ORTHOGONAL PROJECTION AND TOTAL LEAST SQUARES

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Dedicated to Beresford Parlett and William Kahan
on the occasion of their 60th birthdays.

ABSTRACT. When the overdetermined system of linear equations $AX \approx B$ has no solution, compatibility may be restored by an orthogonal projection method. The idea is to determine an orthogonal projection matrix P by some method M such that $[\tilde{A} \ \tilde{B}] = P[A \ B]$, and $\tilde{A}X \approx \tilde{B}$ is compatible. Since both A and B are allowed to be perturbed, denote by X_M the minimum norm total least squares solution by method M (the TLS- M solution) to $\tilde{A}X = \tilde{B}$. In this paper conditions for compatibility of the lower rank approximation and subspace properties of $\tilde{A}$ in relation to the nearest rank- k matrix to A are discussed. We find upper and lower bounds for the difference in the TLS- M solution X_M and the SVD-based TLS-SVD solution X_{SVD} and also provide a perturbation result for the SVD-based TLS method. These results suggest a new algorithm for computing a total least squares solution based on a rank revealing QR factorization and subspace refinement. Numerical simulations are included to illustrate the conclusions.

1. Introduction

In spectral estimation, modern communication and applied fields such as physics one is often faced with determining the linear parameter $X_0 \in \mathbb{R}^{n \times d}$ in the overdetermined system of linear equations

$$A_0 X_0 = B_0 \quad (1.1)$$

where $A_0 \in \mathbb{R}^{m \times n}$ and $B_0 \in \mathbb{R}^{m \times d}$ are known. However, due to ‘noise’ (such sources include human and instrument errors) the linear system at hand

$$AX \approx B \quad (1.2)$$

frequently does not have a solution and one must estimate the relationship between the observation matrix $B \in \mathbb{R}^{m \times d}$ and the data matrix $A \in \mathbb{R}^{m \times n}$. The least squares (LS) and total least squares (TLS) methods are commonly used and each may be reformulated as the problem of finding an orthogonal projection matrix P such that $[\tilde{A} \ \tilde{B}] = P[A \ B]$, and $\tilde{A}X = \tilde{B}$ is compatible. Let $D(:, i : j)$ denote the submatrix of D comprised of the i^{th} through j^{th} columns of D and denote the SVD of the $m \times n$ matrix $A \in \mathbb{R}^{m \times n}$ ($m \geq n$) by

$$A = U' \Sigma' V'^T \quad (1.3)$$

with $U' = [U'_1 \ U'_2]$, $U'_1 = U'(:, 1 : k)$, $U'_2 = U'(:, k + 1 : n)$,

$V' = [V'_1 \ V'_2]$, $V'_1 = V'(:, 1 : k)$, $V'_2 = V'(:, k + 1 : n)$

and $\Sigma' = \text{diag}(\sigma'_1, \dots, \sigma'_n) \in \mathbb{R}^{n \times n}$. Partition the matrix Σ' as

$$\Sigma' = \begin{bmatrix} \Sigma'_1 & 0 \\ 0 & \Sigma'_2 \end{bmatrix},$$

so that $\Sigma'_1 \in \mathbb{R}^{k \times k}$ and $\Sigma'_2 \in \mathbb{R}^{(n-k) \times (n-k)}$.

Denote the SVD of the $m \times (n + d)$ matrix $[A \ B] \in \mathbb{R}^{m \times (n+d)}$ ($m \geq n + d$) by

$$[A \ B] = U \Sigma V^T \quad (1.4)$$

with $U = [U_1 \ U_2]$, $U_1 = U(:, 1 : k)$, $U_2 = U(:, k + 1, n + d)$,
 $V = [V_1 \ V_2]$, $V_1 = V(:, 1 : k)$, $V_2 = V(:, k + 1 : n + d)$ and $\Sigma = \text{diag}(\sigma_1, \dots, \sigma_{n+d}) \in \mathbb{R}^{(n+d) \times (n+d)}$. Partition the matrices V and Σ as

$$V = [V_1 \ V_2] = \begin{bmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{bmatrix} \quad \text{and} \quad \Sigma = \begin{bmatrix} \Sigma_1 & 0 \\ 0 & \Sigma_2 \end{bmatrix},$$

with $V_{11} \in \mathbb{R}^{n \times k}$, $V_{12} \in \mathbb{R}^{n \times (n-k+d)}$, $V_{21} \in \mathbb{R}^{d \times k}$, $V_{22} \in \mathbb{R}^{d \times (n-k+d)}$, $\Sigma_1 \in \mathbb{R}^{k \times k}$ and $\Sigma_2 \in \mathbb{R}^{(n-k+d) \times (n-k+d)}$. The range of a matrix A is denoted $R(A)$ and the nullspace of A by $N(A)$. $\kappa(D) = \|D\| \|D^+\|$ denotes the condition number of the matrix D , where $\|\cdot\|$ denotes the 2-norm. $P_D = DD^+$ denotes the orthogonal projection matrix onto $R(D)$. $\sigma(D)$ denotes the set of singular values of D .

Literature on the computational and statistical aspects of LS is abundant (e.g., [3],[9],[15]). A TLS algorithm based on the singular value decomposition (SVD) is mentioned in [9] and has been used in various disciplines for some time, but only recently has it become well understood. In the field of Numerical Analysis the first significant research on TLS is Golub and Van Loan's (1980) "An Analysis of the Total Least Squares Problem." The work of Golub and Van Loan was extended by Van Huffel and Vandewalle's (1988) "Analysis and Solution of the Nongeneric Total Least Squares Problem" and (1989) "Algebraic Connections Between the Least Squares and Total Least Squares Problems." The insights provided by these articles have generated many new and interesting results and applications. For instance, TLS is used to resolve closely spaced sinusoids in spectral estimation [1], and has been shown to be effective in many other applications. SVD-based methods, however, are not practical for many applications that require a moderate computational workload as well as efficient updating/downdating capabilities, such as in spectral estimation. The SVD, a powerful analytical tool, is known to be very stable but has a high computational demand associated with it [11] as well as high

complexity in its updating/downdating capability [2]. A widely used alternative is QR with ordinary column pivoting (e.g., see [11],[15]). While there are examples to show that this method can fail to reveal the correct near-rank deficiency in a matrix, the algorithm is stable and known to work well in practice [11]. Also, the rank revealing QR algorithm of Chan [4] is viewed as quite a good alternative to the SVD.

The primary objective of this paper is to explore orthogonal projection in computing a TLS solution and determine the intrinsic qualities of a method that make it a viable alternative to the SVD with a general application to rank revealing QR factorizations. A greater understanding of these methods is achieved when they are compared to the well studied SVD method. This paper is organized as follows. In Section 2 we provide a condition for compatibility and examine subspace properties of $\tilde{A}$ in relation to the nearest rank- k matrix to A . In Section 3 we provide lower and upper perturbation bounds for TLS solutions with an emphasis on comparing X_M to X_{SVD} since the properties of the TLS-SVD method are well studied. Then in Section 4 a comparison between the TLS-SVD and TLS-QR solution is made. We also propose a new algorithm for computing a TLS solution based on a rank revealing QR factorization of $[A \ B]$ and subspace refinement. In Section 5 numerical simulations are provided to illustrate the conclusions.

2. Compatibility and Acuteness

Two common orthogonal projection methods are LS and TLS. It is well known that when the data matrix A has $n - k$ small singular values that the computed classical LS solution is subject to high variability due to the inversion of small singular values. To stabilize the solution using truncated LS one solves for

the minimum norm solution X_{LS} such that

$$\|B - A_k X_{LS}\| = \min_{X \in \mathbb{R}^{n \times d}} \|B - A_k X\| \quad (2.1)$$

where $A_k = U_1' \Sigma_1' V_1'^T$ is the nearest rank- k matrix to $A = A_k + \Delta A'$ and $\|A - A_k\| = \sigma'_{k+1}$. $\Delta A'$ is the correction in A which is independent of B . For this method $P = U_1' U_1'^T$ and X_{LS} is the minimum norm solution to $A_k X = PB$. See [12],[13] for more on the properties of this solution.

The computed classical TLS solution, too, is subject to high variability when A is nearly rank- $(n - k)$ deficient. In restoring stability the perturbations of A and B considered by TLS subsume that of truncated LS: choose $[\hat{A} \hat{B}]$ as the minimizer of

$$\text{minimize} \quad \|[A \ B] - [C \ D]\| \quad (2.2)$$

$$\text{subject to} \quad \text{rank}(C) = \text{rank}([C \ D]) = k. \quad (2.3)$$

By the Eckart-Young Theorem [7], a potential solution to the the rank- k matrix approximation problem is

$$[\hat{A} \ \hat{B}] = U_1 \Sigma_1 V_1^T. \quad (2.4)$$

When $\hat{A}X = \hat{B}$ is compatible let $X_{SV D}$ denote the minimum norm TLS-SVD solution. $\Delta \hat{A} = A - \hat{A}$ is the correction of A that is dependent on B and $\|[\Delta \hat{A} \ \Delta \hat{B}]\| = \sigma_{k+1}$. If $P = U_1 U_1^T$ it is easy to verify $[\hat{A} \ \hat{B}] = P[A \ B]$.

In general, let P be an orthogonal projection matrix onto a k -dimensional subspace S and define $[\tilde{A} \ \tilde{B}]$ by

$$[\tilde{A} \ \tilde{B}] = P[A \ B], \quad (2.5)$$

with

$$[\Delta \tilde{A} \ \Delta \tilde{B}] = [A \ B] - [\tilde{A} \ \tilde{B}]. \quad (2.6)$$

Then $[\tilde{A} \tilde{B}]$ is obtained by orthogonal projection and $R([\tilde{A} \tilde{B}]) \subseteq S$. If

$$\tilde{A}X = \tilde{B} \quad (2.7)$$

is compatible, let $X_M \in \mathbb{R}^{n \times d}$ denote the minimum norm TLS-M solution. Denote the i^{th} singular value of $[\tilde{A} \tilde{B}]$ by $\tilde{\sigma}_i$ and the i^{th} singular value of $\tilde{A}$ by σ_i^a with the singular values decreasing for increasing index i . The following result shows under what condition (2.7) is compatible.

Theorem 1 *Let A have the usual SVD and let $[\tilde{A} \tilde{B}]$ be obtained by orthogonal projection as in (2.5). If $\|\Delta \tilde{A}\| < \sigma'_k$, then $\text{rank}(\tilde{A})=k$ and $\tilde{A}X = \tilde{B}$ is compatible.*

Proof:

It is clear that $\text{rank}(\tilde{A}) \leq \text{rank}([\tilde{A} \tilde{B}]) \leq k$, where k is the dimension of subspace S . To show $R(\tilde{B}) \subseteq R(\tilde{A})$, we need only prove $\text{rank}(\tilde{A}) = k$. Since $\tilde{A} = PA$, from [20, p. 34] it follows

$$\sigma'_i \geq \sigma_i^a \quad \text{for } i = 1, \dots, k. \quad (2.8)$$

Since $A - \tilde{A} = \Delta \tilde{A}$ it follows from the perturbation of singular values [3] and (2.8) that

$$\sigma'_i - \sigma_i^a \leq \|\Delta \tilde{A}\| \quad \text{for } i = 1, \dots, k. \quad (2.9)$$

Using the assumption $\|\Delta \tilde{A}\| < \sigma'_k$, this implies $0 < \sigma'_k - \|\Delta \tilde{A}\| \leq \sigma_k^a$. Now $0 < \sigma_k^a \leq \dots \leq \sigma_1^a$ implies $\text{rank}(\tilde{A}) = k$, and hence $R(\tilde{B}) \subseteq R(\tilde{A})$. Therefore, $\tilde{A}X = \tilde{B}$ has a solution $\tilde{X} \in \mathbb{R}^{n \times d}$ and the minimum norm TLS-M solution $X_M \in \mathbb{R}^{n \times d}$ exists. $\square$

In the TLS-SVD case, it is clear that $\|\Delta \hat{A}\| \leq \sigma_{k+1}$. Hence, whenever $\sigma_{k+1} < \sigma'_k$ then it immediately follows from Theorem 1 that $\hat{A}X = \hat{B}$ is compatible. Numerically, this is a mild condition because the interlacing property of singular

values [10] ensures $\sigma_{k+1} \leq \sigma'_k$. Note that Theorem 1 is similar to Theorem 4.2 in [21]. However, we assume the orthogonal projector is rank k , which leads to a compatibility condition that is easier to verify. This assumption is not a serious limitation because if one cannot determine k from the factorization of $[A \ B]$ using method M with little effort, then it is most likely (from a direct computational point of view) to be an undesirable factorization when solving systems of linear equations. As noted in [21], $\tilde{A}X = \tilde{B}$ and $\tilde{A}X \approx B$ have the same solution set.

Further, the condition $\|\Delta\tilde{A}\| < \sigma'_k$ implies that $\tilde{A}$ and A_k are acute, that is, the canonical angles between their column spaces, as well as row spaces, are less than $\pi/2$, as shown below (otherwise, we can expect the pseudoinverses to differ significantly as the lower bound on $\|\hat{A}^+ - A_k^+\|$ may be arbitrarily large [27] and hence the two methods may generate vastly different solutions). Define $E \in \mathbb{R}^{m \times n}$ by

$$\tilde{A} = A_k + E. \quad (2.10)$$

Then $\tilde{A}$ can be viewed as a perturbation of A_k . In the reduced form

$$U'^T A_k V' = \begin{pmatrix} \Sigma'_1 & 0 \\ 0 & 0 \end{pmatrix}, \quad (2.11)$$

$$U'^T E V' = \begin{pmatrix} E_{11} & E_{12} \\ E_{21} & E_{22} \end{pmatrix}, \quad (2.12)$$

and

$$U'^T \tilde{A} V' = \begin{pmatrix} \tilde{\Sigma}_1 & E_{12} \\ E_{21} & E_{22} \end{pmatrix}, \quad (2.13)$$

where $\tilde{\Sigma}_1 = \Sigma'_1 + E_{11}$ and $\Sigma'_1 = \text{diag}(\sigma'_1, \dots, \sigma'_k) \in \mathbb{R}^{k \times k}$. Appealing to Theorem 3.3 [20, p.139], A_k and $\tilde{A}$ are acute if and only if in the reduced form $\tilde{\Sigma}_1$ is nonsingular and $E_{22} = E_{21} \tilde{\Sigma}_1^{-1} E_{12}$. To show $\tilde{\Sigma}_1$ is nonsingular, it suffices to show $\|E_{11}\| < \sigma'_k$.

Rewriting E as

$$E = \Delta A' - \Delta \tilde{A} \quad (2.14)$$

and transforming both sides of (2.14) as in (2.12) yields

$$\begin{pmatrix} E_{11} & E_{12} \\ E_{21} & E_{22} \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & \Sigma'_2 \end{pmatrix} - \begin{pmatrix} \Delta\tilde{A}_{11} & \Delta\tilde{A}_{12} \\ \Delta\tilde{A}_{21} & \Delta\tilde{A}_{22} \end{pmatrix}, \quad (2.15)$$

where

$$U'^T \Delta\tilde{A} V' = \begin{pmatrix} \Delta\tilde{A}_{11} & \Delta\tilde{A}_{12} \\ \Delta\tilde{A}_{21} & \Delta\tilde{A}_{22} \end{pmatrix}. \quad (2.16)$$

From (2.15)-(2.16) and $\|\Delta\tilde{A}\| < \sigma'_k$ it follows

$$\|E_{11}\| = \|\Delta\tilde{A}_{11}\| \leq \|U'^T \Delta\tilde{A} V'\| = \|\Delta\tilde{A}\| < \sigma'_k, \quad (2.17)$$

which implies $\tilde{\Sigma}_1$ is nonsingular. To show $E_{22} = E_{21}\tilde{\Sigma}_1^{-1}E_{12}$, define S by

$$S \equiv E_{22} - E_{21}\tilde{\Sigma}_1^{-1}E_{12}. \quad (2.18)$$

Since $\tilde{\Sigma}_1$ is nonsingular, performing a step of block Gaussian elimination on $U'^T \tilde{A} V'$ gives

$$U'^T \tilde{A} V' = \begin{bmatrix} I_k & 0 \\ E_{21}\tilde{E}_1^{-1} & I_{n-k+d} \end{bmatrix} S_1 \quad (2.19)$$

where

$$S_1 \equiv \begin{bmatrix} \tilde{\Sigma}_1 & E_{12} \\ 0 & S \end{bmatrix}. \quad (2.20)$$

If $S \neq 0$, then $\text{rank}(S_1) \geq k+1$, implying $k = \text{rank}(\tilde{A}) = \text{rank}(U'^T \tilde{A} V') = \text{rank}(S_1) \geq k+1$, a contradiction. Therefore, $S \equiv 0$. This shows that $\|\Delta\tilde{A}\| < \sigma'_k$ implies A_k and $\tilde{A}$ are acute, which means $\tilde{A}^+$ can be considered a continuous function of the perturbation of the elements of A_k . It can also be shown that $\|P_{R(A_k)} - P_{R(\tilde{A})}\| \leq \Delta\tilde{A}/\sigma'_k$ and $\|P_{R(A_k^T)} - P_{R(\tilde{A}^T)}\| \leq \Delta\tilde{A}/\sigma'_k$ so that the compatibility condition is a ‘measure’ of the degree of acuteness.

3. TLS Perturbation Bounds

In this section we first examine how a user-specified approximate nullspace of $[A \ B]$ compares to the “numerical nullspace” of $[A \ B]$, i.e., $R(V_2)$. If $R(Z)$ is the

approximate nullspace, where $Z \in \mathfrak{R}^{(n+d) \times (n-k+d)}$ is a full column rank matrix, we examine the properties Z should possess so that $R(Z)$ and $R(V_2)$ are “close” in some sense. Since $R(V_2)$ is the TLS-SVD solution space, if the approximate nullspace is close to the numerical nullspace then one hopes the total least squares solution using the approximate nullspace is close to the TLS-SVD solution. It will be shown that this is indeed the case. This is desirable because the solution, residual, and singular subspace properties of the SVD-based TLS problem have been examined in [8],[10],[22],[23],[24],[28]. Then the results will be applied to rank revealing QR factorizations of $[A \ B]$ to compute the TLS-QR solution.

Let $Z \in \mathfrak{R}^{(n+d) \times (n-k+d)}$ denote a full column rank matrix with

$$\|[A \ B]Z\| = \epsilon. \quad (3.1)$$

Let Z have the QR decomposition

$$Z = GT \quad (3.2)$$

where $G \in \mathfrak{R}^{(n+d) \times (n-k+d)}$ has orthonormal columns and $T \in \mathfrak{R}^{(n-k+d) \times (n-k+d)}$ is triangular. Let G admit the partition $G = [G_1^T \ G_2^T]^T$ with $G_2 \in \mathfrak{R}^{d \times (n-k+d)}$. Now suppose Z was derived by method M with

$$[\tilde{A} \ \tilde{B}]Z = 0 \quad (3.3)$$

satisfying $\|\Delta \tilde{A}\| < \sigma'_k$. Then the TLS-M solution X_M given by

$$X_M = -G_1 G_2^+ \quad (3.4)$$

is the minimum norm solution to the compatible system

$$\tilde{A}X = \tilde{B}. \quad (3.5)$$

Next it is shown that if $R(Z)$ is sufficiently close to the numerical nullspace $R(V_2)$ then $X_M = -G_1 G_2^+$ will be close to the minimum norm TLS-SVD solution $X_{SV D} = -V_{12} V_{22}^+$. The largest canonical angle θ between $R(Z) = R(G)$ and $R(V_2)$ is the standard measure of “closeness” of the subspaces. The sine of the angle is given by

$$\sin \theta = \text{dist}(R(G), R(V_2)) = \|P_G - P_{V_2}\| = \|V_1^T G\|. \quad (3.6)$$

It is easy to show

$$\begin{bmatrix} X_M \\ -I_d \end{bmatrix} - \begin{bmatrix} \hat{X} \\ -I_d \end{bmatrix} = V_2 V_{22}^+ - G G_2^+. \quad (3.7)$$

This implies

$$V_1^T \left(\begin{bmatrix} X_M \\ -I_d \end{bmatrix} - \begin{bmatrix} \hat{X} \\ -I_d \end{bmatrix} \right) = -V_1^T G G_2^+, \quad (3.8)$$

from which it follows

$$\left\| V_1^T \begin{bmatrix} X_M - X_{SV D} \\ 0 \end{bmatrix} \right\| \leq \|V_1^T G\| \|G_2^+\| \quad (3.9)$$

and

$$\|V_1^T G G_2^+\| \leq \|V_1^T\| \left\| \begin{bmatrix} X_M - X_{SV D} \\ 0 \end{bmatrix} \right\| = \left\| \begin{bmatrix} X_M - X_{SV D} \\ 0 \end{bmatrix} \right\|. \quad (3.10)$$

This leads to the following upper and lower bound on the difference between the TLS-M solution X_M and the ordinary TLS solution $X_{SV D}$.

Theorem 2 *Let A and $[A \ B]$ have the usual SVD. Let $Z \in \Re^{(n+d) \times (n-k+d)}$ have full column rank satisfying (3.1) and (3.3) with the QR decomposition $Z = GT$. If $\max(\|\Delta \tilde{A}\|, \|\Delta \hat{A}\|) < \sigma'_k$ then*

$$\sin \theta \leq \|X_M - \hat{X}\| \leq \sin \theta \|G_2^+\| \|V_{22}^+\| \quad (3.11)$$

where θ is the subspace angle between $R(G)$ and $R(V_2)$.

Proof:

The mild condition $\max(\|\Delta\tilde{A}\|, \|\Delta\hat{A}\|) < \sigma'_k$ ensures both solutions exist. To prove the lower bound, since G_2 is a submatrix of the orthonormal matrix G , all the singular values of G_2 are ≤ 1 . Therefore, $1 \leq \sigma_{\min}(G_2^+)$, hence

$$\sin \theta = \|V_1^T G\| \leq \sigma_{\min}(G_2^+) \|V_1^T G\| \leq \|V_1^T G G_2^+\| \leq \left\| \begin{bmatrix} X_M - X_{SV D} \\ 0 \end{bmatrix} \right\| = \|X_M - X_{SV D}\|.$$

To prove the upper bound, let $E_X \equiv X_M - X_{SV D}$, and let

$$\begin{bmatrix} I_{k-d} & 0 & 0 & 0 \\ 0 & I_d & 0 & C^{-1}S \end{bmatrix} \equiv [I_k \ D].$$

Note that $\sigma_{\min}([I_k \ D]) \geq 1$. Then from the CS Theorem of Paige and Saunders [17] there exist orthogonal matrices H , Y , W and Z of order n , d , k and $n - k + d$ respectively such that

$$\begin{bmatrix} H^T & 0 \\ 0 & Y^T \end{bmatrix} V_1 W = \begin{bmatrix} I_{k-d} & 0 \\ 0 & C \\ 0 & 0 \\ 0 & S \end{bmatrix}, \quad (3.12)$$

which implies

$$V_1^T \begin{bmatrix} E_X \\ 0 \end{bmatrix} = W \begin{bmatrix} I_{k-d} & 0 & 0 & 0 \\ 0 & C & 0 & S \end{bmatrix} \begin{bmatrix} H^T & 0 \\ 0 & Y^T \end{bmatrix} \begin{bmatrix} E_X \\ 0 \end{bmatrix}. \quad (3.13)$$

Thus,

$$\begin{aligned} \left\| V_1^T \begin{bmatrix} E_X \\ 0 \end{bmatrix} \right\| &= \left\| \begin{bmatrix} I_{k-d} & 0 & 0 & 0 \\ 0 & C & 0 & S \end{bmatrix} \begin{bmatrix} H^T E_X \\ 0 \end{bmatrix} \right\| \\ &= \left\| \begin{bmatrix} I_{k-d} & 0 \\ 0 & C \end{bmatrix} \begin{bmatrix} I_{k-d} & 0 \\ 0 & C^{-1} \end{bmatrix} \begin{bmatrix} I_{k-d} & 0 & 0 & 0 \\ 0 & C & 0 & S \end{bmatrix} \begin{bmatrix} H^T E_X \\ 0 \end{bmatrix} \right\| \\ &= \left\| \begin{bmatrix} I_{k-d} & 0 \\ 0 & C \end{bmatrix} \begin{bmatrix} I_{k-d} & 0 & 0 & 0 \\ 0 & I_d & 0 & C^{-1}S \end{bmatrix} \begin{bmatrix} H^T E_X \\ 0 \end{bmatrix} \right\| \end{aligned}$$

$$\begin{aligned}
&\geq \sigma_{\min}(C) \left\| \begin{bmatrix} I_{k-d} & 0 & 0 & 0 \\ 0 & I_d & 0 & C^{-1}S \end{bmatrix} \begin{bmatrix} H^T E_X \\ 0 \end{bmatrix} \right\| \\
&= \|V_{22}^+\|^{-1} \left\| \begin{bmatrix} I_k & D \end{bmatrix} \begin{bmatrix} H^T E_X \\ 0 \end{bmatrix} \right\| \\
&\geq \|V_{22}^+\|^{-1} \sigma_{\min}([I_k \ D]) \left\| \begin{bmatrix} H^T E_X \\ 0 \end{bmatrix} \right\| \\
&\geq \|V_{22}^+\|^{-1} \|E_X\|.
\end{aligned} \tag{3.14}$$

From (3.9) and (3.14) the desired upper bound follows. $\square$

When the subspace angle is sufficiently small and the TLS problem is well conditioned, i.e., $\|V_{22}^+\|$ is not too large, then $\|G_2^+\|$ should be approximately equal to $\|V_{22}^+\|$. This follows because for small θ the orthogonal Procrustes problem [19], [11]

$$\min_{S^T S = I_{n-k+d}} \|G - V_2 S\|$$

can be solved with a small residual. Hence G_1 can be considered an acute perturbation of $V_{12}S$ and G_2 an acute perturbation of $V_{22}S$, and consequently $\|G_2^+\|$ should be correspondingly close to $\|(V_{22}S)^+\| = \|V_{22}^+\|$. Hence, for small θ , since $\|G_2^+\| \approx \|V_{22}^+\|$, then we have

$$\|X_M - \hat{X}\| \leq \sin \theta \|G_2^+\| \|V_{22}^+\| \tag{3.15}$$

$$\approx \sin \theta \|G_2^+\|^2 \tag{3.16}$$

$$= \sin \theta (1 + \|X_M\|^2). \tag{3.17}$$

Equation (3.17) follows from (3.16) using similar arguments as in [8] which show $\|V_{22}^+\| = \sqrt{1 + \|X_{SVD}\|^2}$: one merely “completes the space” so that $[\tilde{G} \ G]$ is an orthogonal matrix and applies the CS Theorem of Paige and Saunders [17] to get

$\|G_2^+\| = \sqrt{1 + \|X_M\|^2}$, which happens to be the “condition number” of the TLS problem for method M. As the TLS solution is orthogonally invariant on the right, $X_{SVD} = -V_{12}V_{22}^+ = -(V_{12}S)(V_{22}S)^+ \approx G_1G_2^+ = X_M$. Thus, Theorem 2 states that if the subspace angle θ is small and the TLS problem is well-conditioned ($\|V_{22}^+\| \approx \|G_2^+\|$ is not too large), then the TLS-M solution X_M will be correspondingly close to the ordinary TLS solution X_{SVD} . It also means that one cannot extract any more accuracy from X_M , as compared to X_{SVD} , than the subspace angle will allow; this will be implicitly assumed as $R\left(\begin{bmatrix} X_M \\ -I_{n-k+d} \end{bmatrix}\right) \subseteq R(G)$ and $R\left(\begin{bmatrix} X_{SVD} \\ -I_{n-k+d} \end{bmatrix}\right) \subseteq R(V_2)$. These conclusions are verified in the numerical simulations for QR with column pivoting in Section 5.

Chan and Hansen [5] obtain a similar upper bound (3.11) for the case when A is full rank. Their total least squares solution X_{RRQR} is deduced from $R(\Pi W)$, where Π and W are matrices obtained from the rank revealing QR algorithm of Chan [4]; they show

$$\|X_{RRQR} - X_{SVD}\| \leq \tan \theta \|V_{22}^{-1}\|^2 (1 + O(\tan \theta)), \quad (3.18)$$

provided A has full rank and $\tan \theta < \|V_{22}^{-1}\|^{-1}$. However, equation (3.11) in Theorem 2 handles the case when A is possibly rank-deficient and applies to *any* total least squares solution, such as X_{RRQR} or a perturbed TLS-SVD problem. The assumption Z has full column rank is not a severe restriction; for reasons of stability and minimum variance a total least squares solution should be deduced from the $(n - k + d)$ -dimensional nullspace of $[\tilde{A} \ \tilde{B}]$ rather than a proper subspace of it.

It should be noted that (3.11) in Theorem 2 also serves as a perturbation result for TLS-SVD. Let $X_{SVD} = -V_{12}V_{22}^+$ denote the TLS-SVD solution to $AX \approx B$ and let $\tilde{X}_{SVD} = -\tilde{V}_{12}\tilde{V}_{22}^+$ denote the TLS-SVD solution to the perturbed problem $(A + \Delta A)X \approx (B + \Delta B)$. Then if $\sin \theta$ is the sine of the subspace angle between

$R\left(\begin{bmatrix} V_{12} \\ V_{22} \end{bmatrix}\right)$ and $R\left(\begin{bmatrix} \tilde{V}_{12} \\ \tilde{V}_{22} \end{bmatrix}\right)$ the same arguments yield

$$\|X_{SVD} - \tilde{X}_{SVD}\| \leq \sin \theta \|V_{22}^+\| \|\tilde{V}_{22}^+\|. \quad (3.19)$$

Now, using singular subspace perturbation theory by Wedin [26], it can be shown that $\sin \theta \leq \|[\Delta A \ \Delta B]\|/(\tilde{\sigma}_k - \sigma_{k+1})$, where $\tilde{\sigma}_k$ is the k^{th} singular value of $[(A + \Delta A) \ (B + \Delta B)]$. This yields

$$\|X_{SVD} - \tilde{X}_{SVD}\| \leq \frac{\|[\Delta A \ \Delta B]\|}{\tilde{\sigma}_k - \sigma_{k+1}} \|V_{22}^+\| \|\tilde{V}_{22}^+\|. \quad (3.20)$$

According to the perturbation theory of singular values [11], $\tilde{\sigma}_k$ can vary from σ_k by at most $\|[\Delta A \ \Delta B]\|$.

For the TLS-M residual defined by $R_M = B - AX_M$, upper and lower bounds can be found in terms of the TLS-M solution X_M and the correction in $[A \ B]$ applied by method M.

Theorem 3 *Let A have the usual SVD and let $[\tilde{A} \ \tilde{B}]$ be a rank- k approximation to $[A \ B]$ from method M. If $\|\Delta \tilde{A}\| \leq \sigma'_k$, then the residual R_M satisfies*

$$\|[\Delta \tilde{A} \ \Delta \tilde{B}]\| \leq \|R_M\| \leq \|[\Delta \tilde{A} \ \Delta \tilde{B}]\| \sqrt{1 + \|X_M\|^2}. \quad (3.21)$$

Proof: The condition $\|\Delta \tilde{A}\| \leq \sigma'_k$ ensures X_M exists. Now, $R_M = B - AX_M$ can be expressed as

$$R_M = \Delta \tilde{B} - \Delta \tilde{A} X_M \quad (3.22)$$

$$= -[\Delta \tilde{A} \ \Delta \tilde{B}] \begin{bmatrix} X_M \\ -I_d \end{bmatrix}. \quad (3.23)$$

It follows

$$\|[\Delta \tilde{A} \ \Delta \tilde{B}]\| \left\| \begin{bmatrix} X_M \\ -I_d \end{bmatrix}^+ \right\|^{-1} \leq \|R_M\| \leq \|[\Delta \tilde{A} \ \Delta \tilde{B}]\| \left\| \begin{bmatrix} X_M \\ -I_d \end{bmatrix} \right\|.$$

The bounds in (3.21) follow as all the singular values of $\begin{bmatrix} X_M \\ -I_d \end{bmatrix}$ are greater or equal to 1 with the largest being $\sqrt{1 + \|X_M\|^2}$. $\square$

Now we will find an upper bound on $\sin \theta$ to determine influencing quantities for the upper bound. Using a generalization of an argument due to Chan [4] we obtain:

$$\begin{aligned}
\sin \theta &= \|V_1^T G\| \\
&= \|\Sigma_1^{-1} U_1^T U_1 \Sigma_1 V_1^T G\| \\
&\leq \|\Sigma_1^{-1}\| \|U_1^T\| \|U_1 \Sigma_1 V_1^T G\| \\
&= \sigma_k^{-1} \|U_1 \Sigma_1 V_1^T G\| \\
&= \sigma_k^{-1} \|\hat{A} \hat{B}\| G\| \\
&= \sigma_k^{-1} \|[A \ B]G - [\Delta \hat{A} \ \Delta \hat{B}]G\| \\
&\leq \sigma_k^{-1} (\|[A \ B]G\| + \|[\Delta \hat{A} \ \Delta \hat{B}]G\|) \\
&\leq \sigma_k^{-1} (\|[A \ B]ZT^{-1}\| + \sigma_{k+1}) \\
&\leq \sigma_k^{-1} (\|[A \ B]Z\| \|T^{-1}\| + \sigma_{k+1}). \tag{3.24}
\end{aligned}$$

This leads to the following general result.

Theorem 4 *Let $[A \ B]$ have the usual SVD. Assume $Z \in \mathbb{R}^{(n+d) \times (n-k+d)}$ has full column rank, satisfies $\|[A \ B]Z\| = \epsilon$, and has QR decomposition $Z = GT$. Then*

$$\sin \theta \leq \frac{\epsilon \|T^{-1}\| + \sigma_{k+1}}{\sigma_k} \tag{3.25}$$

where θ is the subspace angle between $R(G)$ and $R(V_2)$.

Proof: The desired result follows immediately from (3.24) and (3.1). $\square$

This theorem indicates the quality of $R(Z) = R(G)$ depends on several factors: ϵ ,

$\|T^{-1}\|$, σ_{k+1} and σ_k . The subspace angle will be small when Z is a good approximate null-matrix for $[A \ B]$ (ϵ is small), the columns of Z are sufficiently linearly independent ($\|T^{-1}\|$ is not too large), the matrix A has a well defined gap in its singular value spectrum and $AX \approx B$ is not too incompatible ($\sigma_k \geq \sigma'_k$ is moderately sized and σ_{k+1} is small). Because the product of ϵ and $\|T^{-1}\|$ occurs in (3.25), the scaling of Z is only an artificial concern. As T is triangular, one may resort to the wide variety of techniques for the efficient estimation of $\|T^{-1}\|$. An excellent survey is given by Higham [14].

4. Orthogonal Projection via QR Factorization

In this section we consider a QR factorization of $[A \ B]$ to restore compatibility to $AX \approx B$ and give a total least squares solution based on the rank- k approximation of $[A \ B]$.

Let $[A \ B]$ have the QR factorization

$$[A \ B]\Pi = QR = [Q_1 \ Q_2] \begin{bmatrix} R_{11} & R_{12} \\ 0 & R_{22} \end{bmatrix} \quad (4.1)$$

where $\Pi \in \mathbb{R}^{(n+d) \times (n+d)}$ is a permutation matrix that is user-determined, $Q \in \mathbb{R}^{m \times (n+d)}$ has orthonormal columns, $Q_1 \in \mathbb{R}^{m \times k}$, $R \in \mathbb{R}^{(n+d) \times (n+d)}$ is upper triangular, $R_{11} \in \mathbb{R}^{k \times k}$, $R_{22} \in \mathbb{R}^{(n-k+d) \times (n-k+d)}$.

When $\|R_{22}\|$ is small it is well known that $[A \ B]$ must have at least $n-k+d$ small singular values. A reasonable and desirable property of a QR factorization is that it reveals the correct near-rank deficiency of a matrix through a small $\|R_{22}\|$. Using a definition of Chan and Hansen [5], we have an indication whether the QR factorization (4.1) possesses this property.

Definition. Assume $[A \ B]$ has the QR factorization as in (4.1). If $\|R_{22}\| =$

$O(\sigma_{k+1})$ and R_{11} is well-conditioned, then the QR factorization is said to be *rank-revealing* and the *numerical rank* of $[A \ B]$ is k .

Now, define $[\tilde{A} \ \tilde{B}]$ by

$$[\tilde{A} \ \tilde{B}] = P_{Q_1} [A \ B], \quad (4.2)$$

where P_{Q_1} is the orthogonal projection matrix onto $R(Q_1)$. In terms of the QR factors, we have

$$[\tilde{A} \ \tilde{B}] = Q_1 [\underbrace{R_{11}}^k \underbrace{R_{12}}^{n-k+d}] \Pi^T, \quad (4.3)$$

a rank- k approximation to $[A \ B]$. Letting $[\Delta \tilde{A} \ \Delta \tilde{B}] = [A \ B] - [\tilde{A} \ \tilde{B}]$, then

$$\|[\Delta \tilde{A} \ \Delta \tilde{B}]\| = \|R_{22}\|. \quad (4.4)$$

Let X_{QR} denote the minimum norm TLS-QR solution to

$$\tilde{A}X = \tilde{B}, \quad (4.5)$$

or, equivalently,

$$[\tilde{A} \ \tilde{B}] \begin{bmatrix} X \\ -I_d \end{bmatrix} = 0. \quad (4.6)$$

Consider the full column rank matrix $Y \in \Re^{(n+d) \times (n-k+d)}$ given by

$$Y = \begin{bmatrix} R_{11}^{-1} R_{12} \\ -I_{n-k+d} \end{bmatrix}. \quad (4.7)$$

The matrix Y has the property that all of its singular values are ≥ 1 . It is easy to show $[\tilde{A} \ \tilde{B}]\Pi Y = 0$. Therefore $R(\Pi Y)$ is in the $(n - k + d)$ -dimensional nullspace of $[\tilde{A} \ \tilde{B}]$. To compute X_{QR} , we just need a basis for the nullspace of $[\tilde{A} \ \tilde{B}]$. This can be accomplished by first performing a QR decomposition on Y (or using modified Gram-Schmidt orthogonalization on Y):

$$Y = H_Y F, \quad (4.8)$$

where $H_Y \in \mathfrak{R}^{(n+d) \times (n-k+d)}$ has orthonormal columns and $F \in \mathfrak{R}^{(n-k+d) \times (n-k+d)}$ is upper triangular. Defining H by $H = \Pi H_Y$ with the partitioning $H = [H_1^T \ H_2^T]^T$, where $H_2 \in \mathfrak{R}^{d \times (n-k+d)}$, then

$$X_{QR} = -H_1 H_2^+, \quad (4.9)$$

provided H_2 has full row rank. The following corollary gives sufficient conditions for the compatibility of (4.5) and hence the existence of X_{QR} .

Corollary 1 *Assume A has the usual SVD and $[A \ B]$ has the QR decomposition (4.1). If $\|R_{22}\| < \sigma'_k$, then $\tilde{A}X = \tilde{B}$ is compatible and X_{QR} in (4.9) exists.*

Proof:

Follows immediately from (4.4) and Theorem 1. $\square$

At this point we can compare the TLS-QR solution to the TLS-SVD solution. The class of TLS-QR methods may be suboptimal in terms of the problem formulation (2.2)-(2.3); however, the approach can yield acceptable results with a gain in computational efficiency.

Now we can compare $R(\Pi Y)$ and $R(V_2)$ where ΠY (Y as in (4.7)) is annihilated by the rank- k QR approximation $[\tilde{A} \ \tilde{B}]$ in (4.3) and V_2 is annihilated by the rank- k TLS approximation $[\hat{A} \ \hat{B}]$ in (2.4). It can be shown

$$\|[A \ B]\Pi Y\| = \|R_{22}\|. \quad (4.10)$$

From Theorem 4 and (4.10) the sine of the subspace angle between $R(\Pi Y) = R(H)$ and the ordinary TLS solution space $R(V_2)$ is bounded by

$$\sin \theta \leq \frac{\|R_{22}\|}{\sigma_k} (\|F^{-1}\| + 1). \quad (4.11)$$

Further, due to the construction of Y , it follows from Lemma 3.11 [20, p.147]

$$\|F^{-1}\| \leq 1. \quad (4.12)$$

Using the facts $\sigma_k^{-1} \leq \|R_{11}^{-1}\|$ and $\sigma_{k+1} \leq \|R_{22}\|$, this leads to the following corollaries:

Corollary 2 *Assume $[A \ B]$ has the usual SVD and $[\tilde{A} \ \tilde{B}]$ in (4.3) is obtained from the QR factorization of $[A \ B]$ in (4.1). Let Y be defined as in (4.7). If $\|R_{22}\| < \sigma'_k$ then*

$$\sin \theta \leq \frac{2 \|R_{22}\|}{\sigma_k} \quad (4.13)$$

$$\leq 2 \|R_{22}\| \|R_{11}^{-1}\| \quad (4.14)$$

where θ is the subspace angle between $R(\Pi Y)$ and $R(V_2)$.

Corollary 3 *Assume $[A \ B]$ has the usual SVD and $[\tilde{A} \ \tilde{B}]$ in (4.3) is obtained from the QR factorization of $[A \ B]$ as in (4.3). Let X_{QR} be defined as in (4.9). If $\|R_{22}\| < \sigma'_k$ then*

$$\|X_{QR} - X_{SVD}\| \leq \sin \theta \|H_2^+\| \|V_{22}^+\| \quad (4.15)$$

$$\leq \frac{2 \|R_{22}\|}{\sigma_k} \|H_2^+\| \|V_{22}^+\| \quad (4.16)$$

$$\leq 2 \|R_{22}\| \|R_{11}^{-1}\| \|H_2^+\| \|V_{22}^+\| \quad (4.17)$$

where θ is the subspace angle between $R(\Pi Y)$ and $R(V_2)$.

This means that if we have a rank-revealing QR decomposition of $[A \ B]$ and the solution spaces $R(\Pi Y) = R(H)$ and $R(V_2)$ are sufficiently close, i.e., their subspace angle is small, the TLS-QR solution X_{QR} will be correspondingly close to the ordinary TLS solution X_{SVD} . This suggests the following algorithm based on a rank

revealing QR factorization of $[A \ B]$:

Algorithm TLS-QR. Computation of the TLS-QR solution X_{QR} to $AX \approx B$.

Step 1. Given the data $[A \ B]$, compute a rank revealing QR factorization of $[A \ B]$:

$$[A \ B]\Pi = QR = Q \begin{bmatrix} R_{11} & R_{12} \\ 0 & R_{22} \end{bmatrix}$$

Step 2. Use backward elimination to solve $R_{11}W = R_{12}$ and form Y ($O(k^2(n-k+d))$ flops):

$$Y = \begin{bmatrix} W \\ -I_{n-k+d} \end{bmatrix}.$$

Step 3. Compute an orthonormal basis $H_Y \in \Re^{(n+d) \times (n-k+d)}$ for $R(Y)$ using the modified Gram-Schmidt method ($O((n+d)(n-k+d)^2)$ flops).

Step 4. IF $\sin \theta < \delta$ then

set $H = \Pi H_Y$ and compute by Householder transformations an orthogonal matrix P such that

$$HP = \begin{bmatrix} D & Z \\ 0 & \Gamma \end{bmatrix}$$

where $Z \in \Re^{n \times d}$ and $\Gamma \in \Re^{d \times d}$ is upper triangular ($O((n+d)(n-k+d)^2)$ flops).

Then GO TO Step 6.

Step 5. Set $H_0 = H_Y$ and improve the columns of H_0 by means of τ steps of simultaneous inverse iteration using $(R^T R)^{-1}$ to obtain a sequence of estimates $\{H_i\}_{i=1}^{\tau}$ ($O(\tau(n+d)(n-k+d)^2)$ flops). Set $H_Y = H_{\tau}$ and GO TO Step 4.

Step 6. Solve by forward elimination $\Gamma^T S = -Z^T$ for S ($O(nd^2)$ flops). Then $X_{QR} = S^T$.

END OF TLS-QR

Note that the condition $\sin \theta < \delta$ (δ is a user-specified tolerance) can be checked in the first pass by $2\|R_{22}\| \|R_{11}^{-1}\| < \delta$. If this a posteriori bound on $\sin \theta$ is used, the more probable situation is that at least one step of inverse iteration will occur and then one can monitor the subspace angle between $R(H_{i-1})$ and $R(H_i)$ to see if it is sufficiently small. This follows along the lines of Chan and Hansen's subspace iteration algorithm SPIT [6]. The numerical simulations in Section 5 show that one or two subspace iterations (depending on δ) are frequently adequate provided the subspace tolerance is not too demanding.

For subsequent analysis we need to develop conforming expressions for $[A \ B]$, $[\tilde{A} \ \tilde{B}]$, and $[\triangle \tilde{A} \ \triangle \tilde{B}]$ in terms of QR factors. Define $W \in \Re^{(n+d) \times (n+d)}$ by

$$W = \Pi \begin{bmatrix} I_k & 0 \\ (R_{11}^{-1} R_{12})^T & I_{n-k+d} \end{bmatrix} = \begin{bmatrix} W_{11} & W_{12} \\ W_{21} & W_{22} \end{bmatrix} \quad (4.18)$$

where $W_{11} \in \Re^{n \times k}$ and $W_{22} \in \Re^{(n-k+d) \times (n-k+d)}$. To find expressions for A and B ,

$$[A \ B] = [Q_1 \ Q_2] \begin{bmatrix} R_{11} & R_{12} \\ 0 & R_{22} \end{bmatrix} \Pi^T \quad (4.19)$$

$$= [Q_1 \ Q_2] \begin{bmatrix} R_{11} & 0 \\ 0 & R_{22} \end{bmatrix} \begin{bmatrix} I_k & R_{11}^{-1} R_{12} \\ 0 & I_{n-k+d} \end{bmatrix} \Pi^T \quad (4.20)$$

$$= [Q_1 \ Q_2] \begin{bmatrix} R_{11} & 0 \\ 0 & R_{22} \end{bmatrix} \begin{bmatrix} W_{11}^T & W_{21}^T \\ W_{12}^T & W_{22}^T \end{bmatrix} \quad (4.21)$$

$$= \underbrace{[Q_1 R_{11} W_{11}^T + Q_2 R_{22} W_{12}^T]}_n \underbrace{[Q_1 R_{11} W_{21}^T + Q_2 R_{22} W_{22}^T]}_d. \quad (4.22)$$

To find expressions for $\tilde{A}$ and $\tilde{B}$,

$$\begin{aligned} [\tilde{A} \ \tilde{B}] &= Q_1 [R_{11} \ R_{12}] \Pi^T \\ &= Q_1 [R_{11} \ R_{12}] I_{n+d} \Pi^T \end{aligned} \quad (4.23)$$

$$\begin{aligned}
&= [Q_1 \ Q_2] \begin{bmatrix} R_{11} & R_{12} \\ 0 & 0 \end{bmatrix} \begin{bmatrix} I_k & -R_{11}^{-1}R_{12} \\ 0 & I_{n-k+d} \end{bmatrix} \begin{bmatrix} I_k & R_{11}^{-1}R_{12} \\ 0 & I_{n-k+d} \end{bmatrix} \Pi^T \\
&= [Q_1 \ Q_2] \begin{bmatrix} R_{11} & R_{12} \\ 0 & 0 \end{bmatrix} \begin{bmatrix} I_k & -R_{11}^{-1}R_{12} \\ 0 & I_{n-k+d} \end{bmatrix} \begin{bmatrix} W_{11}^T & W_{21}^T \\ W_{12}^T & W_{22}^T \end{bmatrix} \quad (4.24)
\end{aligned}$$

$$= [Q_1 R_{11} \ 0] \begin{bmatrix} W_{11}^T & W_{21}^T \\ W_{12}^T & W_{22}^T \end{bmatrix} \quad (4.25)$$

$$= [\underbrace{Q_1 R_{11} W_{11}^T}_n \ \underbrace{Q_1 R_{11} W_{21}^T}_d]. \quad (4.26)$$

From $[\Delta \tilde{A} \ \Delta \tilde{B}] = [A \ B] - [\tilde{A} \ \tilde{B}]$, (4.22) and (4.26) it follows

$$[\Delta \tilde{A} \ \Delta \tilde{B}] = [\underbrace{Q_2 R_{22} W_{12}^T}_n \ \underbrace{Q_2 R_{22} W_{22}^T}_d]. \quad (4.27)$$

If $\|R_{22}\|/\sigma_k = O(\sigma_{k+1}/\sigma_k)$ is small, that is, there is a well determined gap in the singular value spectrum of A , and $AX \approx B$ is not too incompatible, one would expect the TLS predictor $\hat{A}X_{SV D}$ and the TLS-QR predictor $\tilde{A}X_{QR}$ to be close. That this is true can be seen by the following: using $U_1^T = (\Sigma_1^+)^T V_1^T [A \ B]^T$ from the SVD of $[A \ B]$ and $[A \ B] = [Q_1 R_{11} W_{11}^T + Q_2 R_{22} W_{12}^T \quad Q_1 R_{11} W_{21}^T + Q_2 R_{22} W_{22}^T]$ in (4.22), we have

$$U_1^T Q_2 = (\Sigma_1^+)^T V_1^T \begin{bmatrix} W_{12} \\ W_{22} \end{bmatrix} R_{22}^T. \quad (4.28)$$

Now $[W_{12}^T, W_{22}^T]^T = \Pi[0, I_{n-k+d}]^T$ implies

$$\left\| \begin{bmatrix} W_{12} \\ W_{22} \end{bmatrix} \right\| \leq 1. \quad (4.29)$$

Clearly $\|V_1^T\| \leq 1$. This implies

$$\|U_1^T Q_2\| \leq \|(\Sigma_1^+)^T\| \|V_1^T\| \left\| \begin{bmatrix} W_{12} \\ W_{22} \end{bmatrix} \right\| \|R_{22}^T\| \quad (4.30)$$

$$\leq \|R_{22}\|/\sigma_k. \quad (4.31)$$

Therefore,

$$\|\tilde{A}X_{QR} - \hat{A}X_{SVD}\| = \|(P_{Q_1} - P_{U_1})B\| \quad (4.32)$$

$$\leq \|P_{Q_1} - P_{U_1}\| \|B\| \quad (4.33)$$

$$= \|U_1^T Q_2\| \|B\| \quad (4.34)$$

$$\leq \frac{\|R_{22}\| \|B\|}{\sigma_k}. \quad (4.35)$$

For a rank-revealing QR decomposition, $\|R_{22}\| = O(\sigma_{k+1})$, and it follows

$\|\tilde{A}X_{QR} - \hat{A}X_{SVD}\| \leq \|B\| O(\sigma_k/\sigma_{k+1})$. This means that ordinary TLS and TLS-QR methods will correspondingly “predict” B when $AX = B$ is not too incompatible and the QR decomposition is rank-revealing. Also, from (4.4) and Theorem 3 the following corollary is immediate:

Corollary 4 *Assume A has the usual SVD. Let $[A \ B]$ have the QR factorization as in (4.1) with $[\tilde{A} \ \tilde{B}]$ the rank- k approximation as in (4.3). If $\|R_{22}\| \leq \sigma'_k$, then*

$$\|R_{22}\| \leq \|R_{QR}\| \leq \|R_{22}\| \sqrt{1 + \|X_{QR}\|^2}. \quad (4.36)$$

5. Numerical Simulations: Performance Analysis of TLS-QR

In the previous sections the results concerning the TLS-QR method are independent of the column permutation strategy one might wish to employ. For example, one can use the well known QR with column pivoting algorithm (e.g., see [3],[10, p.164]), the Rank-Revealing QR (RRQR) algorithm of Chan [4] or an *a priori* scheme such as column re-ordering[18]. In this section we consider the QR with column pivoting strategy and compare the method to the TLS-SVD technique.

5.1 TLS-QR without Subspace Refinement

Corollary 3 shows that if the subspace angle is small and the TLS problem is not too ill conditioned, then the TLS-QR solution X_{QR} in (4.9) will be correspondingly close to the TLS solution X_{SVD} . For small θ the orthogonal Procrustes problem

$$\min_{S^T S = I_{n-k+d}} \|H - V_2 S\|$$

can be solved with a small residual. As the ordinary TLS solution is orthogonally invariant, $X_{SVD} = -V_{12}V_{22}^+ = -(V_{12}S)(V_{22}S)^+$. Hence H_1 can be considered an acute perturbation of $V_{12}S$ and H_2 an acute perturbation of $V_{22}S$. Consequently, $\|H_2^+\|$ should be correspondingly close to $\|V_{22}^+\|$, which should not be much larger than the optimal value of 1. The aforementioned conclusions are verified in the following Pro-Matlab [16] simulations.

The coefficient matrix $A_0 \in \mathbb{R}^{50 \times 10}$ has singular values

$$\sigma(A_0) = \{10, 7, 7, 3, 2, 1, \sigma_7(A_0), 0.0005, 0.0001, 0.00005\}$$

where $\sigma_7(A_0) = 0.1$ or 1.0 . Each simulation is characterized by a two-tuple (i, j) , with $i = 1, \dots, 5$ and $j = 1, 2$. Given A_0 , we chose $B_0 \in \mathbb{R}^{50 \times 4}$ such that

$$B_0 = A_0 X_{(i,j)} + Y_j$$

where $X_{(i,j)}$, which depends on both i and j , is a random matrix with entries from the standard normal distribution and the entries of Y_j , which depend only on j , are from the normal distribution with mean zero and standard deviation μ_j ($\mu_1 = 0.0001$, $\mu_2 = 0.01$). For fixed (i, j) we perturbed A_0 and B_0 by random matrices $(\Delta A)_i$ and $(\Delta B)_i$ whose entries have mean zero and standard deviation ω_i ($\omega_1 = 1e - 04$, $\omega_2 = 5e - 04$, $\omega_3 = 1e - 03$, $\omega_4 = 5e - 03$, $\omega_5 = 1e - 02$). The matrices A and B are defined by

$$[A \ B] = [A_0 \ B_0] + [(\Delta A)_i \ (\Delta B)_i].$$

Notice that for $i = 1$ and $j = 1$ the system of equations $AX \approx B$ is only slightly incompatible but as i or j increases the system becomes less compatible. The values shown in the tables are the mean values of 100 independent trials, with γ defined by $\gamma \equiv \|R_{11}^{-1}\| \|H_2^+\| \|V_{22}^+\|$.

In the first simulation we set $\sigma_7(A_0) = 1$. The results without subspace refinement are summarized in Table 5.1. As seen in Table 5.1, the bounds on the norm of the difference in the solutions in terms of the subspace angle are tight, which supports the notion that if the subspaces are “close”, with the subspace angle as a measure of closeness, then the solutions will be correspondingly close. The bound on the difference in the solutions in terms of $\|R_{22}\| \gamma$ does not fare quite as well. In addition, when the TLS problem is not too ill conditioned we see that $\|H_2^+\| \approx \|V_{22}^+\|$, as expected, which is not too large.

We repeat the numerical simulations as explained previously except this time the k^{th} singular value of A_0 is 0.1. The results without subspace refinement are summarized in Table 5.2. As seen in Table 5.2 if the TLS problem is not too ill conditioned, i.e., $\|V_{22}^+\|$ is not too large, then if θ is small the TLS-QR and ordinary TLS solution will be correspondingly close. Also, the bounds on the norm of the difference in the solutions in terms of $\|R_{22}\| \gamma$ rapidly deteriorate as the coefficient matrix becomes more ill conditioned and the size of the perturbations increase so that $AX \approx B$ becomes less compatible.

(i, j)	std dev	$\frac{\ X_{QR} - X_{SVD}\ }{\ X_{SVD}\ }$	$\frac{\sin \theta \ H_2^+\ \ V_{22}^+\ }{\ X_{SVD}\ }$	$\frac{2 \ R_{22}\ \gamma}{\ X_{SVD}\ }$	$\ H_2^+\ $	$\ V_{22}^+\ $
1.1	1.0e-04	3.5617e-07	2.5770e-06	1.9055e-02	4.0242	4.0242
2.1	5.0e-04	3.6109e-06	3.0203e-05	5.4494e-02	3.9074	3.9074
3.1	1.0e-03	4.9318e-05	2.0059e-04	1.4898e-01	3.2407	3.2407
4.1	5.0e-03	9.3495e-04	6.2522e-03	1.3601e+00	3.6518	3.6518
5.1	1.0e-02	3.7749e-03	3.5461e-02	3.0093e+00	3.5799	3.5798
1.2	1.0e-04	2.0155e-04	1.1801e-03	3.5810e-01	4.4817	4.4817
2.2	5.0e-04	3.0704e-04	1.2882e-03	6.8617e-01	3.3704	3.3703
3.2	1.0e-03	2.7372e-04	1.4523e-03	6.3713e-01	3.9303	3.9303
4.2	5.0e-03	1.0284e-03	7.0833e-03	1.1481e+00	4.5981	4.5978
5.2	1.0e-02	4.9603e-03	4.1254e-02	3.7115e+00	4.0263	4.0259

Table 5.1: The mean values of 100 independent trials with $m = 50$, $n = 10$ and $d = 4$. The numerical rank of A_0 is $k = 7$ and $\sigma_7(A_0) = 1$.

(i, j)	std dev	$\frac{\ X_{QR} - X_{SVD}\ }{\ X_{SVD}\ }$	$\frac{\sin \theta \ H_2^+\ \ V_{22}^+\ }{\ X_{SVD}\ }$	$\frac{2 \ R_{22}\ \gamma}{\ X_{SVD}\ }$	$\ H_2^+\ $	$\ V_{22}^+\ $
1.1	1.0e-04	1.5684e-05	2.9320e-05	6.9282e-02	3.5302	3.5302
2.1	5.0e-04	1.1674e-03	3.8587e-03	6.3123e-01	3.1049	3.1047
3.1	1.0e-03	2.6807e-03	1.9210e-02	1.7608e+00	5.3010	5.3042
4.1	5.0e-03	4.5608e-02	1.3279e-01	3.5506e+00	3.6230	3.5639
5.1	1.0e-02	2.7906e-01	1.7380e+00	1.2736e+01	4.5070	4.4015
2.1	1.0e-04	3.6793e-02	1.2604e-01	3.2417e+00	3.6235	3.6173
2.2	5.0e-04	8.0341e-02	6.3297e-01	9.4177e+00	3.8430	3.8374
3.2	1.0e-03	1.1672e-02	1.0151e-01	5.3050e+00	4.0863	4.0885
4.2	5.0e-03	1.5440e+00	5.2355e+00	2.3271e+01	5.0796	3.2296
5.2	1.0e-02	3.8816e-01	1.5600e+00	1.1754e+01	4.2124	3.7755

Table 5.2: The mean values of 100 independent trials with $m = 50$, $n = 10$ and $d = 4$. The numerical rank of A_0 is $k = 7$ and $\sigma_7(A_0) = 0.1$.

5.2 TLS-QR with Subspace Refinement

In this section we show typical results of algorithm TLS-QR with subspace iteration. The subspace iteration process is essentially SPIT [6]. The simulation is designed as follows. The coefficient matrix $A_0 \in \mathbb{R}^{50 \times 10}$ has singular values

$$\sigma(A_0) = \{10, 7, 7, 3, 2, 1, \sigma_7(A_0), 0.0005, 0.0001, 0.00005\}$$

where $\sigma_7(A_0) = 0.1$ or 1.0 . Each simulation is characterized by a three-tuple (i, j, t) , with $i = 1, \dots, 5$ and $j = 1, 2$ and a subspace tolerance δ_t ($t = 1, \dots, 4$). The subspace refinement process is terminated when the subspace angle between two consecutive iterates $R(H_{p-1})$ and $R(H_p)$ is less than δ_t . We defined the tolerance δ_t by

$$\delta_t = \sqrt{n} * \|R\|_1 * eps * 10^{f(t)}$$

where eps is the machine precision (about $2.2e-16$) and $f(t) = 2t+3$ (which lowers the tolerance). Given A_0 , we chose $B_0 \in \mathbb{R}^{50 \times 4}$ such that

$$B_0 = A_0 X_{(i,j)} + Y_j$$

where $X_{(i,j)}$, which depends on both i and j , is a random matrix with entries from the standard normal distribution and the entries of Y_j , which depend only on j , are from the normal distribution with mean zero and standard deviation μ_j ($\mu_1 = 0.0001$, $\mu_2 = 0.001$). For fixed (i, j) we perturbed A_0 and B_0 by random matrices $(\Delta A)_i$ and $(\Delta B)_i$ whose entries have mean zero and standard deviation ω_i :

$$\omega_1 = 1e-04, \omega_2 = 5e-04, \omega_3 = 1e-03, \omega_4 = 5e-03, \omega_5 = 1e-02.$$

The matrices A and B are defined by

$$[A \ B] = [A_0 \ B_0] + [(\Delta A)_i \ (\Delta B)_i].$$

It is important to note that for $i = 1$ and $j = 1$ the system of equations $AX \approx B$ is only slightly incompatible but as i or j increases the system becomes less compatible; further, as t increases the subspace tolerance becomes less demanding. Also, X_{QR} denotes the unrefined TLS-QR solution and X_{REF} denotes the TLS-QR solution after subspace refinement. The values shown in the tables are the mean values of 100 independent trials. The average number of iterations was rounded to the nearest integer.

(i, j, t)	σ_{k+1}/σ_k	$\sin \theta$	$\frac{\ X_{QR} - X_{SVD}\ }{\ X_{SVD}\ }$	$\frac{\ X_{REF} - X_{SVD}\ }{\ X_{SVD}\ }$	iters
1,1,1	6.0616e-04	2.0745e-07	1.4749e-07	3.3814e-15	2
2,1,1	3.5701e-03	1.5006e-05	6.2054e-06	4.1122e-15	2
3,1,1	8.4723e-03	5.8703e-05	2.8643e-05	3.3116e-15	3
4,1,1	2.9339e-02	6.6421e-04	5.5651e-04	1.9596e-13	3
5,1,1	6.2894e-02	3.7569e-03	3.7918e-03	5.0101e-13	4
1,1,2	7.8060e-04	4.2265e-07	2.0095e-07	2.9789e-15	2
2,1,2	3.2441e-03	1.0042e-05	7.8713e-06	4.4279e-15	2
3,1,2	7.8122e-03	4.5567e-05	3.7292e-05	6.9069e-14	2
4,1,2	3.0614e-02	9.8962e-04	7.3393e-04	3.8826e-13	3
5,1,2	7.0267e-02	3.7274e-03	2.0511e-03	1.3843e-10	3
1,1,3	7.6541e-04	3.3999e-07	3.1944e-07	9.4512e-14	1
2,1,3	3.8316e-03	1.1419e-05	1.0659e-05	9.6853e-11	1
3,1,3	7.9057e-03	4.5110e-05	3.3706e-05	7.4426e-14	2
4,1,3	4.0724e-02	1.0718e-03	5.6777e-04	9.6553e-10	2
5,1,3	7.7056e-02	2.0733e-03	1.3035e-03	1.8239e-08	2
1,1,4	7.7235e-04	3.4756e-07	3.2344e-07	9.4272e-14	1
2,1,4	4.0166e-03	8.7286e-06	4.2917e-06	5.3668e-11	1
3,1,4	7.4388e-03	5.1242e-05	2.8398e-05	1.2234e-09	1
4,1,4	3.5960e-02	8.5366e-04	3.3748e-04	2.1780e-07	1
5,1,4	8.3368e-02	5.7827e-03	3.2352e-03	8.7958e-08	2

Table 5.3: The mean values of 100 independent trials with $m = 50$, $n = 10$ and $d = 4$. The numerical rank of A_0 is $k = 7$ and $\sigma_7(A_0) = 1$.

Table 5.3 (with $j = 1$ and $\sigma_7(A_0) = 1$) shows that generally 1 or 2 subspace iterations are frequently adequate for a significant improvement in the solution

provided the subspace tolerance is not too demanding. For this simulation the mean subspace tolerances δ_t ($t = 1, 2, 3, 4$) were:

$$\delta_1 = 8.0355e - 09, \delta_2 = 6.5343e - 07, \delta_3 = 9.1376e - 05, \delta_4 = 6.9339e - 03.$$

The simulation was repeated with $j = 2$, which means $A_0X \approx B_0$ is less compatible and hence σ_{k+1}/σ_k is generally larger. The results are shown in Table 5.4 and it is seen that this does not disproportionately affect the relative accuracy of the refined TLS-QR solution nor the number of iterations required.

(i, j, t)	σ_{k+1}/σ_k	$\sin \theta$	$\frac{\ X_{QR} - X_{SVD}\ }{\ X_{SVD}\ }$	$\frac{\ X_{REF} - X_{SVD}\ }{\ X_{SVD}\ }$	iters
1,2,1	1.5247e-03	1.3701e-06	4.5665e-07	2.9894e-15	2
2,2,1	2.7103e-03	4.4199e-06	4.2178e-06	4.1359e-15	2
3,2,1	7.6512e-03	5.4380e-05	2.7021e-05	8.4930e-15	3
4,2,1	2.4618e-02	3.3540e-04	3.5326e-04	3.8282e-14	3
5,2,1	4.9245e-02	1.7006e-03	2.1179e-03	5.5380e-14	4
1,2,2	2.2991e-03	3.1453e-06	7.9146e-07	3.0459e-15	2
2,2,2	4.0487e-03	1.5733e-05	9.2260e-06	2.9038e-15	2
3,2,2	6.9656e-03	1.8893e-05	1.5766e-05	1.4900e-14	2
4,2,2	4.1016e-02	1.2526e-03	9.7867e-04	2.7738e-12	3
5,2,2	8.0616e-02	3.2117e-03	1.7518e-03	1.4919e-10	3
1,2,3	6.5618e-04	3.5750e-07	2.3921e-07	8.3906e-14	1
2,2,3	2.4692e-03	3.9273e-06	3.2857e-06	1.6162e-11	1
3,2,3	7.2968e-03	5.0082e-05	3.1283e-05	4.8209e-14	2
4,2,3	4.2989e-02	2.3673e-03	1.2357e-03	2.9816e-09	2
5,2,3	5.1375e-02	2.0977e-03	1.6606e-03	7.3525e-09	2
1,2,4	1.9435e-03	3.0454e-06	1.2218e-06	2.6571e-12	1
2,2,4	4.9946e-03	1.6189e-05	5.9909e-06	9.0517e-11	1
3,2,4	8.3138e-03	4.7919e-05	3.0606e-05	1.3856e-09	1
4,2,4	2.8126e-02	5.6113e-04	6.5982e-04	3.1570e-07	1
5,2,4	7.4096e-02	3.6192e-03	1.6327e-03	2.8353e-08	2

Table 5.4: The mean values of 100 independent trials with $m = 50$, $n = 10$ and $d = 4$. The numerical rank of A_0 is $k = 7$ and $\sigma_7(A_0) = 1$.

Table 5.4 shows that generally 1 or 2 subspace iterations are frequently

adequate for a significant improvement in the solution provided the subspace tolerance is not too demanding. For this simulation the mean subspace tolerances δ_t ($t = 1, 2, 3, 4$) were:

$$\delta_1 = 9.0352e - 09, \delta_2 = 6.8948e - 07, \delta_3 = 6.1083e - 05, \delta_4 = 7.3051e - 03.$$

However, in the next set of simulations the coefficient matrix A_0 is more ill conditioned with $\sigma_7(A_0) = 0.1$ and it is seen that this affects the relative accuracy and the number of subspace iterations. The simulations are designed as explained earlier in this section but without $\omega_5 = 1.0e - 02$ or δ_4 due to extreme sensitivity of the TLS problem. The results for $j = 1$ are summarized in Table 5.5.

(i, j, t)	σ_{k+1}/σ_k	$\sin \theta$	$\frac{\ X_{QR} - X_{SVD}\ }{\ X_{SVD}\ }$	$\frac{\ X_{REF} - X_{SVD}\ }{\ X_{SVD}\ }$	iters
1,1,1	9.0109e-03	5.4570e-05	2.9851e-05	1.0774e-13	2
2,1,1	2.1784e-02	2.9460e-04	4.5373e-04	1.9109e-11	3
3,1,1	7.6298e-02	4.6389e-03	2.3703e-03	7.1112e-11	4
4,1,1	3.0974e-01	3.8565e-02	3.2080e-02	4.4380e-09	6
1,1,2	1.1789e-02	8.7330e-05	2.7263e-05	5.6198e-13	2
2,1,2	3.4697e-02	8.3044e-04	4.6674e-04	5.3203e-10	2
3,1,2	2.4920e-02	3.7565e-04	8.8673e-04	2.4775e-10	2
4,1,2	3.2213e-01	7.8794e-02	7.1932e-02	4.6285e-07	5
1,1,3	1.0041e-02	3.7327e-05	2.4065e-05	1.2016e-09	1
2,1,3	2.8095e-02	4.2319e-04	3.2530e-04	2.1527e-07	1
3,1,3	6.4391e-02	4.7150e-03	5.2387e-03	5.4118e-08	2
4,1,3	3.5227e-01	1.1194e-01	6.0103e-02	3.6731e-05	3

Table 5.5: The mean values of 100 independent trials with $m = 50$, $n = 10$ and $d = 4$. The numerical rank of A_0 is $k = 7$ and $\sigma_7(A_0) = 0.1$.

It is seen that the relative accuracy in the solutions as well as the number of subspace iterations are affected by the ill conditioning of the coefficient matrix. The convergence is hampered by the poor ratio σ_{k+1}/σ_k ; a good discussion of the role of this ratio in subspace iteration is given by Watkins in [25]. The results were similar for $j=2$ but are not shown.

6. Conclusions

In this paper we discuss orthogonal projection to restore compatibility to $AX \approx B$. For any method M, a mild condition is given that guarantees the compatibility of $\tilde{A}X = \tilde{B}$ and hence the existence of the minimum norm solution using the method M. This condition not only implies that A_k and $\tilde{A}$ are acute but also the degree of acuteness. It is shown that if the method M yields an approximate nullspace of $[A \ B]$ which is close to the ordinary TLS solution space derived by the SVD, i.e., the subspace angle is small, then the two solutions will be corresponding close. Then it is shown that with an appropriate rotation, as determined by the corresponding orthogonal Procrustes problem, the basis of the approximate nullspace can be viewed as a slight perturbation of the SVD-based TLS basis vectors. Upper and lower bounds are given for an analytical comparison of the TLS technique using the QR decomposition with a user-determined column permutation strategy to the TLS-SVD technique based on the SVD, and leads to a new algorithm TLS-QR based on a rank revealing QR decomposition and subspace refinement. In addition, perturbation bounds are supplied for the TLS-SVD technique. A performance analysis of QR with column pivoting and TLS-SVD is presented. The simulations illustrate that when the subspace angle is small the solutions will be correspondingly close provided the TLS problem is not very ill conditioned and that 1 or 2 simultaneous inverse iterations are frequently adequate provided the subspace tolerance is not too demanding or the ratio σ_{k+1}/σ_k is not too large.

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