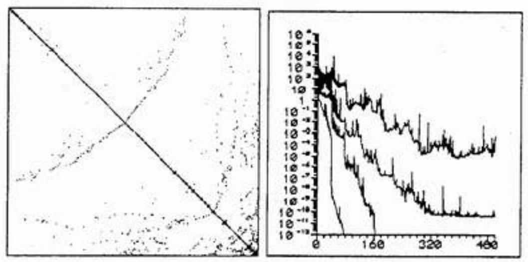
Total least squares problem in linear algebraic systems with multiple right-hand side

< *work in progress* >



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I. Single right-hand side

Consider an orthogonally invariant linear approximation problem

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

where $A \in \mathbb{R}^{m\times n}$, $b \in \mathbb{R}^{m}$, assume $A^T b \neq 0$ and $m > n$.

The **total least square** (**TLS**) **problem** for given A, b:

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

The solution of TLS problem may not exist!

Consider the system

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

then with

$$\left[\, e \,|\, G \,\right] = \left[\begin{array}{c|cc} 0 & 0 & 0 \\ 0 & 0 & \epsilon \end{array}\right], \qquad \epsilon \neq 0$$

the system is compatible

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

Obviously $\| \, [\, e \,|\, G \,] \, \|_F = \epsilon$, thus there is no minimal correction!

I.1 Classical analysis

Consider the singular value decomposition (SVD), $[\, b \,|\, A \,] = U \Sigma V^T$, where σ_j, u_j, v_j, denote the jth singular value, left and right singular vector, respectively, $j = 1, \dots, n+1$. Assuming $\gamma \neq 0$,

$$\left[\frac{-1}{x_{\text{TLS}}}\right] = -\gamma^{-1} v_{n+1} = -\gamma^{-1} \left[\frac{\gamma}{w}\right],$$

$$\left[\, e \,|\, G \,\right] = -u_{n+1} \sigma_{n+1} v_{n+1}^T .$$

Existence? Sufficient condition:

$$\sigma_n'(A) > \sigma_{n+1} \quad \Longrightarrow \quad \gamma \neq 0 .$$

[Golub, Van Loan, 1980]

If $\gamma = 0$, then the solution can not be computed from v_{n+1}.

Compute x_{TLS} from the vector $v_p \equiv \max_j \{ v_j : e_1^T v_j \neq 0 \}$,

$$\begin{bmatrix} -1 \\ \hline x_{\text{TLS}} \end{bmatrix} = -\left(e_1^T v_p \right)^{-1} v_p, \qquad \left[e \,|\, G \right] = -u_p \sigma_p v_p^T .$$

This solves for any A, b, the modified constrained problem

$$\min_{e, G, x} \left\| \left[e \,|\, G \right] \right\|_F \qquad \text{subject to} \qquad (A + G)x = b + e,$$
$$\left[e \,|\, G \right] \left[v_{p+1}, \ldots, v_{n+1} \right] = 0 .$$

[**Van Huffel, Vandewalle, 1991**]: **nongeneric solution**.

Uniqueness

If σ_{n+1} respectively σ_p is not simple, then the solution is nonunique, see [**Golub, Van Loan, 1980**] and [**Van Huffel, Vandewalle, 1991**].

Relationship between the basic and nongeneric solution

The Van Huffel, Vandewalle idea of nongeneric solution is a consistent extension of Golub, Van Loan basic solution.

Consequently: A (possibly nongeneric) solution for any A, b, but two different concepts.

I.2 Data reduction in $A\,x \approx b$

For a given A, b, there are orthogonal matrices P, Q such that

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

The original problem is decomposed into independent subproblems

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

The second subproblem may be nonexistent.

Consider $x_2 = 0$; the first subproblem contains all sufficient information for solving the original problem, $x = Q\,[\,x_1^T \,|\, 0\,]^T$.

[Paige, Strakoš, 2006]

Data reduction based on the SVD of A

Using SVD of A, a suitable choice of a bases of singular vector subspaces gives (after permutation) the decomposition satisfying:

(P1) A_{11} *has full column rank,*
(P2) $[\, b_1 \,|\, A_{11} \,]$ *has full row rank,*
(P3) b_1 *has nonzero projections onto all left singular vector subspaces of* A_{11} *,*
(P4) *singular values of* A_{11} *are simple and nonzero.*

Consequently, the subproblem given by SVD is also minimal; it contains all **necessary and sufficient** information for solving the original problem.

[**Paige, Strakoš, 2006**]

Data reduction based on the Golub-Kahan bidiagonalization

The partial Golub-Kahan iterative bidiagonalization (GK) of A starting from the vector $b/\|b\|_2$ gives a subproblem $\tilde{A}_{11}\,\tilde{x}_1 \approx \tilde{b}_1$ satisfying the properties (P1) and (P2).

The relationship of the GK of A with the Lanczos tridiagonalization of $A\,A^T$ and $A^T\,A$, and the properties of Jacobi matrices gives (P3), (P4), and, moreover

(P5) *singular values of* $[\,\tilde{b}_1 \,|\, \tilde{A}_{11}\,]$ *are simple.*

[**Paige, Strakoš, 2006**], [**Hnětynková, Strakoš, 2006**]

Relationship between these two subproblems

Both subproblems have the properties (P1) – (P4), and thus they are minimal (have minimal dimensions),

both represent the **core subproblem**,
however in different coordinates.

Fundamental data decomposition

- The core subproblem contains all necessary and sufficient information for solving the original problem.
- All irrelevant and redundant information is removed into the matrix A_{22} .

Properties of core problem

From the properties of Jacobi matrices it follows that the core problem always satisfies the Golub-Kahan condition for the existence of the solution of the TLS problem.

Consequently:

- the core problem always has the basic solution,
- the solution of the core problem is always unique,
- the solution of the core problem, transformed to the original coordinates is the (nongeneric) solution of the original problem.

[**Paige, Strakoš, 2006**]

II. Multiple right-hand sides

Consider an orthogonally invariant linear approximation problem

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

where $A \in \mathbb{R}^{m\times n}$, $B \in \mathbb{R}^{m\times d}$, assume $A^T B \neq 0$, $m \geq n + d$, and B has full column rank.

The **total least square (TLS) problem** for given A, B:

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

II.1 Extension of the classical analysis

Consider the SVD, $[\,B\,|\,A\,] = U\,\Sigma\,V^T$, where σ_j, u_j, v_j, denote the jth singular value, left and right singular vector, respectively, $j = 1, \ldots, n+d$. Assuming $\det(\Gamma) \neq 0$,

$$\left[\frac{-I_d}{X_{\mathsf{TLS}}}\right] = -\Gamma^{-1}\left[\, v_{n+1}, \ldots, v_{n+d} \,\right] = -\Gamma^{-1}\left[\frac{\Gamma}{W}\right],$$

$$\left[\; E \,|\, G \;\right] = -\sum_{j=1}^{d} u_i\,\sigma_i\,v_i^T .$$

(A concept of a nongeneric solution has also been developed.)

[**Van Huffel, Vandewalle, 1991**]

Troubles with multiple singular values

[**Van Huffel, Vandewalle, 1991**] analyze special cases (for special distributions of singular values of $[\,B\,|\,A\,]$).

In full generality, the situation with multiple right-hand sides **has not been fully analyzed yet**:

- there is no known general a-priori condition for existence of the solution,
- a meaning of a nongeneric solution is not so clear.

II.2 Data reduction in $A\,X \approx B$

The challenge is: For a given A, B, find orthogonal matrices P, Q, R, such that

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

The original problem is decomposed into independent subproblems

$$A_{11}\,X_1 \approx B_1\,, \qquad \text{and} \qquad A_{22}\,X_2 \approx 0\,.$$

The transformation into the described form always exists (A_{22} may be nonexistent).

Consider $X_2 = 0$; the first subproblem contains all sufficient information for solving the original problem.

Data reduction based on the SVD of A

Using SVD of A, a suitable choice of a bases of singular vector subspaces gives (after permutation) the decomposition satisfying:

(P1) A_{11} *and* B_1 *have full column rank,*

(P2) $[\, B_1 \,|\, A_{11} \,]$ *has full row rank,*

(P3) *projections* $(\, U_j^T B_1 \,)$ *of* B_1 *onto all left singular vector subspaces* U_j *of* A_{11} *have full row rank,*

(P4) *singular values of* A_{11} *are nonzero with multiplicities at most* d *.*

Question: Is the constructed subproblem minimal? Or, equivalently, does this problem contain only necessary information?

Data reduction based on the band generalization of the GK

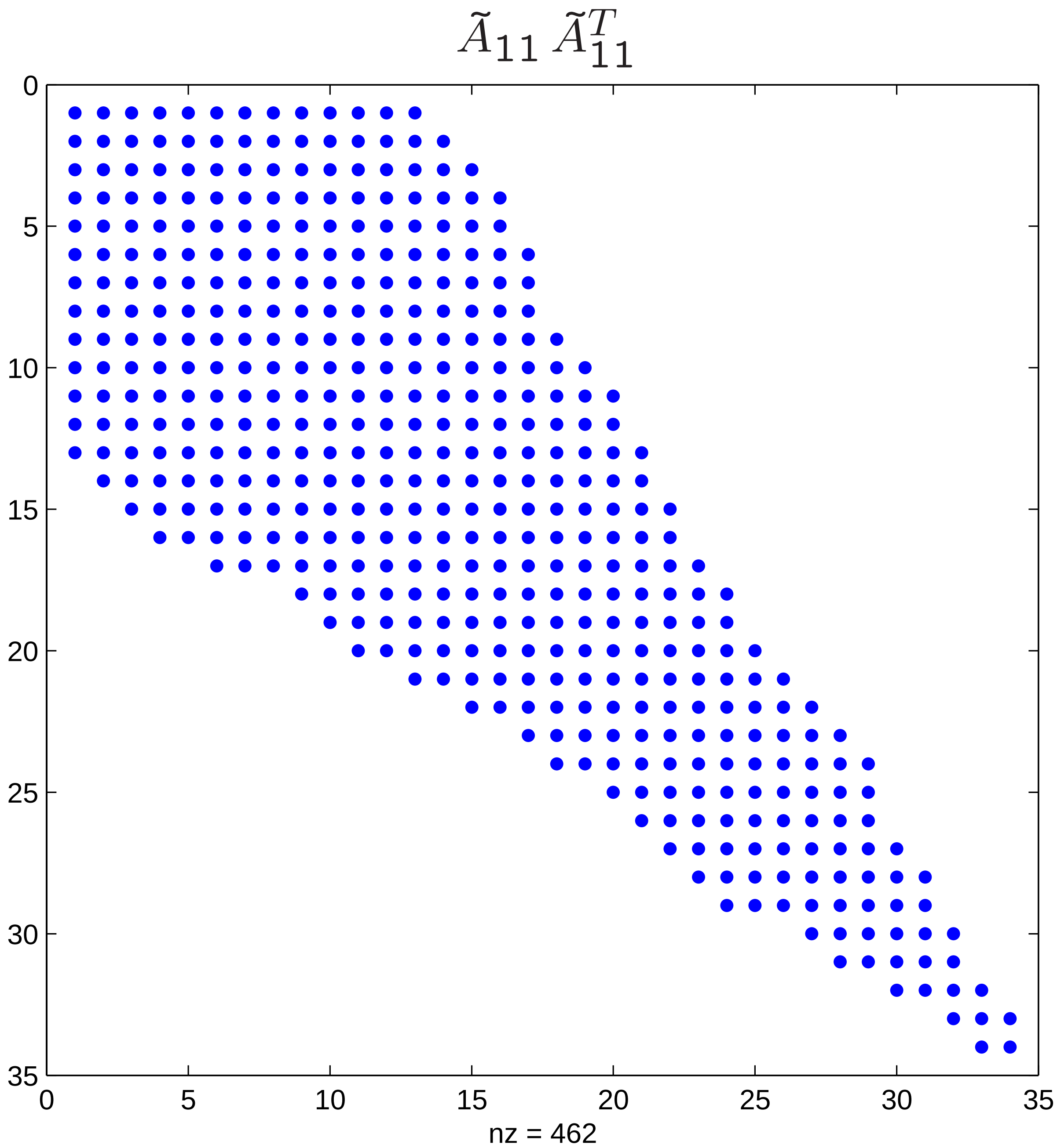
The band generalization of the GK bidiagonalization of A gives a subproblem $\tilde{A}_{11}\,\tilde{X}_1 \approx \tilde{B}_1$ satisfying the properties (P1) and (P2).

Using the properties of the band matrix $\tilde{A}_{11}\,\tilde{A}_{11}^T$, (P4), and, moreover

(P5) *singular values of* $[\,\tilde{B}_1\,|\,\tilde{A}_{11}\,]$ *have multiplicities at most* d,

can be proved.

The property (P3), that projections ($U_j^T\,B_1$) of B_1 onto all left singular vector subspaces of A_{11} have full row rank, is **not proved yet**.



$\tilde{A}_{11}\,\tilde{A}_{11}^T$
0
5
10
15
20
25
30
35
nz = 462

Relationship between these two subproblems

Relationship between the SVD based decomposition and the result of the banded GK generalization is not clear yet.

Definition of the core problem?

III. Future work and open questions

(Q1) Proof of the property (P3) of $[\,\tilde{B}_1\,|\,\tilde{A}_{11}\,]$.

(Q2) Proof of the minimality; definition of the core problem.

(Q3) Relationship of the SVD based decomposition and the banded GK generalization approach.

(Q4) Conditions for existence of the solution.

(Q5) Properties of the core problem.

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THANK YOU
FOR YOUR ATTENTION