Core problem theory

in linear approximation problems

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MOTIVATION

Generalized minimal residuals (GMRES)

$$\| b - A\, x_n \| \; = \; \min_{u \,\in\, x_0 + \mathcal{K}_n(A, r_0)} \; \| b - A\, u \|$$

where

$$\mathcal{K}_n(A, r_0) \equiv span\, \{ r_0, Ar_0, \cdots, A^{n-1} r_0 \} \, .$$

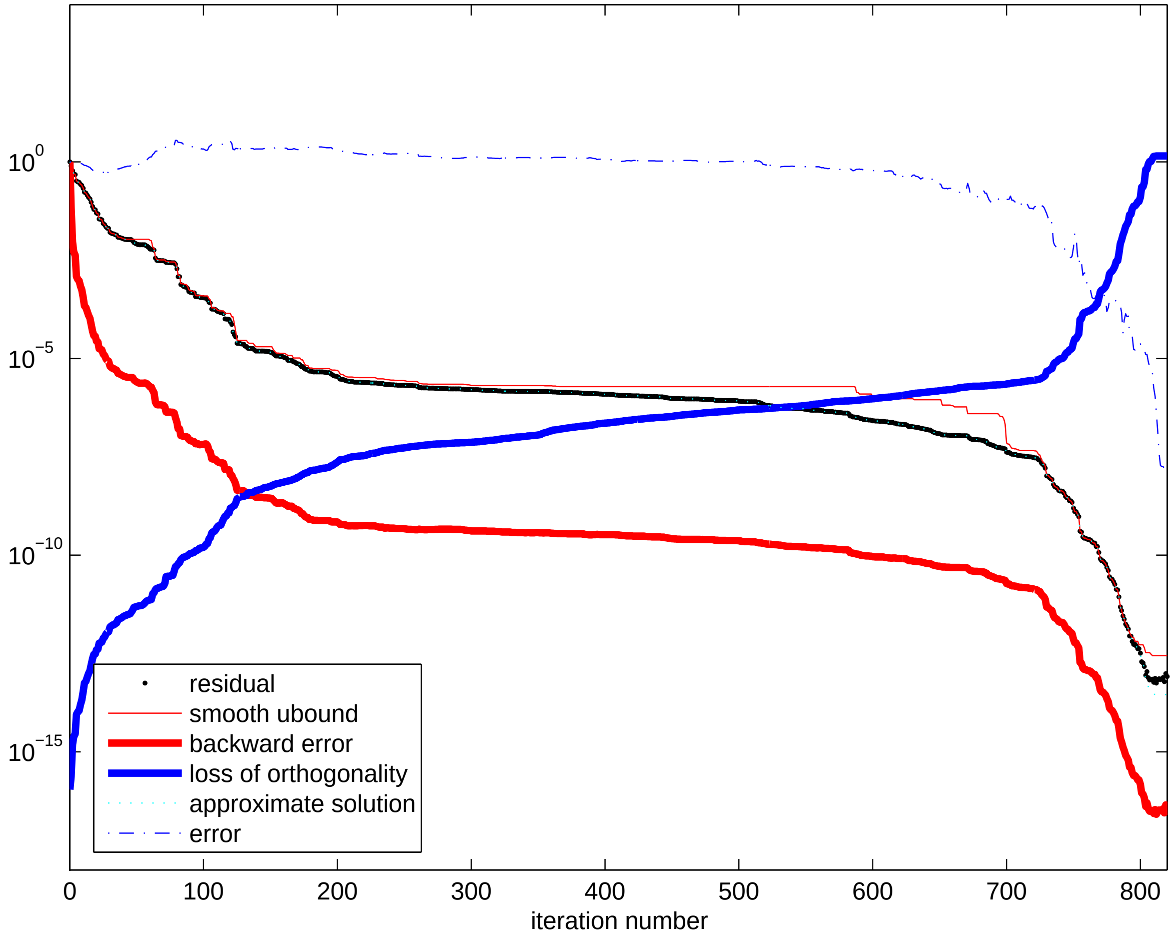
The formulation via the Arnoldi process

$$A\, W_n \; = \; W_{n+1}\, H_{n+1,n}\, , \quad H_{n+1,n} \; = \; W_{n+1}^T(A)\, A\, W_n(A)\, ,$$

and the GMRES approximation given by

$$y_n \; = \; \arg\min_u \; \| \| r_0 \| e_1 - \; H_{n+1,n}\, u \| \, , \quad x_n \; = \; x_0 \, + \, W_n\, y_n \, .$$

MGS GMRES in finite precision



Sherman2 from Matrix market, problem rhs.

Observations

- Despite the loss of orthogonality, the modified Gram-Schmidt implementation is as accurate as the Householder reflections-based implementation.
- There is no delay due to rounding errors.
- Loss of orthogonality seems inversely proportional to the normwise backward error.
- Full loss of orthogonality means that the normwise backward error is proportional to machine precision.

Investigation of the problem

$$\|b - A\,x_n\| \;=\; \min_{u \in x_0 + \mathcal{K}_n(A, r_0)} \|b - A\,u\|$$

$$=\; \min_{y} \|\, \|r_0\|\, w_1 - A\,W_n\,y\| \,.$$

Observation (exact arithmetic): $\|b - A\,x_n\|$ small $\longrightarrow$

w_1 must be well approximated by the columns of $A\,W_n$.

In order to describe the relationship quantitatively while suppressing the influence of $\|b\|,\ \|A\|$ and $\|x_n\|$, it seems convenient to relate

$$\frac{\|b - A\,x_n\|}{\|b\| + \|A\|\|x_n\|} \qquad \text{with} \qquad \kappa\left(\left[w_1, \frac{1}{\|A\|}\,A\,W_n\right]\right) .$$

Updating the smallest singular value

Paige, S (2002, SISC)

$$\frac{1}{\sqrt{2}} \;\leq\; \frac{\|b - A\,x_n\|}{\|b\| + \|A\|\|x_n\|}\;\kappa\left(\left[w_1, \frac{1}{\|A\|}\,A\,W_n\right]\right) \;\leq\; \frac{\sqrt{2}}{1-\delta_n^2}\,,$$

where

$$\delta_n \;=\; \frac{\sigma_{\min}\left(\left[w_1, \frac{1}{\|A\|}\,A\,W_n\right]\right)}{\sigma_{\min}\left(\left[\frac{1}{\|A\|}\,A\,W_n\right]\right)}\,.$$

When does the smallest singular value not change (or change a little) while updating a column? The answer was given in Paige, S (2002, Numerische Math. I + II); S, Hagen (2003) but the story went much further ...

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1 : Approximation problem

$\tilde{A}$ nonzero n by k matrix, $\tilde{b}$ nonzero n-vector.
With no loss of generality $n > k$ (add zero rows if necessary).

Consider an orthogonally invariant linear algebraic approximation problem

$$\tilde{A}\,\tilde{x} \;\approx\; \tilde{b}, \qquad (\tilde{A}^T\tilde{b} \neq 0 \text{ for simplicity}),$$

where $\approx$ typically means using data corrections of the prescribed type in order to get the nearest compatible system.

1 : Examples

- when errors are confined to $\tilde{b}$: **LS**

$$\tilde{A}\,\tilde{x} \;=\; \tilde{b} + \tilde{r}\,, \quad \min \|\tilde{r}\|_2\,;$$

- when errors are contained in both $\tilde{A}$ and $\tilde{b}$: (Scaled) **TLS**

$$(\tilde{A} \,+\, \tilde{E})\,\tilde{x}\,\gamma \;=\; \tilde{b}\,\gamma \,+\, \tilde{r}\,, \quad \min \|[\tilde{r},\; \tilde{E}]\|_F\,,$$

for a given scaling parameter γ;

- when errors are restricted to $\tilde{A}$: **DLS**

$$(\tilde{A} \,+\, \tilde{E})\,\tilde{x} \;=\; \tilde{b}\,, \quad \min \|\tilde{E}\|_F\,.$$

1 : Definition problem – a nonexistent solution

The data $\tilde{A}$, $\tilde{b}$ can suffer from

- multiplicities – the solution may not be unique;
- conceptual difficulties – when there are stronger colinearities among the columns of $\tilde{A}$ than between the columnspace of $\tilde{A}$ and the right hand side $\tilde{b}$, the TLS solution does not exist.

Extreme example: $\tilde{A}$ not full column rank, but $\tilde{b} \notin \mathbf{R}(\tilde{A})$.

It would be ideal to separate the information necessary and sufficient for solving the problem from the rest.

1 : Revealing orthogonal transformation

We prove that this important separation step can always be achieved via some orthogonal transformations providing a revealing block structure. In this sense, any orthogonally invariant linear algebraic approximation problem can be considered structured.

For simplicity of exposition, the presentation is mostly restricted to (unscaled) TLS.

Except for very few exceptions specified below, this presentation assumes exact arithmetic.

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2 : Basic TLS solution

Compatibility condition $(\tilde{A} + \tilde{E})\,\tilde{x} \;=\; \tilde{b} + \tilde{r}$ is equivalent to

$$\left([\tilde{b}, \tilde{A}] \;+\; [\tilde{r}, \tilde{E}]\right) \begin{bmatrix} -1 \\ \tilde{x} \end{bmatrix} \;=\; 0\,.$$

Look for the smallest perturbation $[\tilde{r}, \tilde{E}]$ of $[\tilde{b}, \tilde{A}]$ which makes the last matrix rank deficient. If the right singular vector corresponding to the smallest singular value of $[\tilde{b}, \tilde{A}]$ has a nonzero first component, then scaling it so that the first component is -1 gives the basic TLS solution.

Theorem

If $\sigma_{\min}(\tilde{A}) > \sigma_{\min}([\tilde{b}, \tilde{A}])$, then the Algorithm GVL gives the unique solution,

$$[\tilde{b}, \tilde{A}] = \tilde{U}\tilde{\Sigma}\tilde{V}^T = \sum_{i=1}^{k+1} \tilde{u}_i \tilde{\sigma}_i \tilde{v}_i^T, \quad \tilde{v}_{k+1} = \begin{bmatrix} \nu \\ w \end{bmatrix},$$

$$\tilde{x} = -\frac{1}{\nu} w, \quad [\tilde{r}, \tilde{E}] = -\tilde{u}_{k+1} \tilde{\sigma}_{k+1} \tilde{v}_{k+1}^T.$$

Golub and Reinsch (1970), Golub (1973), van der Sluis (1975), Golub and Van Loan (1980), Golub, Hoffman and Stewart (1987) contain much more, in particular,

2 : Golub and Van Loan founding paper

- Scaling of columns and weighting of rows;
- Minimum 2-norm solution;
- Scaled TLS solution $\longrightarrow$ LS solution as $\gamma \searrow 0$;
- TLS sensitivity analysis;
- Enlightening comments on possible numerical difficulties.

2 : Minimum norm solution $\left([\tilde{b}\,,\ \tilde{A}] = \tilde{U}\,\tilde{\Sigma}\,\tilde{V}^T \right)$

$$\tilde{\sigma}_j > \tilde{\sigma}_{j+1} = \ldots = \tilde{\sigma}_{k+1}\,, \quad \begin{aligned} V' &= [\tilde{v}_{j+1}\,,\ \ldots\,,\ \tilde{v}_{k+1}]\,, \\ U' &= [\tilde{u}_{j+1}\,,\ \ldots\,,\ \tilde{u}_{k+1}]\,. \end{aligned}$$

If $e_1^T V' \neq 0$, then take Q', $Q'^T Q' = Q' Q'^T = I$ such that

$(e_1^T V')\, Q' = \nu\, e_1^T$; set $\tilde{v} = (V' Q')\, e_1 = \begin{bmatrix} \nu \\ w \end{bmatrix}$, $\tilde{u} = U' Q' e_1$.

The solution is given by

$$x = -\frac{1}{\nu}\, w\,, \quad [\tilde{r}\,,\ \tilde{E}] = -\,\tilde{u}\ \tilde{\sigma}_{k+1}\,\tilde{v}^T\,.$$

2 : Related optimization problem

$$\| [\tilde{r}\,,\ \tilde{E}] \|_F \quad = \quad \sigma_{\min}\left([\tilde{b}\,,\ \tilde{A}]\right)$$

$$= \quad \min_{\tilde{x}} \frac{\| [\tilde{b}, \tilde{A}]\,(-1, \tilde{x}^T)^T \|}{\| (-1, \tilde{x}^T)^T \|}$$

$$= \quad \min_{\tilde{x}} \frac{\| \tilde{b} - \tilde{A}\,\tilde{x} \|}{\sqrt{1 + \|\tilde{x}\|^2}}\,,$$

but there remains a principal difficulty hidden in the formulation of the TLS problem.

2 : Remaining difficulty

The condition $\sigma_{\min}(\tilde{A}) > \sigma_{\min}([\tilde{b}, \tilde{A}])$ is sufficient,

but not necessary:

If $\sigma_{\min}(\tilde{A}) = \sigma_{\min}([\tilde{b}, \tilde{A}])$,

then there might be a solution, or it *can* happen that

$$\tilde{v}_{k+1} = \begin{bmatrix} 0 \\ w \end{bmatrix}$$

and the TLS formulation does not have a solution.

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3 : Nonpredictive collinearities

If $e_1^T V' = 0$, i.e. no column of V' has a nonzero first component, then the corresponding directions in the columnspace of $\tilde{A}$ bear no information whatsoever about the “observation” or “response” $\tilde{b}$. In other words, the correlations between the columns of $\tilde{A}$ are stronger than the correlations between the columnspace of $\tilde{A}$ and the vector $\tilde{b}$.

Van Huffel, Vandewalle (1991):

Eliminate some unwanted directions in the columnspace of $\tilde{A}$ (nonpredictive colinearities) uncorrelated with the vector $\tilde{b}$.

3 : Nongeneric TLS concept

Consider the splitting

$$[\tilde{b}\,,\ \tilde{A}] \;=\; \sum_{i=1}^{q} \tilde{u}_i\,\tilde{\sigma}_i\,\tilde{v}_i^T \;+\; \sum_{i=q+1}^{k+1} \tilde{u}_i\,\tilde{\sigma}_i\,\tilde{v}_i^T\,,$$

where q is the maximal value of i such that $e_1^T\,\tilde{v}_i \;\neq\; 0$.

The *nongeneric* TLS formulation uses the additional restriction:

$$(\tilde{A} + \tilde{E})\,\tilde{x} \;=\; \tilde{b} + \tilde{r}\,, \quad \min \|\,[\tilde{r}\,,\ \tilde{E}]\,\|_F \quad \text{subject to}$$

$$[\tilde{r}\,,\ \tilde{E}]\,[\tilde{v}_{q+1}\,,\ \ldots\,,\ \tilde{v}_{k+1}] \;=\; 0\,.$$

Theorem

The (minimum norm) nongeneric TLS solution always exists and is unique.

The whole construction is linked with the basic condition

$$\sigma_{\min}\,(\tilde{A}) \;>\; \sigma_{\min}\,([\tilde{b},\, \tilde{A}])\,.$$

The fact that the condition is sufficient but not necessary complicates both the theory and computation.

3 : Computation

Any decision as to whether the problem is generic or nongeneric can be made only in the process of computation and it is based on the intermediate computed results.

Moreover, the computation does not remove all directions in the column space of $\tilde{A}$ uncorrelated with the vector $\tilde{b}$, nor all redundant information.

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4 : Fundamental block structure

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

so that the problem $Ax \approx b$ can be rewritten as two independent approximation problems

$$\begin{aligned} A_{11}\,x_1 &\approx b_1\,, \\ A_{22}\,x_2 &\approx 0\,, \end{aligned}$$

with the solution $x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$.

4 : A meaningful solution

But $A_{22}\, x_2 \approx 0$ says x_2 lies approximately in the null space of A_{22}, and no more. Thus, unless there is a reason not to, we can set $x_2 = 0$.

Now since we have obtained b with the intent to estimate x, and since x_2 does not contribute to b in any way,

the best we can do is estimate x_1 from $A_{11}\, x_1 \approx b_1$.

4 : Well justified restriction on A_{11}, b_1

We need only consider the case where $Ax \approx b$ is incompatible.
Then $A_{11}x_1 \approx b_1$ is also incompatible.

We will show later that we can get:

- A_{11} is a $(p+1) \times p$ matrix with no zero or multiple singular values,
- b_1 has nonzero components in all left singular vector subspaces of A_{11}. That is if $A_{11} = U_{11}\Sigma_1 V_{11}^T$, then $U_{11}^T b_1$ has no zero entry.

As a consequence we will have the desired basic condition:

- $\sigma_{\min}(A_{11}) > \sigma_{\min}([b_1, A_{11}])$, see Paige, S (2002, NM I).

4 : SVD – based analysis

The SVD of $[b, \ A]$ is the direct sum of the SVDs of $[b_1, \ A_{11}]$ and A_{22}. Indeed,

$$\left[\begin{array}{c||c|c} b_1 & A_{11} & 0 \\ \hline 0 & 0 & A_{22} \end{array}\right] = \left[\begin{array}{c|c} U_1 \, \Sigma_1 \, V_1^T & 0 \\ \hline 0 & U_2 \, \Sigma_2 \, V_2^T \end{array}\right],$$

then extend the singular vectors by zeros.

4 : Standard TLS theory

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

- $\sigma_{\min}(A_{22}) > \sigma_{\min}([b_1, A_{11}])$ implies $\sigma_{\min}(A) > \sigma_{\min}([b, A])$ and the algorithm of Golub-Van Loan finds the unique solution.

- $\sigma_{\min}(A_{22}) = \sigma_{\min}([b_1, A_{11}])$ implies $\sigma_{\min}(A) = \sigma_{\min}([b, A])$; $\sigma_{\min}([b, A])$ is multiple, but $e_1^T V' \neq 0$. Consequently, the unique minimum norm solution follows in a standard way.

- $\sigma_{\min}(A_{22}) < \sigma_{\min}([b_1, A_{11}])$ implies $\sigma_{\min}(A) = \sigma_{\min}([b, A])$ and $e_1^T V' = 0$. The problem is considered by GVL unsolvable. The nongeneric TLS concept of VHV has to be applied.

4 : The if and only if condition

With the block structure above, the basic TLS concept and its minimum norm extension does not have a solution if and only if

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

The nongeneric TLS concept projects out (by imposing the additional condition) “the part of the block” A_{22} with singular values below $\sigma_{\min}([b_1, A_{11}])$. Then it solves the projected problem using the standard (minimum norm) TLS concept.

The nonexistence of the TLS solution is illustrated on a simple example.

4 : Example

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

$$\text{SVD of} \quad [b_1\,,\ A_{11}] =$$

$$\left[\begin{array}{cc} 0.8507 & -0.5257 \\ 0.5257 & 0.8507 \end{array}\right] \left[\begin{array}{cc} 1.618 & 0 \\ 0 & 0.618 \end{array}\right] \left[\begin{array}{cc} 0.5257 & -0.8507 \\ 0.8507 & 0.5257 \end{array}\right]^T$$

- If $\omega \geq \sigma_{\min}([b_1, A_{11}]) = 0.618$, then all is fine.
- If $\omega < \sigma_{\min}([b_1, A_{11}]) = 0.618$, then we see the trouble:

Take any z, define $r_1 = b_1 - A_{11} z$.

Then for any $\theta > 0$, (denoting v_2 , u_2 the singular vectors corresponding to $\sigma_{\min}(A_{22}) \equiv \sigma_2$, here $v_2 = 1$, $u_2 = 1$, $\sigma_{\min}(A_{22}) = \omega$)

$$\left[\begin{array}{c||c|c} b_1 & A_{11} & r_1 \, \theta^{-1} \, v_2^T \\ \hline 0 & 0 & A_{22} - u_2 \, \sigma_2 \, v_2^T \end{array} \right] \left[\begin{array}{c} -1 \\ z \\ v_2 \, \theta \end{array} \right] \equiv$$

$$\left[\begin{array}{c||c|c} b_1 & A_{11} & r_1 \theta^{-1} \\ \hline 0 & 0 & 0 \end{array} \right] \left[\begin{array}{c} -1 \\ z \\ \theta \end{array} \right] = 0 ,$$

4 : Meaningless solution approximation

$$\|[r\,,\;E]\|_F^2 \;=\; \|r_1\|^2\,\theta^{-2} \,+\, \sigma_{\min}^2\,(A_{22}) \;=\; \|r_1\|^2\,\theta^{-2} \,+\, \omega^2\,.$$

For large θ we have $\|[r\,,\;E]\|_F \;\longrightarrow\; \sigma_{\min}\,([A_{22}]) \;=\; \omega$ and
"close to optimal solution vector"

$$\begin{bmatrix} z \\ v_2\,\theta \end{bmatrix} \equiv \begin{bmatrix} z \\ \theta \end{bmatrix}$$

which is absolutely meaningless, since it couples the blocks and reflects no useful information whatsoever.

The nongeneric TLS concept requires $[r\,,\;E]\;[0\,,\;0\,,\;1]^T \;=\; 0$,
and constructs the unique nongeneric solution from the block $[b_1\,,\;A_{11}]$.

4 : The block structure is not restrictive

In this section, the problem was structured so that the difficulty was clearly revealed and the solution was transparent.

The crucial point:

We claim and show that the given block structure, which represents fundamental decomposition of the original data, fully determined by the multiplicities and irelevant information in the data $\tilde{b}$, $\tilde{A}$, can always be found via proper orthogonal transformations.

The solution can then be found by ignoring all multiplicities and irelevant information (i.e. block A_{22}).

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5 : The goal

Our suggestion is to find an orthogonal transformation

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

so that A_{11} has minimal dimensions, and $A_{11}x_1 \approx b_1$ can be solved by the algorithm given by Golub and Van Loan. Then solve $A_{11}x_1 \approx b_1$, and take the original problem solution to be

$$\tilde{x} \;=\; Q \begin{bmatrix} x_1 \\ 0 \end{bmatrix}.$$

5 : The transformation (compatible case)

Such an orthogonal transformation is given by reducing $[\tilde{b}, \tilde{A}]$ to an upper bidiagonal matrix. In fact, A_{22} need not be bidiagonalized, $[b_1, A_{11}] = P_1^T\,[\tilde{b},\ \tilde{A}\,Q_1]$ has nonzero bidiagonal elements and is either

$$[b_1,\ A_{11}] = \left[\begin{array}{c|cccc} \beta_1 & \alpha_1 & & & \\ & \beta_2 & \alpha_2 & & \\ & & \cdot & \cdot & \\ & & & \beta_p & \alpha_p \end{array}\right], \quad \beta_i\alpha_i \neq 0, \quad i = 1, \ldots, p$$

if $\beta_{p+1} = 0$ or $p = n$, (where $\tilde{A}$ is $n \times k$), or

5 : The transformation (incompatible case)

$$[b_1,\ A_{11}] = \left[\begin{array}{c|ccccc} \beta_1 & \alpha_1 & & & & \\ & \beta_2 & \alpha_2 & & & \\ & & \cdot & \cdot & & \\ & & & \beta_p & \alpha_p & \\ & & & & \beta_{p+1} & \end{array}\right], \quad \beta_i\alpha_i \neq 0\,,\ \beta_{p+1} \neq 0$$

if $\alpha_{p+1} = 0$ or $p = k$ (where $\tilde{A}$ is $n \times k$).

In both cases: $[b_1, A_{11}]$ has full row rank and A_{11} has full column rank.

Technique: Householder reflections or Golub-Kahan bidiagonalization.

Theorem: Core problem characteristics

(a) A_{11} has no zero or multiple singular values, so any zero singular values or repeats that $\tilde{A}$ has must appear in A_{22}.

(b) A_{11} has minimal dimensions, and A_{22} maximal dimensions, over all orthogonal transformations of the form given above.

(c) All components of b_1 in the left singular vector subspaces of A_{11} are nonzero. Consequently, the solution of the TLS problem $A_{11}x_1 \approx b_1$ can be obtained by the algorithm of Golub and Van Loan.

5 : Theory justifies computation

The core problem approach consists of three steps:

1. Orthogonal transformation $[b,\ A] \;=\; P^T\,[\tilde{b}\,,\ \tilde{A}\,Q]\,,$ where the upper bidiagonal block $[b_1,\ A_{11}]$ is as above, A_{22} is not bidiagonalized. All irrelevant and multiple information is filtered out to A_{22} .

2. Solving the minimally dimensioned $A_{11}\,x_1 \;\approx\; b_1$ by the algorithm of Golub and Van Loan (minimization problem).

3. Setting $\tilde{x} \;=\; Q\,x \;\equiv\; Q \begin{bmatrix} x_1 \\ 0 \end{bmatrix}$, (if we take $x_2 = 0$).

5 : Computational efficiency

The core problem approach is computationally efficient.
When the bidiagonalization stops, we use only the necessary (and sufficient) information for computing the solution.

The approximation problems for the original data $[\tilde{b}, \tilde{A}]$ and the orthogonally transformed data $[b, A]$ are equivalent. Consequently, the core problem approach always gives meaningful solutions by setting $x_2 = 0$.

Theorem

The core problem approach gives in exact arithmetic the minimum norm (Scaled) TLS solution of $\tilde{A}\tilde{x} \approx \tilde{b}$ determined by the algorithm of Golub and Van Loan, if it exists. If such a solution does not exist, then the core problem approach gives the nongeneric minimum norm (Scaled) TLS solution determined by the algorithm of Van Huffel and Vandewalle.

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Start with the SVD of $\tilde{A}$:

$$[\tilde{b}, \tilde{A}] = \left[\tilde{b} \,\middle|\, U \left[\begin{array}{c|c} S & 0 \\ \hline 0 & 0 \end{array} \right] V^T \right] = U \left[\begin{array}{c||c|c} \tilde{c} & S & 0 \\ \hline d & 0 & 0 \end{array} \right] \left[\begin{array}{c|c} 1 & 0 \\ \hline 0 & V^T \end{array} \right]$$

Use orthogonal transformations from the left and right in order to

- transform nonzero d to δe_1;
- create as many zeros in $\tilde{c}$ as possible;
- move out all zeros in $\tilde{c}$,
- and so move out all multiplicities and unneeded elements in S.

6 : Analysis based on SVD

Result (with new U, V):

$$U^T\,[\,\tilde{b}\,,\,\tilde{A}\,V\,] = \left[\begin{array}{c||c|c} b_1 & A_{11} & 0 \\ \hline 0 & 0 & A_{22} \end{array}\right] = \left[\begin{array}{c||c|c} c & S_1 & 0 \\ \delta & 0 & 0 \\ \hline 0 & 0 & S_2 \end{array}\right],$$

δ is nonzero (and the corresponding row exists) if and only if the system is incompatible. Size of the core problem ($p \times p$ or $(p+1) \times p$) is given by the number of the left singular subspaces of $\tilde{A}$, corresponding to distinct nonzero singular values, in which $\tilde{b}$ has a nonzero component.
(c has all its components nonzero, singular values in S_1 are distinct and nonzero).

Obtaining this structure from bidiagonalization

Upper bidiagonalization of $[\tilde{b}, \tilde{A}]$. Then, using $A_{11} = U_{11} S_1 V_{11}^T$, (obtaining $A_{22} = U_{22} S_2 V_{22}^T$ is unnecessary),

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

$$\left[\begin{array}{cc|c} U_{11} & r_1 & 0 \\ \hline 0 & 0 & U_{22} \end{array}\right] \left[\begin{array}{c||c|c} c & S_1 & 0 \\ \delta & 0 & 0 \\ \hline 0 & 0 & S_2 \end{array}\right] \left[\begin{array}{c|c|c} 1 & 0 & 0 \\ 0 & V_{11}^T & 0 \\ \hline 0 & 0 & V_{22}^T \end{array}\right]$$

where $c \equiv U_{11}^T b_1$, $\delta \equiv \|w\| \equiv \|b_1 - U_{11} c\|$, and, if $\delta \neq 0$, $r_1 \equiv w/\delta$.

6 : Alternative proof

Hnětynková and S (2007), Hnětynková, Plešinger and S (2006):
Relationship between

the Golub-Kahan bidiagonalization of $\tilde{A}$ starting with $\tilde{b}/\|\tilde{b}\|$

and

the Lanczos tridiagonalization of $\tilde{A}^T\tilde{A}$ starting with $\tilde{A}^T\tilde{b}/\|\tilde{A}^T\tilde{b}\|$

respectively

the Lanczos tridiagonalization of $\tilde{A}\tilde{A}^T$ starting with $\tilde{b}/\|\tilde{b}\|$.

6 : It gives the standard concept solutions

Orthogonal transformations do not change the problem. Therefore, consider the (partial) upper bidiagonal form in the incompatible case (the compatible case is obvious)

$$[b, A] = \left[\begin{array}{c||c|c} b_1 & A_{11} & 0 \\ \hline 0 & 0 & A_{22} \end{array}\right] = \left[\begin{array}{c||cccc|c} \beta_1 & \alpha_1 & & & & \\ & \beta_2 & \ddots & & & 0 \\ & & \ddots & \alpha_p & & \\ & & & \beta_{p+1} & & \\ \hline 0 & & 0 & & & A_{22} \end{array}\right]$$

6 : Proof

Case 1: $\sigma_{\min}(A) > \sigma_{\min}([b, A]) > 0$.

Case 2: $\sigma_j([b, A]) > \sigma_{j+1}([b, A]) = \ldots = \sigma_{k+1}([b, A])$,

$$V' = [\tilde{v}_{j+1}, \tilde{v}_{j+2}, \ldots, \tilde{v}_{k+1}],$$

Case 2a: $e_1^T V' \neq 0$.

Case 2b: $e_1^T V' = 0$.

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4. When TLS solution does not exist
5. Core problem within $\tilde{A}\,\tilde{x} = \tilde{b}$
6. Techniques, if time permits
7. Further work

7 : Numerical issues and regularization

Numerically, determining b_1 , A_{11} , A_{22} will depend on some (application related) threshold criterion.

If the problem is ill-posed and the data are corrupted by noise, then determining and solving the numerical core problem should also incorporate some way of determining what we can of a meaningful solution, such as regularization.

A survey of regularization in connection with TLS is given in Hansen and O'Leary (1997), Fierro, Golub, Hansen and O'Leary (1997), Hansen (1998), Golub, Hansen and O'Leary (1999), Sima, Van Huffel and Golub (2004), see also Kilmer and O'Leary (2001), Kilmer, Hansen and Espanol (2006), ..., Beck and Ben Tal (2006)

Also in computational statistics, and the Russian school inspired by Tikhonov, see Zhdanov et al. (1986, 89, 90, 91).

7 : Truncated TLS

$$(\tilde{A} + \tilde{E})\,\tilde{x} \;=\; \tilde{b} \,+\, \tilde{r}, \qquad \min \|\,[\tilde{r}, \tilde{E}]\,\|_F \quad \text{subject to}$$

$$(\text{rank}\;([\tilde{b} + \tilde{r},\; \tilde{A} + \tilde{E}]) \equiv) \quad \text{rank}\;(\tilde{A} + \tilde{E}) \;\leq\; m\,.$$

Its (minimum norm nongeneric) TLS solution is constructed by considering the smallest singular values equal and set to zero, while preserving the singular vectors. With the restriction of the rank, the T-TLS distance is (unlike in the nongeneric TLS problem) the square root of the sum of squares of the neglected singular values.

Suggested in van Huffel and Vandewalle (1991), Section 3.6.1.
Analyzed in Fierro and Bunch (1994), Fierro and Bunch (1996), Wei (1992), see also Stewart (1984), van der Sluis and Veltkamp (1979).

7 : Golub-Kahan Truncated TLS

Golub-Kahan bidiagonalization of $[\tilde{b}\,,\ \tilde{A}]$. Then compute approximate truncated TLS solution by applying TLS to the bidiagonal system with the $(k+1) \times k$ matrix at each step k (which represents the truncated approximation of the core problem). Stopping criterion is based on the TLS solution of the $(k+1)$ by k bidiagonal problem.

Fierro, Golub, Hansen and O'Leary (1997), Sima and Van Huffel (2005, 06), Sima (2006)

Hnětynková, Plešinger and S (2006): Bidiagonalization itself can provide useful information about the level of noise in b.

Hansen, Kilmer and Kjeldsen (2006)

7 : In ill-posed LS problems

Paige and Saunders (1982 I+II) classics contains, in addition to LSQR for solving least squares problems, also stopping criteria, approximation to truncated SVD - regularization, see also Golub and Kahan (1965), relationship to other methods like CGLS, Craig, PLS Wold (1980), see Eldén (2004), numerical stability issues, code.

Regularization by projection: Eldén (1977), Björck and Eldén (1979 rep.), Björck (1980 rep.), Varah (1979), van der Sluis and van der Vorst (1986, 1990), Golub and Urs von Matt (1991), Hansen and O'Leary (1993), Hanke, Nagy and Plemmons (1993), Björck, Grimme and Van Dooren (1994), Vogel and Wade (1994), Hanke (1995), Vogel (1997), Hansen (1998), Calvetti, Golub and Reichel (1999), Simon and Zha (2000), Calvetti and Reichel (2002) ...

Projection with subsequent regularization: O'Leary and Simmons (1980), Björck (1988 paper!), Hanke and Hansen (1993), Hanke (2001), Kilmer and O'Leary (2001), Kilmer, Hansen and Espanol (2006) ...

7 : A nonzero x_2 component

Consider, noisy ill-posed LS problems and Modified TSVD
Hansen, Sekii and Shibahaski (1992)

$$\min \; \| L\tilde{x} \|_2 \quad \text{subject to} \quad \min \; \| \tilde{A}\tilde{x} - \tilde{b} \| \,.$$

If L is a general matrix with full row rank, then one can consider $x_2 \neq 0$ for numerically determined A_{22}. This does not alter the core problem concept theoretically or computationally,

cf. Fierro, Golub, Hansen and O'Leary (1997), Section 5.

For more general case see Kilmer, Hansen, and Espanol (2006).

Extension of the core problem theory and computation?

Björck (2005, 06): generalization of the bidiagonalization to band Lanczos

Sima (2006): generalization of the SVD analysis

Hnětynková, Plešinger, Sima, S and van Huffel (2007?): the minimum dimensional decomposition of data and definition of the core problem, work in progress ...

Closing remarks

The core problem approach represents a clear computationally efficient concept which in exact arithmetic gives in all cases (Scaled) TLS solutions identical to the minimum norm solutions given by the standard concepts of Golub and Van Loan, Van Huffel and Vandewalle.

Theoretically, it simplifies and extends the previous (Scaled) TLS analysis.

Computationally, it can lead to interesting numerical questions and applications. A close connection to regularization.

Extension to multiple right hand sides seems to be in progress in the sense of decomposition of data and the core problem definition, with interesting ideas also in the sense of computation.

Here the analysis using linear algebra tools is crucial for understanding of the subtleties of the possible formulations via optimization.

THANK YOU!