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A projection method for general form linear least-squares problems

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ABSTRACT

One of the possible approaches for the solution of underdetermined linear least-squares problems in general form, for a chosen regularization operator L, projects the problem in the null space of L and in its orthogonal complement. In this paper, we show that the projected problem cannot be solved by the generalized singular value decomposition, and propose some approaches to overcome this issue. Numerical experiments ascertain the stability of the new procedures.

1. Introduction

We are concerned with the computation of the solution of linear least-squares problems

$$\min_{\boldsymbol{x}\in\mathbb{R}^n} \|A\boldsymbol{x}-\boldsymbol{b}\|^2, \tag{1}$$

where $\|\cdot\|$ denotes the Euclidean norm, $A\in\mathbb{R}^{m\times n}$, $\boldsymbol{x}\in\mathbb{R}^n$, $\boldsymbol{b}\in\mathbb{R}^m$ is a known vector, and $\operatorname{rank}(A)=r\leq\min(m,n)$. In the following we will denote by $\mathcal{N}(A)$ the null space of A.

If the solution of (1) is not unique, e.g., if $m<n$ or A is rank deficient, a common choice is to compute the minimal-L-norm solution

$$\begin{cases} \min\limits_{\boldsymbol{x}\in\mathbb{R}^n} \|L\boldsymbol{x}\|^2 \\ \boldsymbol{x}\in\left\{\arg\min\limits_{\boldsymbol{x}\in\mathbb{R}^n}\|A\boldsymbol{x}-\boldsymbol{b}\|^2\right\}, \end{cases} \tag{2}$$

where $L\in\mathbb{R}^{p\times n}$, with $\operatorname{rank}(L)=p$, is referred to as the regularization operator and the two following equivalent conditions hold true

$$\mathcal{N}(A)\cap\mathcal{N}(L)=\{\mathbf{0}\}, \qquad \operatorname{rank}\left(\begin{bmatrix}A\\L\end{bmatrix}\right)=n. \tag{3}$$

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The matrix L incorporates desirable properties for the solution. It is typically a diagonal weighting matrix or a discrete approximation of a derivative operator, in which case L is banded with full row rank. For example, the matrices

$$D_1 = \begin{bmatrix} -1 & 1 & & \\ & \ddots & \ddots & \\ & & -1 & 1 \end{bmatrix} \in \mathbb{R}^{(n-1)\times n} \quad \text{and} \quad D_2 = \begin{bmatrix} 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \end{bmatrix} \in \mathbb{R}^{(n-2)\times n}$$

are approximations to the first and second derivatives. Regularization operators of this form are often referred to as smoothing operators. An effective choice of L is such that the solution $\boldsymbol{x}$ is (at least approximately) in the null space $\mathcal{N}(L)$. In fact, $\mathcal{N}(D_1)$ and $\mathcal{N}(D_2)$ include constant and linearly varying vectors, respectively. A classical solution method for the problem (2) employs the singular value decomposition (SVD) of A, if $L = I_n$, otherwise the generalized SVD of the matrix pair (A, L).

The singular value decomposition is a matrix factorization of the form

$$A = U\Sigma V^T,$$

where $U = [\boldsymbol{u}_1, \dots, \boldsymbol{u}_m] \in \mathbb{R}^{m\times m}$ and $V = [\boldsymbol{v}_1, \dots, \boldsymbol{v}_n] \in \mathbb{R}^{n\times n}$ are matrices with orthonormal columns. The non-zero elements of the diagonal matrix $\Sigma \in \mathbb{R}^{m\times n}$ are the *singular values* $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0$, with $r = \operatorname{rank}(A) \leq \min(m, n)$; see [1] for details.

Let $A \in \mathbb{R}^{m\times n}$ and $L \in \mathbb{R}^{p\times n}$ be matrices with $\operatorname{rank}(A) = r$ and $\operatorname{rank}(L) = p \leq n$. Assume that $m+p \geq n$ and conditions (3) are met. Then, the generalized SVD (GSVD) [1] of the matrix pair (A, L) is defined by the factorizations

$$A = U\Sigma_A W^{-1}, \qquad L = V\Sigma_L W^{-1}, \tag{4}$$

where $U \in \mathbb{R}^{m\times m}$ and $V \in \mathbb{R}^{p\times p}$ have orthonormal columns $\boldsymbol{u}_i$ and $\boldsymbol{v}_i$, respectively, $W \in \mathbb{R}^{n\times n}$ is nonsingular, $\Sigma_A \in \mathbb{R}^{m\times n}$, and $\Sigma_L \in \mathbb{R}^{p\times n}$. The matrices Σ_A and Σ_L are diagonal matrices which assume different forms depending on $m \geq n \geq r$ or $r \leq m < n$; see [2,3] for explicit expressions of Σ_A and Σ_L.

A solution method which expresses the solution subspace as the direct sum of the null space of L and its orthogonal complement has been introduced in [4] for the solution of large linear discrete ill-posed problems. It has been applied in [5] coupled to the truncated SVD, and it has been employed in [6,7] in iterative methods for solving large scale Tikhonov minimization problems with a linear regularization operator in general form.

The method is very effective when a basis for $\mathcal{N}(L)$ is available, but in the present paper it is proved that it cannot be applied to problem (2) in conjunction with the generalized SVD.

In Section 2, we revise the method and show the reason for its failure when it is applied to the solution of (2). We propose some approaches for its practical implementation in Section 3 and investigate, in Section 4, their numerical performance. Future research developments are discussed in Section 5.

2. Problem setting

Let $A \in \mathbb{R}^{m\times n}$ and $L \in \mathbb{R}^{p\times n}$ be defined as above. Assuming A is fairly conditioned, we consider the minimization problem (2) when either $r = \operatorname{rank}(A) = m < n$ or $r < \min(m, n)$. The case $m \geq n = r$ is trivial, as the minimization of the residual admits only one solution, and minimizing $\|L\boldsymbol{x}\|$ has no effect.

In the following we describe an approach, firstly proposed in [4,5], which explicitly determines a solution component in $\mathcal{N}(L)$, that is, a component which is not damped by L. The approach is applicable when a basis for $\mathcal{N}(L)$ is known and has a fairly small cardinality.

Let the orthonormal columns of the matrix $B = [\boldsymbol{b}_1, \dots, \boldsymbol{b}_d] \in \mathbb{R}^{n\times d}$, with $d = n - p$, span $\mathcal{N}(L)$. If $L = D_1$ or $L = D_2$, they can be obtained by orthonormalizing the bases

$$\{(1, \dots, 1)^T\} \quad \text{and} \quad \{(1, \dots, 1)^T, (1, 2, \dots, n)^T\}$$

for $\mathcal{N}(D_1)$ and $\mathcal{N}(D_2)$, respectively. Introduce the QR factorization

$$AB = QR, \tag{5}$$

where $Q \in \mathbb{R}^{m\times d}$ has orthonormal columns and $R \in \mathbb{R}^{d\times d}$ is upper triangular and nonsingular, as $\mathcal{N}(A) \cap \mathcal{N}(L) = \{\mathbf{0}\}$, and define the orthogonal projectors

$$\mathcal{P}_B = BB^T, \qquad \mathcal{P}_B^{\perp} = I_n - BB^T, \qquad \mathcal{P}_Q = QQ^T, \qquad \mathcal{P}_Q^{\perp} = I_m - QQ^T. \tag{6}$$

Then, using that $I_n = \mathcal{P}_B + \mathcal{P}_B^{\perp}$ and $\mathcal{P}_Q^{\perp} A \mathcal{P}_B = 0$, we decompose the solution $\boldsymbol{x}$ of (2) as

$$\boldsymbol{x} = \boldsymbol{x}' + \boldsymbol{x}'', \qquad \boldsymbol{x}' = \mathcal{P}_B \boldsymbol{x}, \qquad \boldsymbol{x}'' = \mathcal{P}_B^{\perp} \boldsymbol{x},$$

and we split the residual according to

$$\begin{aligned} \|A\boldsymbol{x} - \boldsymbol{b}\|^2 &= \|\mathcal{P}_Q A\boldsymbol{x} - \mathcal{P}_Q \boldsymbol{b}\|^2 + \|\mathcal{P}_Q^{\perp} A\boldsymbol{x} - \mathcal{P}_Q^{\perp}\boldsymbol{b}\|^2 \\ &= \|\mathcal{P}_Q A \mathcal{P}_B \boldsymbol{x} - (\mathcal{P}_Q \boldsymbol{b} - \mathcal{P}_Q A \mathcal{P}_B^{\perp}\boldsymbol{x})\|^2 + \|\mathcal{P}_Q^{\perp} A \mathcal{P}_B^{\perp} \boldsymbol{x} - \mathcal{P}_Q^{\perp}\boldsymbol{b}\|^2. \end{aligned}$$

Letting $\boldsymbol{y} = B^T\boldsymbol{x}$, we obtain

$$\|\mathcal{P}_Q A \mathcal{P}_B \boldsymbol{x} - (\mathcal{P}_Q \boldsymbol{b} - \mathcal{P}_Q A \mathcal{P}_B^{\perp}\boldsymbol{x})\|^2 = \|R\boldsymbol{y} - Q^T(\boldsymbol{b} - A\boldsymbol{x}'')\|^2. \tag{7}$$

Since R is nonsingular, we can determine, for any $\boldsymbol{x}'' = \mathcal{P}_B^{\perp}\boldsymbol{x}$, a vector $\boldsymbol{y} \in \mathbb{R}^d$ so that the expression in the right-hand side of (7) vanishes. This yields the component $\boldsymbol{x}' = B\boldsymbol{y}$ in $\mathcal{N}(L)$ of the solution. Then, the solution component $\boldsymbol{x}''$ in $\mathcal{N}(L)^{\perp}$ is computed by solving

$$\min_{\boldsymbol{x}\in\mathbb{R}^n} \|\mathcal{P}_Q^{\perp} A \mathcal{P}_B^{\perp}\boldsymbol{x} - \mathcal{P}_Q^{\perp}\boldsymbol{b}\|^2.$$

We remark that since $\mathcal{P}_Q^{\perp} A \mathcal{P}_B = 0$, in the above residual we can write $\mathcal{P}_Q^{\perp} A$ in place of $\mathcal{P}_Q^{\perp} A \mathcal{P}_B^{\perp}$, i.e., we do not require the computed solution to be in the range of $\mathcal{P}_B^{\perp}$. If the problem has infinitely many solutions, we first solve the constrained problem

$$\begin{cases} \min\limits_{\boldsymbol{x}\in\mathbb{R}^n} \|L\boldsymbol{x}\|^2 \\ \boldsymbol{x} \in \left\{\arg \min\limits_{\boldsymbol{x}\in\mathbb{R}^n} \|\mathcal{P}_Q^{\perp} A\boldsymbol{x} - \mathcal{P}_Q^{\perp}\boldsymbol{b}\|^2\right\}, \end{cases} \tag{8}$$

then determine $\boldsymbol{x}'' = \mathcal{P}_B^{\perp}\boldsymbol{x}$ and substitute it in (7) to obtain $\boldsymbol{x}' = B\boldsymbol{y}$. Finally, the solution is $\boldsymbol{x}' + \boldsymbol{x}''$.

In this situation, it would be natural to solve (8) by computing the GSVD of the matrix pair $(\mathcal{P}_Q^{\perp} A, L)$, but this cannot be done as the intersection of the corresponding null spaces is non-trivial, i.e., they do not fulfill condition (3). In fact, we will prove that the two null spaces are coincident.

First we characterize a subset of the range $\mathcal{R}(Q)$ of the orthogonal matrix Q.

Lemma 2.1. *Let $Q \in \mathbb{R}^{m\times d}$ be the matrix defined in (5). If $\boldsymbol{x} \in \mathcal{N}(L)$, then $A\boldsymbol{x} \in \mathcal{R}(Q)$, i.e.,*

$$\{\boldsymbol{z} \in \mathbb{R}^m : \boldsymbol{z} = A\boldsymbol{x},\ \boldsymbol{x} \in \mathcal{N}(L)\} \subset \mathcal{R}(Q).$$

Conversely, if $A\boldsymbol{x} \in \mathcal{R}(Q)$, then $\boldsymbol{x} \in \mathcal{N}(L)$.

Proof. Let $B \in \mathbb{R}^{n\times d}$ be the matrix whose orthonormal columns form a basis for $\mathcal{N}(L)$. Then, for any $\boldsymbol{x} \in \mathcal{N}(L)$ there exists $\boldsymbol{y} \in \mathbb{R}^d$ such that $\boldsymbol{x} = B\boldsymbol{y}$. From (5), it follows

$$A\boldsymbol{x} = AB\boldsymbol{y} = QR\boldsymbol{y},$$

that is, $A\boldsymbol{x} \in \mathcal{R}(Q)$. Conversely, if $A\boldsymbol{x} \in \mathcal{R}(Q)$, then we can write $A\boldsymbol{x} = Q\boldsymbol{z}$ with $\boldsymbol{z} \in \mathbb{R}^d$. Considering the nonsingular matrix R of (5), there exists $\boldsymbol{y} \in \mathbb{R}^d$ such that $\boldsymbol{z} = R\boldsymbol{y}$. It follows that $\boldsymbol{x} = B\boldsymbol{y} \in \mathcal{N}(L)$. $\square$

Theorem 2.2. *Let $A \in \mathbb{R}^{m\times n}$, $L \in \mathbb{R}^{p\times n}$, and $\mathcal{P}_Q^\perp$ be the projector defined in (6). Then,*

$$\mathcal{N}(L) = \mathcal{N}(\mathcal{P}_Q^\perp A).$$

Proof. First we prove that $\mathcal{N}(L) \subset \mathcal{N}(\mathcal{P}_Q^\perp A)$. Let $\boldsymbol{x} = B\boldsymbol{y} \in \mathcal{N}(L)$ for $\boldsymbol{y} \in \mathbb{R}^d$. Then, by (5),

$$\mathcal{P}_Q^\perp A\boldsymbol{x} = \mathcal{P}_Q^\perp AB\boldsymbol{y} = \mathcal{P}_Q^\perp QR\boldsymbol{y} = \mathbf{0},$$

that is, $\boldsymbol{x} \in \mathcal{N}(\mathcal{P}_Q^\perp A)$. To prove that $\mathcal{N}(\mathcal{P}_Q^\perp A) \subset \mathcal{N}(L)$, consider $\boldsymbol{x} \in \mathcal{N}(\mathcal{P}_Q^\perp A)$. Hence,

$$\mathbf{0} = \mathcal{P}_Q^\perp A\boldsymbol{x} = A\boldsymbol{x} - QQ^T A\boldsymbol{x},$$

that is, $A\boldsymbol{x} = QQ^T A\boldsymbol{x} \in \mathcal{R}(Q)$. From Lemma 2.1 we conclude that $\boldsymbol{x} \in \mathcal{N}(L)$. □

In the next section we develop two numerical schemes to solve (8).

3. Solving the problem (8)

Let us consider the constrained least-squares problem (8). We extend the matrix $B = [\boldsymbol{b}_1, \ldots, \boldsymbol{b}_d]$, whose columns span $\mathcal{N}(L)$, by adding p columns to obtain an orthonormal basis for $\mathbb{R}^n$

$$[B\ \widetilde{B}] = [\boldsymbol{b}_1, \ldots, \boldsymbol{b}_d, \boldsymbol{b}_{d+1}, \ldots, \boldsymbol{b}_n]. \tag{9}$$

This implies $\mathcal{N}(L)^\perp = \operatorname{span}\{\boldsymbol{b}_{d+1}, \ldots, \boldsymbol{b}_n\}$.

Since in (8) $\boldsymbol{x} \in \mathcal{N}(L)^\perp$, then $\boldsymbol{x} = \widetilde{B}\boldsymbol{z}$ with $\boldsymbol{z} \in \mathbb{R}^p$, and the problem becomes

$$\begin{cases} \min\limits_{\boldsymbol{z}\in\mathbb{R}^p} \|L\widetilde{B}\boldsymbol{z}\|^2 \\ \boldsymbol{z} \in \left\{\arg\min\limits_{\boldsymbol{z}\in\mathbb{R}^p} \|\mathcal{P}_Q^\perp A\widetilde{B}\boldsymbol{z} - \mathcal{P}_Q^\perp \boldsymbol{b}\|^2\right\}, \end{cases} \tag{10}$$

whose solution yields the component of the solution in $\mathcal{N}(L)^\perp$, i.e., $\boldsymbol{x}'' = \widetilde{B}\boldsymbol{z}$.

Theorem 3.1. *Let $L \in \mathbb{R}^{p\times n}$, with $p < n$, and let $\widetilde{B} \in \mathbb{R}^{n\times p}$ be the matrix defined in (9). Then, $L\widetilde{B}$ is a square invertible matrix of size p.*

Proof. To prove nonsingularity it suffices to show that the dimension of the null space of $L\widetilde{B}$ is zero. If we assume that $\dim(\mathcal{N}(L\widetilde{B})) \neq 0$, then there exists some vector $\boldsymbol{x} \neq \mathbf{0}$ such that $L\widetilde{B}\boldsymbol{x} = \mathbf{0}$. On the other hand, $\widetilde{B}\boldsymbol{x}$ is in $\mathcal{N}(L)^\perp$, so that $L\widetilde{B}\boldsymbol{x} \neq \mathbf{0}$. This is a contradiction, and the rank-nullity theorem implies that $\operatorname{rank}(L\widetilde{B}) = p$. □

Since $L\widetilde{B}$ is a square invertible matrix of size p, we have

$$\operatorname{rank}\left(\begin{bmatrix} \mathcal{P}_Q^\perp A\widetilde{B} \\ L\widetilde{B} \end{bmatrix}\right) = p = n - d.$$

This means that the matrix pair $(\mathcal{P}_Q^\perp A\widetilde{B}, L\widetilde{B})$ fulfills the condition (3) and the problem (10) can be solved by the GSVD of $(\mathcal{P}_Q^\perp A\widetilde{B}, L\widetilde{B})$; see Eq. (4).

A slight simplification of problem (10) can be obtained by considering a different, but equivalent, regularization matrix. The matrix L is generally designed so that a meaningful component of the solution $\boldsymbol{x}$ is not damped by the term $\|L\boldsymbol{x}\|$. This is accomplished by choosing L in order that its null space contains such component. For this reason, we propose to set $L = \widetilde{B}^T$. In this case, $L\widetilde{B} = I_p$ and the problem (10) becomes

$$\begin{cases} \min_{\boldsymbol{z}\in\mathbb{R}^p} \|\boldsymbol{z}\|^2 \\ \boldsymbol{z} \in \left\{\arg\min_{\boldsymbol{z}\in\mathbb{R}^p} \|\mathcal{P}_Q^{\perp} A\widetilde{B}\boldsymbol{z} - \mathcal{P}_Q^{\perp}\boldsymbol{b}\|^2\right\}, \end{cases} \tag{11}$$

which can be solved by the SVD of the matrix $\mathcal{P}_Q^{\perp} A\widetilde{B}$.

The above approaches produce the minimal-L-norm solution of (1) when the matrix A has a small condition number, compared to the accuracy of the data. When A is ill-conditioned, both (10) and (11) yield a regularized solution if they are solved by the truncated GSVD and the truncated SVD, respectively, while applying the truncated GSVD directly to problem (2) would be unfeasible.

4. Numerical experiments

In order to investigate the accuracy of the proposed new approach, we performed a large number of numerical experiments organized as follows. Chosen a test matrix and a model solution, we generated the exact right-hand side for the corresponding linear system, and contaminated it by additive Gaussian noise with standard deviation δ. Then, we solved problems (2) and (10) by GSVD, and (11) by SVD. Since the chosen matrices are strongly ill-conditioned, we employed truncated SVD/GSVD, selecting the truncation parameter in order to minimize the ℓ_2-norm error with respect to the exact solution. In this way, we are comparing the best solutions that each method can produce.

The test matrices were Baart, Deriv2, Foxgood, Gravity, Heat, Phillips, and Shaw, from [8], Hilbert, Lotkin, and Prolate, from the `gallery` function of Matlab. We chose 7 model functions with different degree of regularity, and three regularization matrices, the discretization of the first, second, and third derivatives. The square linear systems were generated at two different dimensions, $n = 40{,}100$, and three noise levels were adopted, $\delta = 10^{-3}, 10^{-2}, 10^{-1}$, leading to 1260 test problems. Each experiment was repeated 5 times with different realizations of the Gaussian noise, producing 6300 numerical tests; see [9–11], where a similar experimental dataset was used.

The two new formulations (10) and (11) proved to be substantially equivalent to the standard approach (2). Indeed, in all numerical test the best error produced by the three methods differed by less that 0.01%. The same result was obtained by solving rectangular underdetermined systems of dimension $m \times n$, with $n = 40{,}100$ and $m = n/2$.

This shows that the additional transformations required by the two new approaches do not introduce instability in the computation, and encourages its application to more complicate regularization operators, other than the discrete approximations of the derivatives, as well as to the solution of large scale problems by iterative methods, where a standard approach to deal with general form regularization is not available.

While the three considered methods perform similarly when the truncation parameter is chosen so as to minimize the error in the solution, the situation is different when the regularization parameter is determined by an automatic estimation algorithm, as it is done in real applications. In this case, we observed that some examples exhibit a better performance of the methods (10) and (11) with respect to the standard GSVD formulation.

In Fig. 1 we consider the test problem Deriv2 from [8] (setting the "example" parameter to 2), with a noisy right-hand side with noise level $\delta = 10^{-2}$. The problem is solved by applying the truncated GSVD to both problems (2) and to (10), estimating the truncation parameter the L-curve method, introduced in [12]. The estimation algorithm is the one described in [13] and available in the `corner` routine from [8]; see [11] for a comparison of methods for estimating a discrete regularization parameter. It is evident that in this particular example the regularization parameter estimated by the L-curve for the LSNSB method produces a much better solution than when the same estimation algorithm is applied to (2).

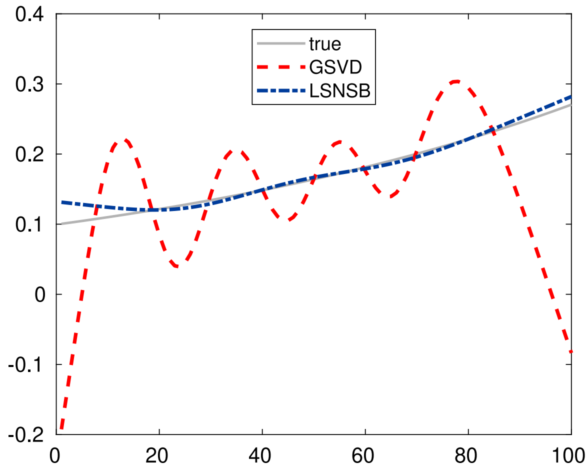

Fig. 1. Solutions of DERIV2 test problem from [8] computed by the truncated GSVD applied to (2) and to (10), labeled as LSNSB in the legend. The truncation parameter has been estimated by the L-curve; the noise level is $\delta = 10^{-2}$.

5. Conclusions

Solving underdetermined least-squares problems by computing the minimal-L-norm solution, for a chosen regularization matrix L, is a common practice when sufficient information is available about the space that contains a desirable solution.

In this paper we proved that the solution method introduced in [4,5], which makes explicit use of a basis for the null space of L, cannot be applied to the underdetermined least-squared problem in general form (2) by means of the GSVD. We also propose two computational schemes to overcome this difficulty.

Numerical experiments show that the new approaches are as stable as the standard one, and suggest that in some situation it may be more effective to apply regularization parameter estimation methods to the newly introduced formulations of the problem. Further research will investigate this aspect as well as the application of the main idea of the method to iterative algorithms for the regularized solution of large scale discrete ill-posed problems.

Data availability

No data was used for the research described in the article.

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