle|\,\Sigma_A\,S_R\,\right] = \left[\,S_L^T\,\widetilde{C}\,\middle|\,\Sigma_A\,\right].$$

The matrix $(\,S^T\,\widetilde{C}\,)$ contains exactly r_j nonzero rows corresponding to the singular value (and to the zero block), e.g.,

$$\left[\,S^T\,\widetilde{C}\,\middle|\,\Sigma_A\,\right] = \left[\begin{array}{c||c|c||c|c}
D_1 & \varsigma_1'\,I_{r_1} & & & \\
\hline
0 & & \varsigma_1' & & \\
\vdots & & \ddots & & \\
0 & & \varsigma_1' & & \\
\hline\hline
D_2 & & & \varsigma_2'\,I_{r_2} & \\
\hline
0 & & & & \varsigma_2' \\
\vdots & & & & \ddots \\
0 & & & & \varsigma_2'
\end{array}\right].$$

Step 3: Final permutation

The nonzero rows in $(S_L^T \, \tilde{C} \,)$ are permuted up such that

$$\left[\, S^T \, \tilde{C} \, \middle| \, \Sigma_A \, \right] \qquad \longrightarrow \qquad \Pi_L^T \left[\, S_L^T \, \tilde{C} \, \middle| \, \Sigma_A \, \Pi_R \, \right] =$$

$$= \left[\begin{array}{c|c} \begin{array}{c||c|c|c} D_1 & \varsigma_1' \, I_{r_1} & & \\ \hline \vdots & & \ddots & \\ \hline D_k & & & \varsigma_k' \, I_{r_k} \\ \hline \hline D_{k+1} & & 0 & \end{array} & 0 \\ \hline 0 & \begin{array}{c|c|c||c} \varsigma_1' \, I_{(m_1 - r_1)} & & & \\ \hline & \ddots & & 0 \\ \hline & & \varsigma_k' \, I_{(m_k - r_k)} & \\ \hline \hline & 0 & & 0 \end{array} \end{array} \right] \equiv$$

$$\equiv \left[\begin{array}{c||c|c} B_1 & A_{11} & 0 \\ \hline 0 & 0 & A_{22} \end{array} \right] ,$$

where the red block contains only ς_j' for which $r_j > 0$.

Summary of the SVD-based reduction:

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

where

$$P \equiv U'\,S_L\,\Pi_L\,, \qquad Q \equiv V'\,S_R\,\Pi_R\,, \qquad R \equiv V_B\,.$$

Matrices

V_B	arises from SVD of B	(in Step 0),
$U'\,,\ V'$	arise from SVD of A	(in Step 1),
$S_L\,,\ S_R$	arise from the partitioning of $\tilde{C} = U'^T\,C$	(in Step 2),
$\Pi_L\,,\ \Pi_R$	are permutation matrices	(in Step 3).

Dimensions of $A_{11}X_1 \approx B_1$ are *minimal*.

II.5 Generalized Golub-Kahan algorithm

The generalized GK of A starting with B gives a subproblem, e.g.,

$$\left[\, \widetilde{B}_1 \,\middle|\, \widetilde{A}_{11} \,\right] = \left[\begin{array}{ccc||ccccccc} \gamma_1 & \beta_{12} & \beta_{13} & \alpha_1 & & & & & & \\ & \gamma_2 & \beta_{23} & \beta_{24} & \alpha_2 & & & & & \\ & & \gamma_3 & \beta_{34} & \beta_{35} & \alpha_3 & & & & \\ & & & \gamma_4 & \beta_{45} & \beta_{46} & \alpha_4 & & & \\ & & & & & \gamma_5 & \beta_{57} & \alpha_5 & & \\ & & & & & & \gamma_6 & \beta_{68} & & \\ & & & & & & & \gamma_7 & \alpha_6 & \\ & & & & & & & & \gamma_8 & \alpha_7 \\ & & & & & & & & & \gamma_9 \end{array}\right],$$

where $\alpha_j > 0$, $\gamma_\ell > 0$.

Proposed by Björck in several talks. Manuscript(s) [Hnětynková, P., Strakoš, 2012-3?].

Analysis of properties of the subproblem $[\,\widetilde{B}_1\,|\,\widetilde{A}_{11}\,]$

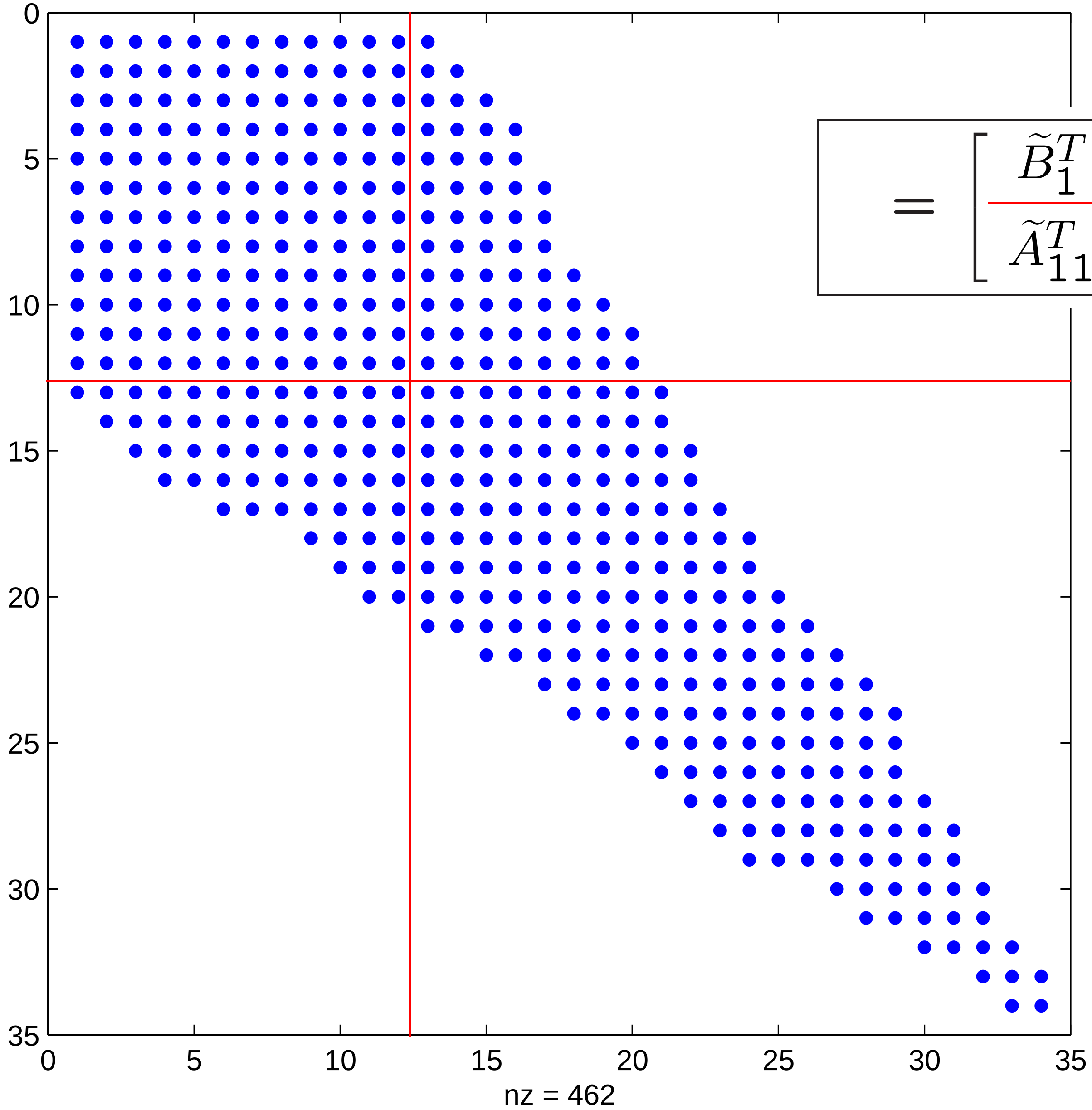
is based on it relationship to the so-called "wedge-shaped" matrix

$$\left[\,\widetilde{B}_1\,|\,\widetilde{A}_{11}\,\right]^T\left[\,\widetilde{B}_1\,|\,\widetilde{A}_{11}\,\right] \qquad \text{and it submatrix} \qquad \widetilde{A}_{11}^T\,\widetilde{A}_{11}\,.$$

The "wedge-shaped" matrices represent generalization of the (tridiagonal) Jacobi matrices.

Manuscript(s) [Hnětynková, P., Strakoš, 2012-3?].

"Wedge-shaped" matrix $[\,\widetilde{B}_1 \,|\, \widetilde{A}_{11}\,]^T [\,\widetilde{B}_1 \,|\, \widetilde{A}_{11}\,] =$



$$= \left[\begin{array}{c|c} \widetilde{B}_1^T \widetilde{B}_1 & \widetilde{B}_1^T \widetilde{A}_{11} \\ \hline \widetilde{A}_{11}^T \widetilde{B}_1 & \widetilde{A}_{11}^T \widetilde{A}_{11} \end{array} \right]$$

II.6 TLS solution of a core problem

Let

$$P^T[B|A]\left[\begin{array}{cc} R & 0 \\ 0 & Q \end{array}\right] = \left[\begin{array}{c|c||c|c} B_1 & 0 & A_{11} & 0 \\ \hline 0 & 0 & 0 & A_{22} \end{array}\right]$$

and let $\mathtt{X}$, $\mathtt{X}_1$ be the matrices returned by the TLS algorihtm applied on the original problem and its core problem, respectively. Then

$$\mathtt{X} = Q\left[\begin{array}{cc} \mathtt{X}_1 & 0 \\ 0 & 0 \end{array}\right].$$

The core problem reduction does not change the output of the TLS algoritm.

The original is in one of the four classes $\mathcal{F}_\ell$, $\ell = 1, 2, 3$, $\mathcal{S}$.

And the core problem?

Example (decomposable core problem):

Let

$$\left[\, B_1 \,\middle|\, A_{11} \,\right] = \left[\begin{array}{c|c||c|c} B_{1,I} & 0 & A_{11,I} & 0 \\ \hline 0 & B_{1,II} & 0 & A_{11,II} \end{array}\right],$$

be a problem with the two *independent* subproblems (components)

$$A_{11,I}\, X_{1,I} \approx B_{1,I}\,, \qquad A_{11,II}\, X_{1,II} \approx B_{1,II}.$$

The composed problem represents a core problem *if and only if* both subproblems represent core problems.

Let both, the red and the blue components be problems with *single* right hand side, i.e.,

- both belong to the set $\mathcal{F}_1$,
- both have the *uniqe TLS solution*,
- these solutions are computed by the TLS algoritm.

Depending on the relationship between the singular values of both components, the *core problem*

$$A_{11} X_1 \approx B_1 \in \mathcal{F}_1,\ \ \mathcal{F}_2, \text{ or } \mathcal{S}.$$

Composition of three single right-hand side core problems can form a core problem from the set $\mathcal{F}_3$.

Consequently:

- The core problem with multiple right-hand side can belong in *any* of the four classes $\mathcal{F}_\ell$, $\ell = 1, 2, 3$, $\mathcal{S}$,
- and thus it *does not have* a TLS solution in general.

(It can be, however, shown, that any core problem that belongs to the class $\mathcal{F}_1$ has the *unique* TLS solution.)

For example, if

$$\sigma_{\min}([\, B_{1,I} \,|\, A_{11,I}]) \;>\; \sigma_1([\, B_{1,II} \,|\, A_{11,II}]) \,,$$

then the core problem $A_{11}\, X_1 \approx B_1$ *does not have the TLS solution*.

Moreover, the TLS algoritm returns

$$\mathtt{X}_1 = \left[\begin{array}{c|c} \mathtt{X}_{1,I} & 0 \\ \hline 0 & 0 \end{array}\right], \qquad \text{indstead of expected} \qquad \left[\begin{array}{c|c} \mathtt{X}_{1,I} & 0 \\ \hline 0 & \mathtt{X}_{1,II} \end{array}\right].$$

The second (small) subproblem is *neglected* by the algorithm (regularization).

Consequently:

- The composition of core problems and does not preserve the output of the TLS algoritm.

Summary

In the single right hand-side case, the problem core reduction yields the subproblem having the unique (basic) solution, which allows to define the solution for the original problem, for any data b, A. Moreover, this solution is identical to one of the output of the TLS algorithm, which makes the whole theory clear and consistent with the computational approach.

In the multiple right hand-sides, the core problem reduction does not ensure existence of unique (basic) solution of the resulting subproblem. The core problem can belong in any of the four classes.

The main open question

How to detect decomposable core problem?

Conjecture:

Any core problem that belongs to class $\mathcal{F}_2$, $\mathcal{F}_3$, or $\mathcal{S}$ is decomposable, i.e. the core problem:

- has the unique TLS solution
- or it is decomposable.

References

Björck: *Bidiagonal Decomposition and Least Squares*, Talk, Canberra, 2005.
Björck: *A Band-Lanczos Generalization of Bidiagonal Decomp.*, Talk, Stockholm, 2006.
Golub, Van Loan: *An analysis of the total least squares problem*, Numer. Anal., 1980.
Hnětynková, P., Strakoš: *Lanczos tridiagonalization, GK bidiag. and core problem*, PAMM, 2006.
Hnětynková, Strakoš: *Lanczos tridiagonalization and core problems*, LAA, 2007.
Hnětynková, P., Sima, Strakoš, Van Huffel: *The TLS pb. in $AX \approx B$: A new classification*, SIMAX 2011.
Hnětynková, P., Strakoš: *On a core pb. within linear approx. pbs. $AX \approx B$ with multiple rhs.*, Manuscript 2012-3?
Hnětynková, P., Strakoš: *Band gen. of GK bidiag., generalized Jacobi matrices, and the core pb.*, Manuscript 2012-3?
Paige, Strakoš: *Scaled TLS fundamentals*, Numerische Mathematik, 2002.
Paige, Strakoš: *Unifying LS, TLS and DLS*, in TLS and EIV Modelling, 2002.
Paige, Strakoš: *Core problem in lin. alg. systems*, SIMAX, 2006.
Van Huffel, Vandewalle: *The TLS Problem: Computational aspects and analysis*, SIAM, 1991.

Related works

Sungwoo Park: *Matrix reduction in numerical optimization*, Dept of CS, Uni of Maryland, 2011.
Jörg Lampe: *Solving Regularized TLS Based on Eigenproblems*, TU Hamburg-Harburg, 2010.

THANK YOU

FOR YOUR ATTENTION