A note on the recursive calculation of dominant singular subspaces

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Abstract

A recursive procedure for computing an approximation of the left and right dominant singular subspaces of a given matrix is proposed in [1]. The method is particularly suited for matrices with many more rows than columns. The procedure consists of a few steps. In one of these steps a Householder transformation is multiplied to an upper triangular matrix. The following step consists in recomputing an upper triangular matrix from the latter product. In [1] it is said that the latter step is accomplished in $O(k^3)$ operations, where k is the order of the triangular matrix. In this short note we show that this step can be accomplished in $O(k^2)$ operations.

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A note on the recursive calculation of dominant singular subspaces *

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A recursive procedure for computing an approximation of the left and right dominant singular subspaces of a given matrix is proposed in [1]. The method is particularly suited for matrices with many more rows than columns. The procedure consists of a few steps. In one of these steps a Householder transformation is multiplied to an upper triangular matrix. The following step consists in recomputing an upper triangular matrix from the latter product. In [1] it is said that the latter step is accomplished in $O(k^3)$ operations, where k is the order of the triangular matrix. In this short note we show that this step can be accomplished in $O(k^2)$ operations.

Keywords: Householder matrix, Givens matrix, QR factorization, URV factorization, updating, singular value decomposition

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1. Introduction

In [1], a recursive procedure is designed for computing an approximation of the left and right dominant singular subspaces of a matrix, whose columns are produced incrementally. The method is particularly suited for matrices with many more rows than columns. The procedure consists of a few steps. In one of these steps a Householder transformation is multiplied to an upper triangular matrix. The following step consists in recomputing an upper triangular matrix from the latter product. In [1] it is said that the latter step is accomplished in $O(k^3)$ operations, where k is the order of the triangular matrix. In this short note we show that this step can be accomplished in $O(k^2)$ operations. Moreover, the exploitation of the matrix structure in the latter step allows to reduce the computational complexity from $O(k^3)$ to $O(k^2)$ if also the right dominant singular subspace is required.

The note is organized as follows. In section 2 the algorithm proposed in [1] is described and the proposed modification is described in section 3.

2. Recursive calculation of dominant singular subspaces

In this section we shortly describe the algorithm proposed in [1] to recursively compute dominant singular subspaces, whose columns are known incrementally, i.e., at each step one more column is added to the matrix. The algorithm is particularly suited for matrices $A \in \mathbb{R}^{m \times n}$, $m \gg n$.

At each recursion, the following steps are performed:

Step 1. Known the orthogonal matrix $U \in \mathbb{R}^{m \times k}$, and the upper triangular matrix $R \in \mathbb{R}^{k \times k}$ of the URV factorization of the matrix $\tilde{A} \in \mathbb{R}^{m \times k}$, $k < n \ll m$, $\tilde{A} = URV$, with $V \in \mathbb{R}^{k \times k}$ orthogonal (V does not need to be known), a new column b is added to $\tilde{A}$,

$$\hat{A} = [\tilde{A}, b].$$

Step 2. Update the URV factorization of the extended matrix $\hat{A}$ via Gram–Schmidt orthogonalization,

$$\begin{aligned} r &= U^T b, \\ \hat{b} &= b - Ur, \\ \rho &= \|\hat{b}\|_2, \\ \hat{u} &= \frac{\hat{b}}{\rho}. \end{aligned}$$

Then

$$[\tilde{A}|b] = [UR|b] \left[\begin{array}{c|c} V & \\ \hline & 1 \end{array} \right] = [U|\hat{u}] \left[\begin{array}{c|c} R & r \\ \hline & \rho \end{array} \right] \left[\begin{array}{c|c} V & \\ \hline & 1 \end{array} \right] = [U|\hat{u}] \hat{R} \left[\begin{array}{c|c} V & \\ \hline & 1 \end{array} \right].$$

Step 3. Let σ_{k+1} be the smallest singular value of $\widehat{R}$ and u_{k+1} the corresponding left singular vector. Let G_u be an orthogonal matrix such that

$$G_u^T u_{k+1} = e_{k+1} = [0, \dots, 0, 1]^T,$$

and compute

$$G_u^T \widehat{R} = \widehat{S},$$

with $\widehat{S} \in \mathbb{R}^{(k+1) \times (k+1)}$ no more upper triangular.

Step 4. Compute the RQ factorization of $\widehat{S}$,

$$\widehat{S} = \widetilde{R} \widetilde{H},$$

where $\widetilde{R}$ and $\widetilde{H}$ are upper triangular and orthogonal matrices of order $(k+1)$, respectively. It turns out that

$$\widetilde{R} = \left[\begin{array}{c|c} R_n & \\ \hline & \sigma_{k+1} \end{array} \right].$$

Step 5. Update the orthogonal matrix U

$$U \leftarrow U G_u, \quad V \leftarrow \widetilde{H}^T V,$$

and set

$$\widetilde{A} = U(:, 1:k) R_n V(1:k, :).$$

Remark. It is not necessary to update the matrix V , as stated in [1], if only the left dominant singular subspaces are needed.

The matrix G_u in step 3 could be either a product of k Givens rotations or a Householder matrix. If the product of k Givens rotations is chosen, step 4 can be accomplished in $O(k^2)$ operations in a way similar to the one described in [2], and the matrix $\widetilde{H}$ is given by the product of k different Givens rotations.

However, the costly part of the algorithm is the update of the matrix U , and hence it is preferable to choose G_u to be a Householder transformation. In fact, the cost of the latter product $U G_u$ is $4mk + 2m$ if G_u is a Householder transformation, whereas the cost is $6mk$ if the orthogonal matrix G_u is given by the product of k Givens rotations. In [1] is said that the price to pay choosing G_u a Householder transformation is that the RQ factorization in step 4 is computed in $O(k^3)$ operations.

In the next section we show that the latter factorization can be accomplished in $O(k^2)$ operations.

3. Computation of the RQ factorization of the matrix $\widehat{S}$

Let $G_u = I - \beta z z^T$ be the Householder transformation such that $G_u^T u_{k+1} = e_{k+1}$. Let us denote by $\hat{s}_i, i = 1, \dots, k+1$, the i th column of $\widehat{S}$. Similarly, we use the notation $\hat{r}_i$ for the i th column of the matrix $\widehat{R}$.

The product $G_u^T \widehat{R}$ can be written as

$$G_u^T \widehat{R} = [G_u^T \hat{r}_1, G_u^T \hat{r}_2, \dots, G_u^T \hat{r}_{k+1}].$$

We observe that

$$G_u^T \hat{r}_i = (I - \beta z z^T) \hat{r}_i = \hat{r}_i - (\beta z^T \hat{r}_i) z.$$

Since $\widehat{R}$ is an upper triangular matrix, the i th column of $\widehat{S}$ below the main diagonal is a multiple of z , i.e.,

$$\hat{s}_i(i+1 : k+1) = (G_u^T \hat{r}_i)(i+1 : k+1) = -(\beta z^T \hat{r}_i) z(i+1 : k+1).$$

In other words, the strictly lower triangular part of $\widehat{S}$ is the strictly lower triangular part of a rank-one matrix. Therefore, the retriangularization of $\widehat{S}$ can be accomplished applying only $2k - 1$ Givens rotations to the right, with $O(k^2)$ operations as described below.

We observe that the strictly lower triangular part is not explicitly computed, since the entries of the i th column below the main diagonal are given by $-\beta z^T \hat{r}_i z(k)$, $k > i$, where $z(k)$ is the k th entry of the vector z . Therefore, for any column it is only needed to store the values $\gamma(i) = \beta z^T \hat{r}_i, i = 1, \dots, k$.

Let us suppose, for simplicity, that $k = 5$, and denote with $\boxtimes$ the entries of $\widehat{S}$ belonging to the strictly lower triangular part:

$$\widehat{S} = \begin{bmatrix} \times & \times & \times & \times & \times & \times \\ \boxtimes & \times & \times & \times & \times & \times \\ \boxtimes & \boxtimes & \times & \times & \times & \times \\ \boxtimes & \boxtimes & \boxtimes & \times & \times & \times \\ \boxtimes & \boxtimes & \boxtimes & \boxtimes & \times & \times \\ \boxtimes & \boxtimes & \boxtimes & \boxtimes & \boxtimes & \times \end{bmatrix}.$$

Applying a Givens rotation G_1 to the right in order to annihilate the entry $(3, 1)$, the whole column below this entry is annihilated, since both the columns are a multiple of the vector z below the main diagonal:

$$\widehat{S}G_1 = \begin{bmatrix} \times & \times & \times & \times & \times & \times \\ \boxtimes & \times & \times & \times & \times & \times \\ \boxtimes & \boxtimes & \times & \times & \times & \times \\ \boxtimes & \boxtimes & \boxtimes & \times & \times & \times \\ \boxtimes & \boxtimes & \boxtimes & \boxtimes & \times & \times \\ \boxtimes & \boxtimes & \boxtimes & \boxtimes & \boxtimes & \times \end{bmatrix} G_1 = \begin{bmatrix} \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ \boxtimes & \times & \times & \times & \times & \times \\ \boxtimes & \boxtimes & \times & \times & \times & \times \\ \boxtimes & \boxtimes & \boxtimes & \times & \times & \times \\ \boxtimes & \boxtimes & \boxtimes & \boxtimes & \times & \times \end{bmatrix}.$$

Let c_1 and s_1 be the Givens coefficients of G_1 , i.e.,

$$G_1 = \begin{bmatrix} c_1 & s_1 \\ -s_1 & c_1 \end{bmatrix}, \quad c_1 = \frac{z^T \hat{r}_2}{\sqrt{(z^T \hat{r}_1)^2 + (z^T \hat{r}_2)^2}}, \quad s_1 = \frac{z^T \hat{r}_1}{\sqrt{(z^T \hat{r}_1)^2 + (z^T \hat{r}_2)^2}}.$$

Of course, it is not necessary to compute $\hat{S}G_1$ below the upper Hessenberg part of the matrix. In fact the entries of the first column with row indexes greater than 2 are zero. Moreover, the entries of the second column with row indexes greater than 2 are given by

$$\beta z(i) \sqrt{(z^T \hat{r}_1)^2 + (z^T \hat{r}_2)^2}, \quad i > 2.$$

Therefore it is only needed to update the value $\gamma(2) = \beta \sqrt{(z^T \hat{r}_1)^2 + (z^T \hat{r}_2)^2}$.

In the same manner, applying a Givens rotation G_2 to the right in order to annihilate the entry (4, 2), the whole row below this entry is annihilated.

$$\hat{S}G_1G_2 = \begin{bmatrix} \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ & \boxtimes & \times & \times & \times & \times \\ & \otimes & \boxtimes & \times & \times & \times \\ & \boxtimes & \boxtimes & \boxtimes & \times & \times \\ & \boxtimes & \boxtimes & \boxtimes & \boxtimes & \times \end{bmatrix} G_2 = \begin{bmatrix} \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ & \times & \times & \times & \times & \times \\ & & \boxtimes & \times & \times & \times \\ & & \boxtimes & \boxtimes & \times & \times \\ & & \boxtimes & \boxtimes & \boxtimes & \times \end{bmatrix}.$$

Also in this case, only the upper Hessenberg part of columns 2 and 3 and the coefficient $\gamma(3)$ need to be updated.

Proceeding in this way, after $k - 1$ multiplications to the right by Givens rotations, the original matrix is transformed into an upper Hessenberg one with $O(k^2)$ operations,

$$\hat{S}G_1G_2 \cdots G_{k-1} = \begin{bmatrix} \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ & \times & \times & \times & \times & \times \\ & & \times & \times & \times & \times \\ & & & \times & \times & \times \\ & & & & \times & \times \end{bmatrix}.$$

To reduce the latter Hessenberg matrix to upper triangular form, apply k Givens rotations $\hat{G}_i$, $i = k, k - 1, \dots, 2, 1$, to the right in order to annihilate the entries $(k + 1, k)$, $(k, k - 1), \dots, (2, 1)$. The whole transformation is depicted in figure 1. Therefore the reduction of the matrix $\hat{S}$ into triangular form can be made in $O(k^2)$ operations.

If one is interested also in the right singular dominant subspace, the latter construction of the RQ factorization of the matrix $\hat{S}$ allows to reduce the computational complexity from $O(k^3)$ to $6k^2$ flops because the updated matrix of the right singular vectors is given by

$$Q \left[\begin{array}{c|c} V & \\ \hline & 1 \end{array} \right] = \hat{G}_1^T \hat{G}_2^T \cdots \hat{G}_{k-1}^T \hat{G}_k^T G_{k-1}^T G_{k-2}^T \cdots G_2^T G_1^T \left[\begin{array}{c|c} V & \\ \hline & 1 \end{array} \right].$$

Figure 1. Multiplication of $\hat{R}$ to the left by a Householder transformation followed by a sequence of $2k - 1$ multiplications by Givens rotations to the right in order to retrieve the upper triangular structure. With $\otimes$ is denoted the entry of the matrix to be annihilated by a Givens transformation.

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