An answer to an open question in the incremental SVD

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Abstract

Incremental singular value decomposition (SVD) was proposed by Brand to efficiently compute the SVD of a matrix. The algorithm needs to compute thousands or millions of orthogonal matrices and to multiply them together. However, the multiplications may corrode the orthogonality. Hence many reorthogonalizations are needed in practice. In [Linear Algebra and its Applications 415 (2006) 20–30], Brand asked “It is an open question how often this is necessary to guarantee a certain overall level of numerical precision; it does not change the overall complexity.” In this paper, we answer this question and the answer is we can avoid computing the large amount of those orthogonal matrices and hence the reorthogonalizations are not necessary by modifying his algorithm. We prove that the modification does not change the outcomes of the algorithm. Numerical experiments are presented to illustrate the performance of our modification.

1 Introduction

The singular value decomposition (SVD) of a matrix has many applications, such as proper orthogonal decomposition model order reduction and principal component analysis.

One drawback of the SVD is the cost of its computation. Let \( U \) be a \( m \) by \( n \) dense matrix of low rank \( r \), the computational complexity of traditional methods is \( O(mn^2 + m^2n + n^3) \) time, which is unfeasible for a large size matrix. Lanczos methods [2] yield thin svds and the complexity is \( O(mnr^2) \) time, but we need to know the rank in advance. These methods are referred to as batch methods because they need to store the matrix.

In some scenarios the data sets will be produced incrementally, such as the snapshots of a time dependent partial differential equations (PDEs). It may be advantageous to perform the SVD as the columns of a matrix become available, instead of waiting until all data sets are available before doing any computation. These characteristics on the availability of data sets have given rise to a class of incremental methods.

In 2002, Brand [3] proposed a new algorithm to find the SVD of a matrix incrementally. Given the SVD of a matrix \( U = Q\Sigma R^\top \), the goal is to update the SVD of the related matrix \( [U \mid c] \), by using the SVD of \( U \) and the new adding vector \( c \). Then the SVD of \( [U \mid c] \) can be constructed by

1. letting \( e = c - QQ^\top c \) and \( p = \|e\| \),

2. finding the full SVD of \( \begin{bmatrix} \Sigma & Q^\top c \\ 0 & p \end{bmatrix} = Q\Sigma R^\top \), and then

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3. updating the SVD of \([U \mid c]\) by

\[
[U \mid c] = ( [Q \mid e/p] \tilde{Q} ) \tilde{\Sigma} \begin{pmatrix} R & 0 \\ 0 & 1 \end{pmatrix} \tilde{R}^T.
\]

For many of the motivating applications, only the dominant singular vectors and values of \(U\) are needed. Hence, in practice, we perform truncation when \(p\) or the last singular value of \(\tilde{\Sigma}\) is small. The incremental SVD has been applied to many different areas; see [8, 10–12] for more details. There are many other incremental methods, see [1] for a survey.

There are two ways to update the left and right singular subspace. The first way is very straightforward and the update is given by

\[
Q \leftarrow [Q \mid e/p] \tilde{Q}, \quad \Sigma \leftarrow \tilde{\Sigma}, \quad R \leftarrow \begin{bmatrix} R & 0 \\ 0 & 1 \end{bmatrix} \tilde{R}.
\] (1.1)

However, this update has two defects:

1. The computational cost of (1.1) is expensive since the updates involves a very tall thin matrix \(Q\) and \(R\).
2. Reorthogonalizations are needed for \(Q\) almost after each update. Theoretically, the matrix \([Q \mid e/p] \tilde{Q}\) is orthogonal. However, in practice, small numerical errors cause a loss of orthogonality. Without a reorthogonalization, the decomposition of the incremental SVD algorithm is not orthogonal. Therefore, the singular values are not true and truncation is not reliable. Hence a reorthogonalization is needed and the computational cost can be high if the rank of the matrix is not extremely low. Specifically, Fareed et al. recommended a Gram-Schmidt orthogonalization [7] while Oxberry et al. chose thin QR in [13].

Numerical experiments in Example 1 show that the above two items take the majority of the CPU time.

To avoid the huge computational cost, Brand [4] suggested to update the matrix \(Q\) and \(R\) indirectly. His idea is to leave the SVD decomposed into the five matrices

\[
U = Q_{old} \tilde{Q}_{old} \Sigma_{old} \tilde{R}_{old} R_{old}^T
\]

with orthonormal \(Q_{old} \tilde{Q}_{old}\), \(R_{old} \tilde{R}_{old}\), \(Q_{old}\) and \(\tilde{Q}_{old}\) (but not \(\tilde{R}_{old}\) or \(R_{old}^T\)). The large outer matrices only record the span of the left and right subspaces and are built by appending columns to \(Q_{old}\) and rows to \(R_{old}\). The updates only involve with the small matrices \(\tilde{Q}_{old}\) and \(\tilde{R}_{old}\). This makes the update much faster.

However, over thousands or millions of updates, the multiplications may erode the orthogonality of through numerical error; see the right figure in Figure 3. Hence reorthogonalizations are needed for these small orthonormal matrices. In [4], Brand asked: “It is an open question how often this is necessary to guarantee a certain overall level of numerical precision; it does not change the overall complexity.” We also note that only reorthogonalize the small matrix \(\tilde{Q}\) is not enough for some data sets. In Example 2, we show that without reorthogonalizations for the larger outside matrix \(Q_{old}\), the algorithm provides untruthful SVD.

In this paper, we first answer the open question, and the answer is we can avoid computing the large amount of those orthogonal matrices and hence the reorthogonalizations for those small orthonormal matrices are not necessary by modifying Brand’s algorithm. Second, we proposed an efficient reorthogonalization for the larger out matrix \(Q_{old}\); numerical experiments in Examples 2 and 3 show that the reorthogonalization works well in practice. Third, we prove that our modification does not change the outputs of Brand’s algorithm.
2 Incremental SVD (I)

We begin by introducing notation needed throughout the paper. Let $I_k$ be a $k \times k$ identity matrix and the $W$-weighted inner product:

$$(a, b)_W = a^\top W b, \quad a, b \in \mathbb{R}^m.$$  

Let $U$ be a $m$ by $n$ dense matrix and $u_j$ denote the $j$-th column of $U$, i.e.,

$$U = [u_1 \mid u_2 \mid \cdots \mid u_n].$$

For convenience, we adopt Matlab notation herein. We use both $U(:, 1: \ell)$ and $U_{\ell}$ to denote the first $\ell$ columns of $U$, and $U(1: \ell, 1: \ell)$ be the $\ell$-th leading principal minor of $U$. The function $\text{diag}: \mathbb{R}^k \to \mathbb{R}^{k \times k}$ takes as input a vector and outputs a square, diagonal matrix with that vector’s entries on its main diagonal as follows: if $\alpha = (a_1, a_2, \ldots, a_k)^\top$, then

$$\text{diag}(\alpha) = \begin{bmatrix} a_1 & 0 & \cdots & 0 \\ 0 & a_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & a_k \end{bmatrix}.$$  

If the data arising from a Galerkin-type simulation of a PDE, one has to deal with Cholesky factorization of a weighted matrix if one directly apply Brand’s algorithm. To avoid this, Fareed et al. [7] extended Brand’s algorithm to accommodate data of this type without computing Cholesky factorization. More specifically, if the data lies in a finite element space and is expressed using a collection of basis functions. Then the SVD of the data is equivalent to find a so-called core SVD of their coefficient matrix.

Definition 1. [7] A core SVD of a matrix $U \in \mathbb{R}^{m \times n}$ is a decomposition $U = Q\Sigma R^\top$, where $Q \in \mathbb{R}^{m \times d}$, $\Sigma \in \mathbb{R}^{d \times d}$, and $R \in \mathbb{R}^{n \times d}$ satisfy

$$Q^\top W Q = I, \quad R^\top R = I, \quad \Sigma = \text{diag}(\sigma_1, \ldots, \sigma_d),$$

where $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_d > 0$. The values $\{\sigma_i\}$ are called the (positive) singular values of $U$ and the columns of $Q$ and $R$ are called the corresponding singular vectors of $U$.

We note that if $W = I$, the above core SVD is reduced to the standard SVD of the matrix $U$. In [7], $W$ is the standard finite element mass or stiffness matrix. For more information about the incremental SVD in a weighted norm setting, see [5,6].

Next, we introduce Brand’s incremental SVD algorithm and follow the discussions in [7].

Step 1: Initialization. Assume that the first column of $U$ is nonzero, i.e., $u_1 \neq 0$, we initialize the core SVD of $u_1$ by setting

$$\Sigma = (u_1^\top W u_1)^{1/2}, \quad Q = u_1 \Sigma^{-1}, \quad R = 1.$$  

The algorithm is shown in Algorithm 1.

Step 2: Core SVD of $U_\ell$. Suppose we already have a rank-$k$ truncated core SVD of $U_\ell$:

$$U_\ell = Q\Sigma R^\top,$$  

with $Q^\top W Q = I_k$, $R^\top R = I_k$, $\Sigma = \text{diag}(\sigma_1, \ldots, \sigma_k), \quad \Sigma = \diag(\sigma_1, \ldots, \sigma_k), \quad (2.1)$

where $\Sigma \in \mathbb{R}^{k \times k}$ is a diagonal matrix with the $k$ (ordered) singular values of $U_\ell$ on the diagonal, $Q \in \mathbb{R}^{m \times k}$ is the matrix containing the corresponding $k$ left singular vectors of $U_\ell$, and $R \in \mathbb{R}^{\ell \times k}$ is the matrix of the corresponding $k$ right singular vectors of $U_\ell$.  

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Algorithm 1 (Initialize incremental SVD)

Input: \( u_1 \in \mathbb{R}^m, W \in \mathbb{R}^{m \times m} \)

1: \( \Sigma = (u_1^T W u_1)^{1/2}, Q = u_1 \Sigma^{-1}; R = 1; \)
2: return \( Q, \Sigma, R \)

Step 3: Updates the core SVD of \( U_{\ell+1} \). Our goal next is to update the above SVD, i.e., we want to find the core SVD of \( U_{\ell+1} \) by using the core SVD of \( U_{\ell} \) and the new adding vector \( u_{\ell+1} \).

To do this, let \( e \in \mathbb{R}^m \) be the residual of \( u_{\ell+1} \) onto the space spanned by the columns of \( Q \) with the weighted inner product \((\cdot, \cdot)\). Therefore,

\[
e = u_{\ell+1} - QQ^T W u_{\ell+1}.
\]

Let \( p \) be the magnitude of \( e \), i.e., \( p = (e^T W e)^{1/2} \). If \( p > 0 \), we let \( \tilde{e} \) be the unit vector in the direction of \( e \), i.e., \( \tilde{e} = e/p \). If \( p = 0 \), we set \( \tilde{e} = 0 \). Then we have the fundamental identity:

\[
U_{\ell+1} = [U_\ell \mid u_{\ell+1}] = [Q \Sigma R^T \mid u_{\ell+1}] = [Q \mid \tilde{e}] [\begin{bmatrix} 0 & Q^T W u_{\ell+1} \cr \Sigma & p \end{bmatrix} Y \begin{bmatrix} R & 0 \cr 0 & 1 \end{bmatrix}]^T. \tag{2.2}
\]

We can find the SVD of the updated matrix \( U_{\ell+1} \) by finding the full SVD of the matrix \( Y \) in the right hand side of the above identity.

1) If \( p < \text{tol} \), we approximate and set \( p = 0 \) and \( \tilde{e} = 0 \). Let \( Q_Y \Sigma_Y R_Y^T \) be the full SVD of \( Y = \begin{bmatrix} \Sigma & Q^T W u_{\ell+1} \\ 0 & 0 \end{bmatrix} \). Then the core SVD of \( U_{\ell+1} \in \mathbb{R}^{m \times (\ell+1)} \) is given by

\[
U_{\ell+1} = [U_\ell \mid u_{\ell+1}] = ([Q \mid \tilde{e}] \Sigma_Y) \left( \begin{bmatrix} R & 0 \\ 0 & 1 \end{bmatrix} R_Y \right)^T.
\]

This suggests the following update

\[
Q \leftarrow QQ_Y (1 : k, 1 : k), \quad \Sigma \leftarrow \Sigma_Y (1 : k, 1 : k), \quad R \leftarrow \begin{bmatrix} R & 0 \\ 0 & 1 \end{bmatrix} R_Y(:, 1 : k). \tag{2.3}
\]

2) If \( p \geq \text{tol} \), we let \( Q_Y \Sigma_Y R_Y^T \) be the full SVD of the middle matrix \( Y \) in (2.2), and then update the SVD of \( U_{\ell+1} \) by

\[
Q \leftarrow [Q \mid \tilde{e}] Q_Y \quad \Sigma \leftarrow \Sigma_Y \quad R \leftarrow \begin{bmatrix} R & 0 \\ 0 & 1 \end{bmatrix} R_Y. \tag{2.4}
\]

In [7], the authors considered a data from the simulation of 2D laminar flow around a cylinder with circular cross-section. The incremental SVD algorithms kept computing very small singular values (near machine precision) - these required huge computational cost and these values were not needed in their application. Hence, they suggested another truncation in [7, Algorithm 4] if the last few singular values are less than a tolerance. That is, find the minimal \( r \) such that \( \Sigma_Y (r, r) \geq \text{tol} \) and \( \Sigma_Y (r+1, r+1) \geq \text{tol} \) and set the following truncation:

\[
Q \leftarrow Q(:, 1 : r), \quad \Sigma \leftarrow \Sigma(1 : r, 1 : r), \quad R \leftarrow R(:, 1 : r). \tag{2.5}
\]
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Algorithm 2 (Update Incremental SVD (I))

Input: $Q \in \mathbb{R}^{m \times k}$, $\Sigma \in \mathbb{R}^{k \times k}$, $R \in \mathbb{R}^{\ell \times k}$, $u_{\ell+1} \in \mathbb{R}^m$, $W \in \mathbb{R}^{m \times m}$, $\text{tol}$

1. Set $d = Q^\top (Wu_{\ell+1})$; $e = u_{\ell+1} - Qd$; $p = (e^\top We)^{1/2}$;
2. if $p < \text{tol}$ then
3. Set $p = 0$;
4. else
5. Set $e = e/p$;
6. end if
7. Set $Y = \begin{bmatrix} \Sigma & d \\ 0 & p \end{bmatrix}$;
8. $[Q_Y, \Sigma_Y, R_Y] = \text{svd}(Y)$;
9. if $p < \text{tol}$ then
10. Set $Q = QQ_Y(1 : k, 1 : k)$, $\Sigma = \Sigma_Y(1 : k, 1 : k)$, $R = \begin{bmatrix} R & 0 \\ 0 & 1 \end{bmatrix} R_Y(:, 1 : k)$;
11. else
12. Set $Q = \begin{bmatrix} Q | e \end{bmatrix} Q_Y$, $\Sigma = \Sigma_Y$, $R = \begin{bmatrix} R & 0 \\ 0 & 1 \end{bmatrix} R_Y$.
13. if $\Sigma(r, r) \geq \text{tol} \& \& \Sigma(r + 1, r + 1) \geq \text{tol}$ then
14. Set $Q = Q(:, 1 : r)$, $\Sigma = \Sigma(1 : r, 1 : r)$, $R = R(:, 1 : r)$;
15. end if
16. end if
17. return $Q, \Sigma, R$

where $Q, \Sigma$ and $R$ were defined in (2.4). Now we summarize the above discussions in Algorithm 2.

Next, we discuss the complexity of Brand’s algorithm (Algorithm 2) with $W = I$ and note that $U \in \mathbb{R}^{m \times n}$ with low rank $r$. The total time complexity is $O((m + n)r^2)$ and the details are shown below.

1. Line 1: this needs to be executed $n$ times and the computational cost of each time is about $O(mr)$, the whole complexity is $O(mnr)$.

2. Lines 8: since $Y$ is a one-column bordered diagonal matrix, then it can be bidiagonalized in $O(r^2)$ time and the whole time is $O(nr^2)$.

3. Lines 10-12: the computational cost of each time is about $O(mr^2 + \ell r^2)$, hence the total complexity is about $O(\sum_{\ell=1}^{n}(mr^2 + \ell r^2)) = O((m + n)mr^2)$.

Step 4: Reorthogonalization. Theoretically, the above SVD update yields orthonormal left and right singular vectors. However, in practice, small numerical errors cause a loss of orthogonality. Then the incremental SVD algorithm is a non-orthogonal decomposition, and the singular values are not true hence truncation is not reliable. Therefore a reorthogonalization is needed and the computational cost can be high if the rank of the matrix is not extremely low. Specifically, Brand recommended a Gram-Schmidt orthogonalization \[3\] while Oxberry et al. chose thin QR in \[13\]. Our numerical test show that thin QR is faster than the Gram-Schmidt when the weighted matrix is an identity, see Example 1. However, since there is no thin QR with a weighted norm setting at hand, Fareed et al. in \[7\] use the $W$-weighted Gram–Schmidt for the reorthogonalization.
Algorithm 3 (Reorthogonalization)

Input: $Q \in \mathbb{R}^{m \times k}$, $W \in \mathbb{R}^{m \times m}$, tol

1: if $|(Q(:,1))^{\top}WQ(:,1)| > \text{tol}$ then
2:  for $i = 1$ to $k$ do
3:    Set $\alpha = Q(:,i)$;
4:    for $j = 1$ to $i - 1$ do
5:      $Q(:,i) = Q(:,i) - (\alpha^{\top}WQ(:,j))Q(:,j)$;
6:    end for
7:    Set $\text{norm} = ((Q(:,i))^{\top}WQ(:,i))^{1/2}$;
8:    Set $Q(:,i) = Q(:,i) / \text{norm}$;
9:  end for
10: end if
11: return $Q$

We do not discuss the time complexity of the reorthogonalization since there is no clue that how many times we need to execute the Algorithm 3. However, numerical experiments in Example 1 show that the orthogonalization step described above is a large part of the computational cost of the incremental SVD algorithm.

Finally we conclude the full implementation of the incremental SVD with the $W$-weighted Gram–Schmidt for the reorthogonalization in Algorithm 4.

Algorithm 4 (Fully incremental SVD (I))

Input: $W \in \mathbb{R}^{m \times m}$, tol

1: Get $u_1$;
2: $[Q, \Sigma, R] =$ InitializeISVD ($u_1$, $W$); % Algorithm 1
3: for $\ell = 2, \ldots, n$ do
4:  Get $u_\ell$;
5:  $[Q, \Sigma, R] =$ UpdateISVD1 ($Q, \Sigma, R, u_\ell, W$, tol); % Algorithm 2
6:  $Q =$ Reorthogonalization ($Q, W$, tol); % Algorithm 3
7: end for
8: return $Q, \Sigma, R$

Example 1. In this example, we test the Algorithm 4. We let $\Omega \subset \mathbb{R}^2$ be an unit square and we partition it into 524288 uniform triangles. Let $\{\varphi_i\}_{i=1}^m$ be the standard linear finite element basis functions. Next we let $\{(x_i, y_j)\}_{i,j=1}^m$ be the grids of $\Omega$, $\{t_i\}_{i=1}^n$ be an equally space grid in $[0, 10]$ and time step $\Delta t = 1/10^3$. Define

$$f(t, x, y) = \cos(t(x + y)), \quad b_i = [(f(t_i), \varphi_j)]_{j=1}^m, \quad B = [b_1 | b_2 | \ldots | b_n],$$

$$M = [(\varphi_j, \varphi_i)]_{i,j=1}^m, \quad u_k = [f(t_k, x_i, y_j)]_{i,j=1}^m, \quad U = [u_1 | u_2 | \ldots | u_n].$$

Here $M$ is the finite element mass matrix and $u_k$ is the coefficient of the linear Lagrange interpolation of $f(t, x, y)$ at $t = t_k$. We compute the SVD of the matrix $B$ with $W = I$ and of the matrix $U$ with $W = M$ by setting tol $= 10^{-12}$. Let $\|A\|_F$ be the Frobenius norm of matrix $A$, and we use

$$\mathcal{E}_W = \|I - Q^{\top}WQ\|$$

to measure the error of the orthogonality of the orthonormal matrix $Q$ under the weight inner product $(\cdot, \cdot)_W$.  

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In Figure 1 we show the orthogonality of the left singular matrix $Q$ with different weighted norms. For the case $W = M$, the orthogonality of $Q$ is eroded (even with reorthogonalizations).

![Figure 1: Example 1 Left: $W = I$. Right: $W = M$.](image)

The whole simulations take about 154 and 4000 seconds for $W = I$ and $W = M$, respectively. Next, we show the CPU time (seconds) of the main part of the Algorithm 4 in Table 1. We see that the orthogonalization step is a large part of the computational cost of the incremental SVD algorithm, especially for the case $W = M$.

|       | Line 1 in Algorithm 2 | Lines 9-13 in Algorithm 2 | Algorithm 3 |
|-------|------------------------|-----------------------------|-------------|
| $W = I$ | 32.034                | 60.213                      | 60.129      |
| $W = M$ | 110.58                | 115.96                      | 3761.6      |

Table 1: The CPU time (seconds) for different weighted inner products.

3 Incremental SVD (II)

Algorithm 4 is easy to implement while the computational cost is high, especially for the weighted norm setting. For a $m \times n$ dense matrix with low rank $r$, the time complexity of Algorithm 4 is $O(m(m + n)r^2)$. In [4], Brand reduced the complexity to $O(mnr)$. However, to update the left singular space, one has to compute thousands or millions of orthogonal matrices and multiply them together. It is more complicated to update the right singular space which need to compute the pseudo-inverse of a matrix for thousands or millions times.

Next, we follow [4] to extend Brand’s improvements to compute the core SVD of $U \in \mathbb{R}^{m \times n}$ with respect to the weighted inner product $(\cdot, \cdot)_W$. Instead of updating the large singular vector matrices as prescribed in (2.3) or (2.4), we suppose the core SVD of $U_\ell \in \mathbb{R}^{m \times \ell}$ can be written into the following five matrices

$$U_\ell = Q_{\text{old}} \tilde{Q}_{\text{old}} \Sigma_{\text{old}} \tilde{R}_{\text{old}}^T \tilde{R}_{\text{old}}^T. \quad (3.1)$$

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1 All the code for all examples in the paper has been made by the author using MATLAB R2020b and has been run on a laptop with MacBook Pro, 2.3 Ghz8-Core Intel Core i9 with 64GB 2667 Mhz DDR4.
Here $Q_{old} \in \mathbb{R}^{m \times k}$ is a orthonormal matrix under the weighted inner product, $\tilde{Q}_{old}$ and $\tilde{R}_{old}^T R_{old}^T$ are standard orthonormal matrices, but $\tilde{R}_{old}^T$ and $R_{old}^T$ are not. The large outer matrices only record the span of the left and right subspaces and are built by appending columns to $Q_{old}$ and rows to $R_{old}$. And the update only relates to the small matrices $\tilde{Q}_{old}$ and $\tilde{R}_{old}$, this makes the update much faster.

Next, we consider the core SVD of $U_{\ell+1} = [U_{\ell} | u_{\ell+1}] \in \mathbb{R}^{m \times (\ell+1)}$. Similar to Section 2, we let $e \in \mathbb{R}^m$ be the residual of $u_{\ell+1}$ onto the space spanned by the columns of $Q_{old}Q_{old}$ with the weighted inner product $(\cdot, \cdot)_W$, i.e.,

$$e = u_{\ell+1} - (Q_{old} \tilde{Q}_{old})(Q_{old} \tilde{Q}_{old})^T W u_{\ell+1} = u_{\ell+1} - Q_{old} Q_{old}^T W u_{\ell+1}.$$ 

Let $p = (e^T W e)^{1/2}$. If $p > 0$, we let $\tilde{e} = e/p$, otherwise we set $\tilde{e} = 0$. Then by (3.1) and the fundamental identity (2.2) we have

$$U_{\ell+1} = [Q_{old} \tilde{Q}_{old} | \tilde{e}] \begin{bmatrix} \Sigma_{old} & 0 \\ 0 & p \end{bmatrix} \begin{bmatrix} \tilde{R}_{old} \tilde{R}_{old} & 0 \\ 0 & 1 \end{bmatrix}_Y.$$

Assume that $Q_Y \Sigma_Y R_Y^T$ be the full SVD of $Y$, then the core SVD of $U_{\ell+1}$ is given by

$$U_{\ell+1} = \left( [Q_{old} \tilde{Q}_{old} | \tilde{e}] Q_Y \right) \Sigma_Y \left( [\tilde{R}_{old} \tilde{R}_{old} & 0 \\ 0 & 1] R_Y \right)^T.$$

(1) If $p < tol$, we set $p = 0$ and $\tilde{e} = 0$, then the update is not rank-increasing. We update the small orthonormal matrix $Q_{new} \in \mathbb{R}^{m \times k}$ and the diagonal matrix $\Sigma_{new} \in \mathbb{R}^{k \times k}$ by

$$\tilde{Q}_{new} \leftarrow \tilde{Q}_{old} Q_Y (1 : k, 1 : k), \quad \Sigma_{new} \leftarrow \Sigma_Y (1 : k, 1 : k).$$

(2) If $p \geq tol$, we then update the large outer matrix $Q_{new}$ by adding the vector $\tilde{e}$ to $Q_{old}$, and update the small orthonormal matrix $\tilde{Q}_{new} \in \mathbb{R}^{m \times (k+1)}$ and the diagonal matrix $\Sigma_{new} \in \mathbb{R}^{(k+1) \times (k+1)}$ by

$$Q_{new} \leftarrow [Q_{old} | \tilde{e}], \quad \tilde{Q}_{new} \leftarrow \begin{bmatrix} \tilde{Q}_{old} & 0 \\ 0 & 1 \end{bmatrix} Q_Y, \quad \Sigma_{new} \leftarrow \Sigma_Y.$$

The time complexity of (3.3) or (3.4) is about $O(r^2)$ since the update of the left singular vector matrix is completed by the multiplication of two small orthonormal matrices. This is a major difference comparing to (2.3) or (2.4).

However, we have to update the small orthonormal matrices over thousands or millions of times, the multiplications may erode the orthogonality of $Q$ through numerical error. Hence reorthogonalizations are needed when the inner product between the first and last left singular vectors of $Q$ is greater than some tolerance.

In [4], Brand asked “It is an open question how often this is necessary to guarantee a certain overall level of numerical precision; it does not change the overall complexity”. In the next section, we answer this question and the answer is we can avoid computing the large amount of those orthogonal matrices and those multiplications are not necessary. Hence, the reorthogonalizations are not needed.
Remark 1. Theoretically, the new adding vector $\tilde{e}$ is orthogonal to each column of $Q_{old}$. However, in practice, the matrix $[Q_{old} \mid \tilde{e}]$ loss its orthogonality very quickly for some data sets. Hence reorthogonalizations are needed for this matrix. We note that in [4], Brand did not include this. In Example 2, we show how this is important and in the next section we propose a very efficient way to remedy this issue.

The updates of right singular vector matrix $R_{new}$ and $\tilde{R}_{new}$ are more complicated because of adding rows to $R_{old}$ while guaranteeing that the columns of the product $R_{new} \tilde{R}_{new}$ are orthonormal. From the fundamental identity (2.2) and (3.2), the right-side update must satisfy

$$R_{new} \tilde{R}_{new} = \begin{bmatrix} R_{old} \tilde{R}_{old} & 0 \\ 0 & 1 \end{bmatrix} R_Y.$$

In the following updates, we need to compute the pseudo-inverse of $R_{old}$ and a sub-matrix of $R_Y$. We use $X^+$ to denote the pseudo-inverse of $X$.

(3) If $p < tol$, the rank does not increase, the last column of $R_Y$ represents an unused subspace dimension and should be suppressed. Let $R_1 = R_Y(1 : k, 1 : k)$, $R_2 = R_Y(k + 1, 1 : k)$,

$$\tilde{R}_{new} \leftarrow \tilde{R}_{old} R_1, \quad \tilde{R}_{new}^+ \leftarrow R_1^+ \tilde{R}_{old}^+, \quad R_{new} \leftarrow \begin{bmatrix} R_{old} \\ R_2 \tilde{R}_{new}^+ \end{bmatrix} .$$

(4) If $p \geq tol$, the update is rank-increasing. We update the small orthonormal matrix $\tilde{Q}_{new} \in \mathbb{R}^{m \times k}$ and the diagonal matrix $\Sigma_{new} \in \mathbb{R}^{k \times k}$ by

$$\tilde{R}_{new} \leftarrow \begin{bmatrix} \tilde{R}_{old} & 0 \\ 0 & 1 \end{bmatrix} R_Y, \quad \tilde{R}_{new}^+ \leftarrow R_Y^T \begin{bmatrix} \tilde{R}_{old}^+ & 0 \\ 0 & 1 \end{bmatrix}, \quad R_{new} \leftarrow \begin{bmatrix} R_{old} & 0 \\ 0 & 1 \end{bmatrix} .$$

The implementation of this incremental SVD algorithm is shown in Algorithms 5 and 6.
Algorithm 5 (Incremental SVD (II))

Input: \( Q \in \mathbb{R}^{m \times k}, \Sigma \in \mathbb{R}^{k \times k}, \bar{R} \in \mathbb{R}^{k \times \ell}, u_{t+1} \in \mathbb{R}^m, W \in \mathbb{R}^{m \times m}, \text{tol}, \bar{Q}, \bar{R}, \bar{R}^+ \)

1. Set \( d = Q^\top (Wu_{t+1}); e = u_{t+1} - Qd; p = (e^\top We)^{1/2} \);
2. if \( p < \text{tol} \) then
   3. Set \( Y = \begin{bmatrix} \Sigma & d \\ 0 & 0 \end{bmatrix} \);
   4. \([Q_Y, \Sigma_Y, R_Y] = \text{svd}(Y)\);
   5. Set \( \tilde{Q} = \bar{Q}Q_Y, \quad \Sigma = \Sigma_Y, \quad \mathcal{R}_1 = R_Y(1 : k, 1 : k), \quad \mathcal{R}_2 = R_Y(k + 1 : k, \cdot) \), \( \bar{R} = \tilde{Q}^\top \)
   6. \( \bar{R}_+ = \mathcal{R}_1^\top \bar{R}_1^+, \quad R = \begin{bmatrix} R & 0 \\ \mathcal{R}_2^\top \bar{R}_1^+ & 0 \end{bmatrix} \);
7. else
8. Set \( e = e/p \);
9. Set \( Y = \begin{bmatrix} \Sigma & d \\ 0 & p \end{bmatrix} \);
10. \([Q_Y, \Sigma_Y, R_Y] = \text{svd}(Y)\);
11. Set \( \tilde{Q} = \begin{bmatrix} Q & 0 \\ 0 & 1 \end{bmatrix} Q_Y, \quad Q = [Q \mid e], \quad \Sigma = \Sigma_Y, \quad R = \begin{bmatrix} R & 0 \\ 0 & 1 \end{bmatrix} \);
12. \( \bar{R} = \begin{bmatrix} \tilde{Q} & 0 \\ 0 & 1 \end{bmatrix} R_Y, \quad \bar{R}_+ = \mathcal{R}_Y^\top \begin{bmatrix} \bar{R}_1^+ & 0 \\ 0 & 1 \end{bmatrix} \);
13. end if
14. if \( |(\bar{Q}(\cdot, 1))^\top \cdot \bar{Q}(\cdot, \text{end})| > \text{tol} \) then
  15. Apply Gram-Schmidt to Reorthogonalize the matrix \( \bar{Q} \);
16. end if
17. return \( Q, \Sigma, R, \bar{Q}, \bar{R}, \bar{R}^+ \)

Algorithm 6 (Fully incremental SVD (II))

Input: \( W \in \mathbb{R}^{m \times m}, \text{tol} \)

1. Get \( u_1 \);
2. \([Q, \Sigma, R] = \text{InitializeISVD}(u_1, W)\); % Algorithm 1
3. Set \( \tilde{Q} = \bar{R} = 1 \);
4. for \( \ell = 2, \ldots, n \) do
5. Get \( u_\ell \)
6. \([Q, \Sigma, R, \tilde{Q}, \bar{Q}, \bar{R}, \bar{R}^+] = \text{UpdateISVD2}(Q, \Sigma, R, \tilde{Q}, \bar{Q}, \bar{R}, \bar{R}^+, u_\ell, W, \text{tol})\); % Algorithm 5
7. end for
8. return \( Q, \Sigma, R, \tilde{Q}, \bar{Q}, \bar{R} \)

Example 2. In this example, we first show that the reorthogonalizations are needed for the matrix \( Q \) in [Algorithm 5]. Let \( \Omega \subset \mathbb{R}^2 \) be an unit square and partition it into 512 uniform triangles. Let \( \{\varphi_j\}_{j=1}^m \) be the standard linear finite element basis functions, \( \{t_i\}_{i=1}^n \) be an equally space grid in \([0, 10]\) and time step \( \Delta t = 1/10^2 \). Define

\[
  f(t, x, y) = \cos(t(x + y)), \quad b_i = [(f(t_i), \varphi_j)]_{j=1}^m, \quad B = [b_1 \mid b_2 \mid \ldots \mid b_n].
\]

We then use the [Algorithm 6] to compute the SVD of \( B \) with the weighted matrix \( W = I \). To make a comparison, we use the MATLAB built-in function \texttt{svd()} to find the “exact” singular values of \( B \). From [Figure 2] we see that Brand’s algorithm provides unrelated singular values.
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Figure 2: Singular values of $B$: Left: Algorithm 6 Right: MATLAB built-in function \texttt{svd}().

Next, we add reorthogonalizations (details will be given in the next section) to Algorithm 6 and plot the errors (left in Figure 3) between the modified Algorithm 6 and the MATLAB built-in function \texttt{svd}(). We see that the new adding reorthogonalizations works well in practice.

Finally, we test the orthogonality of the small orthonormal matrices $\tilde{Q}$ at each update, we use $\mathcal{E}_r(\tilde{Q}) = \|I - \tilde{Q}^\top \tilde{Q}\|$ to measure the orthogonality of $\tilde{Q}$, which is shown in the right of Figure 3, we see that the matrix $\tilde{Q}$ loss its orthogonality quickly after $n = 600$ even performed the reorthogonalizations.

Figure 3: Example 2 Left: the errors of the first 34 singular values of $B$ by adding the reorthogonalizations. Right: the error of the orthogonality of $\tilde{Q}$ at each update.

4 Our improvements

As it is pointed in Section 3, the Algorithm 6 needs to update the small orthonormal matrices $\tilde{Q}$ over thousands or millions of times, the multiplications may erode the orthogonality of $\tilde{Q}$ through
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numerical error. To overcome this issue, Brand proposed reorthogonalizations when the inner product between the first and last left singular vectors of $\tilde{Q}$ is greater than some tolerance. However, as we have seen in Example 2, even we performed the reorthogonalizations, the orthonormal matrix $\tilde{Q}$ could still lose its orthogonality. Furthermore, to update the right singular space, the Algorithm 6 needs to compute the pseudo-inverse of a matrix for thousands or millions of times.

First, we summarize our contributions in this section.

1. We answer the question that Brand asked in [4]: “It is an open question how often this is necessary to guarantee a certain overall level of numerical precision; it does not change the overall complexity”.

2. We prove that the output of our new algorithm is the same with Brand’s.

3. We show that it is not necessary to compute thousands or millions of the pseudo-inverse of a matrix to update the right singular subspace.

4. We propose a reorthogonalization for the matrix $[Q_{\text{old}} \mid e]$, we note that this step is not in the original algorithm in [4]. In Example 2 we have showed that the reorthogonalizations are necessary.

To begin, we introduce the following lemma:

**Lemma 1.** Let $A \in \mathbb{R}^{k \times k}$, $\alpha \in \mathbb{R}^k$, and let $Q_1 \Sigma_1 R_1^\top$ be a thin SVD of $[A \mid \alpha]$, then

$$
\begin{bmatrix}
Q_1 & 0 \\
0 & 1
\end{bmatrix}
\begin{bmatrix}
\Sigma_1 & 0 \\
0 & 0
\end{bmatrix}
\begin{bmatrix}
R_1^\top \\
r_{k+1}^\top
\end{bmatrix}
$$

is a SVD of $[A \alpha \mid 0]$, where $r_{k+1} \in \mathbb{R}^{k+1}$ is an unit vector and orthogonal to each column of $R_1$.

Next, we use Lemma 1 to modify the updates of the left singular subspace if the rank does not increase. Assume that $Q \Sigma R^\top$ is a rank $k$ truncated core SVD of $U_\ell$, the norm of $u_{\ell+1} - QQ^\top W u_{\ell+1}$ is very small and we approximate it by 0. Therefore,

$$
U_{\ell+1} = [U_\ell \mid u_{\ell+1}] = Q \left[ \begin{array}{c|c}
\Sigma & Q^\top W u_{\ell+1} \\
0 & 1
\end{array} \right] R^\top.
$$

Let $Q_1 \Sigma_1 R_1^\top$ be a thin SVD of $[\Sigma \mid Q^\top W u_{\ell+1}]$, then the core SVD of $U_{\ell+1}$ is given by

$$
U_{\ell+1} = QQ_1 \Sigma_1 R_1^\top \left[ \begin{array}{c}
R \\
0
\end{array} \right].
$$

Hence the following update

$$
Q \leftarrow QQ_1, \quad \Sigma = \Sigma_1, \quad R = \left[ \begin{array}{c}
R \\
0
\end{array} \right] R_1,
$$

is exactly the same with (2.3) due to Lemma 1.

Next, we consider a more general situation. Assume that the matrix $C$ has $s$ columns, and the norm of $C - QQ^\top W C$ is zero or very small, then we approximate it by 0 and we then have the following fundamental identity:
In this paper we use the MATLAB built-in function \texttt{svd(Y, 'econ')} to find the SVD of \( Y \) since the matrix \( Y \) is always short-and-fat.

### 4.1 Update the left and right singular spaces

Since we assume that the matrix \( U \) is low rank, then it is reasonable to anticipate that most vectors of \( \{u_{\ell+1}, u_{\ell+2}, \ldots, u_n\} \) are linear dependent or almost linear dependent with the vectors in \( Q \in \mathbb{R}^{m \times k} \). Without loss of generality, we assume that the next 2 vectors, \( u_{\ell+1} \) and \( u_{\ell+2} \), their residuals are less than the \texttt{tol} in [Algorithm 4] when project them onto the space spanned by the columns of \( Q \). In other words, we assume that

\[
\|u_{\ell+1} - QQ^\top Wu_{\ell+1}\|_W < \texttt{tol}, \quad \|u_{\ell+2} - QQ^\top Wu_{\ell+2}\|_W < \texttt{tol}. \tag{4.6}
\]

We then follow Brand’s algorithm to find the SVD of \( U_{\ell+2} \) incrementally:

1. Find the SVD of \( \begin{bmatrix} \Sigma & Q^\top Wu_{\ell+1} \end{bmatrix} \), and we assume

\[
\begin{bmatrix} \Sigma & Q^\top Wu_{\ell+1} \end{bmatrix} = Q(1)\Sigma(1)R(1)^\top, \tag{4.7}
\]

where \( Q(1) \in \mathbb{R}^{k \times k} \), \( \Sigma(1) \in \mathbb{R}^{k \times k} \), \( R(1) \in \mathbb{R}^{(k+1) \times k} \) and \( Q(1)^\top Q(1) = Q(1)Q(1)^\top = I_k \).

2. Update the SVD of \( U_{\ell+1} \) by

\[
Q_{\ell+1} = QQ(1), \quad \Sigma_{\ell+1} = \Sigma(1), \quad R_{\ell+1} = \begin{bmatrix} R & 0 \\ 0 & 1 \end{bmatrix} R(1). \tag{4.8}
\]

By the above discussion, the update (4.8) is exactly the same with (2.3). Next, according to [Algorithm 4], we should check the magnitude of the residue of \( u_{\ell+2} \) when project onto the space spanned by the columns of \( Q_{\ell+1} \). To do this, we introduce the following lemma.

**Lemma 2.** Let \( Q \in \mathbb{R}^{k \times k} \) be an orthonormal matrix, then for any \( x \in \mathbb{R}^m \), \( Q \in \mathbb{R}^{m \times k} \) we have

\[
QQ^\top x = (QQ)(QQ)^\top x.
\]

Since \( Q(1) \) is an orthonormal matrix, then by Lemma 2 and (4.6) we have

\[
\|u_{\ell+2} - Q_{\ell+1}Q_{\ell+1}^\top Wu_{\ell+2}\|_W = \|u_{\ell+2} - QQ^\top Wu_{\ell+2}\|_W < \texttt{tol}.
\]

Next we follow the same arguments as in the above steps (1) and (2) to deal with \( u_{\ell+2} \).

3. Find the SVD of \( \begin{bmatrix} \Sigma_{\ell+1} & Q_{\ell+1}^\top Wu_{\ell+2} \end{bmatrix} \), and we assume

\[
\begin{bmatrix} \Sigma_{\ell+1} & Q_{\ell+1}^\top Wu_{\ell+2} \end{bmatrix} = Q(2)\Sigma(2)R(2)^\top, \tag{4.9}
\]

where \( Q(2) \in \mathbb{R}^{k \times k} \), \( \Sigma(2) \in \mathbb{R}^{k \times k} \), \( R(2) \in \mathbb{R}^{(k+1) \times k} \) and \( Q(2)^\top Q(2) = Q(2)Q(2)^\top = I_k \).
(4) By (4.8) we update the SVD of $U_{\ell+2}$ by

$$Q_{\ell+2} = Q_{\ell+1}Q(2) = QQ(1)Q(2),$$
$$\Sigma_{\ell+2} = \Sigma(2),$$
$$R_{\ell+2} = \begin{bmatrix} R_{\ell+1} & 0 \\ 0 & 1 \end{bmatrix} R(2) = \begin{bmatrix} R & 0 \\ 0 & I(1) \\ 0 & 1 \end{bmatrix} R(2).$$  \hspace{1cm} (4.10)

Algorithm 4 updates the left singular matrix $Q_{\ell+2}$ by computing $Q_{\ell+1} = QQ(1)$ first and then compute $Q_{\ell+2} = Q_{\ell+1}Q(2)$. The drawback of this update is its high computational cost. To avoid this, Brand proposed to compute $\tilde{Q} = Q(1)Q(2)$ first and then update the matrix $Q$ by computing $\tilde{Q}Q$; see the details in Algorithm 6. For the right singular space, Algorithm 4 updates $R_{\ell+2}$ by computing $R_{\ell+1} = \begin{bmatrix} R & 0 \\ 0 & 1 \end{bmatrix} R(1)$ first and then $R_{\ell+2} = \begin{bmatrix} R_{\ell+1} & 0 \\ 0 & 1 \end{bmatrix} R(2)$. To save the CPU time, one can use Brand’s algorithm to update the right singular subspace, but has to compute the pseudo-inverse of the sub-matrix of $R(1)$ and $R(2)$.

From Examples 1 and 2, we have seen that both algorithms have suffered in loss of the orthogonality of the left singular vector matrix.

Our new algorithm below can avoid the above issue without changing the complexity of Algorithm 6. To describe our new algorithm, we need the following fundamental identity.

\[
\begin{bmatrix}
A & 0 \\
0 & I_2 \\
0 & 1
\end{bmatrix}
\begin{bmatrix} B & 0 \\
0 & 1
\end{bmatrix} = \begin{bmatrix} A & 0 \\
0 & I_2 \\
0 & 1
\end{bmatrix} \begin{bmatrix} B & 0 \\
0 & 1
\end{bmatrix}, \quad A \in \mathbb{R}^{m \times n}, \quad B \in \mathbb{R}^{(n+1) \times n}. \hspace{1cm} (4.11)
\]

By the fundamental identity (4.11) we can rewrite $R_{\ell+2}$ as

$$R_{\ell+2} = \begin{bmatrix} R & 0 \\ 0 & I_2 \\
0 & 1
\end{bmatrix} \begin{bmatrix} R(1) & 0 \\ 0 & 1
\end{bmatrix} R(2).$$

By (4.10) we know that the SVD of $U_{\ell+2}$ is given by

$$U_{\ell+2} = QQ(1)Q(2)\Sigma(2)R^T(2) \begin{bmatrix} R(1) & 0 \\ 0 & 1 \end{bmatrix}^T \begin{bmatrix} R & 0 \\ 0 & I_2 \end{bmatrix}^T. \hspace{1cm} (4.12)$$

Motivated by (4.12), if we can compute $Q(1)Q(2)$ and $\begin{bmatrix} R(1) & 0 \\ 0 & 1 \end{bmatrix} R(2)$ directly, then the updates of the SVD of $U_{\ell+2}$ can possibly avoid many matrix-multiply-matrix operations.

**Theorem 1.** Let $\tilde{Q} = Q(1)Q(2)$, $\tilde{\Sigma} = \Sigma(2)$ and $\tilde{R} = \begin{bmatrix} R(1) & 0 \\ 0 & 1 \end{bmatrix} R(2)$, then $\tilde{Q}\tilde{\Sigma}\tilde{R}^T$ is a thin SVD of

\[
\begin{bmatrix} \Sigma & Q^TW_{\ell+1} & Q^TW_{\ell+2} \end{bmatrix}.
\]

**Proof.** First, by using (4.7) we have

\[
\begin{bmatrix} \Sigma & Q^TW_{\ell+1} & Q^TW_{\ell+2} \end{bmatrix} = \begin{bmatrix} Q(1)\Sigma(1)R^T(1) & Q^TW_{\ell+2} \end{bmatrix}.
\]
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Note that $Q_{(1)}^T Q_{(1)} = Q_{(1)} Q_{(1)}^T = I_k$ and by the fundamental identity (4.5) we have

$$
\begin{bmatrix}
\Sigma & Q^T W u_{\ell+1} \\
Q^T W u_{\ell+2}
\end{bmatrix}
= Q_{(1)} \begin{bmatrix}
\Sigma_{(1)} & Q_{(1)}^T W u_{\ell+2}
\end{bmatrix}
\begin{bmatrix}
R_{(1)} \\
0 \\
1
\end{bmatrix}^T
= Q_{(1)} \begin{bmatrix}
\Sigma_{\ell+1} & Q_{\ell+1}^T W u_{\ell+2}
\end{bmatrix}
\begin{bmatrix}
R_{(1)} \\
0 \\
1
\end{bmatrix}^T,
$$

where we used the first two identities in (4.8). Next we use (4.9) to obtain:

$$
\begin{bmatrix}
\Sigma & Q^T W u_{\ell+1} \\
Q^T W u_{\ell+2}
\end{bmatrix}
= Q_{(1)} Q_{(2)} \Sigma_{(2)} R_{(2)}^T \begin{bmatrix}
R_{(1)} \\
0 \\
1
\end{bmatrix} = \tilde{Q} \Sigma \tilde{R}^T.
$$

Theorem 1 implies that we can update the SVD of $U_{\ell+2}$ by computing a thin SVD of

$$
\begin{bmatrix}
\Sigma & Q^T W u_{\ell+1} \\
Q^T W u_{\ell+2}
\end{bmatrix} := \tilde{Q} \Sigma \tilde{R}^T
$$

first, and then update them by

$$
Q_{\ell+2} = Q \tilde{Q}, \quad \Sigma_{\ell+2} = \tilde{\Sigma}, \quad R_{\ell+2} = \begin{bmatrix}
R \\
0 \\
I_s
\end{bmatrix} \tilde{R}.
$$

(4.13)

Now we extend the above discussions to a more general situation.

**Theorem 2.** Let $\Sigma_{\ell+1} R_{\ell+1}^T$ be a rank $k$ truncated core SVD of $U_\ell$, $u_{\ell+j}$ be the $(\ell+j)$-th column of $U$, $j = 1, 2, \ldots, s$. If their residuals are less than $\text{tol}$ in Algorithm 4 when project them onto the space spanned by the columns of $Q$. Let $\tilde{Q} \Sigma \tilde{R}^T$ be the standard thin SVD of

$$
\begin{bmatrix}
\Sigma & Q^T W u_{\ell+1} \\
Q^T W u_{\ell+2} & \cdots & Q^T W u_{\ell+s}
\end{bmatrix} \in \mathbb{R}^{k \times (k+s)}.
$$

(4.14)

Then we suggest the following updates

$$
Q \leftarrow Q \tilde{Q}, \quad \Sigma \leftarrow \tilde{\Sigma}, \quad R \leftarrow \begin{bmatrix}
R \\
0 \\
I_s
\end{bmatrix} \tilde{R}.
$$

(4.15)

Moreover, the updates in (4.15) are exactly the same with the output of Algorithm 4.

**Remark 2.** In real computations, we do not compute $Q \tilde{Q}$, only need to store $Q$ and $\tilde{Q}$ for future updates. Since we only need to compute $Q$ for $r$ times, then we do not loss the orthogonality of their multiplications. Hence, our answer to Brand’s question in [4] is that the reorthogonalizations to $\tilde{Q}$ are not needed. Furthermore, to update the right singular subspace, we do not compute the pseudo-inverse of a matrix. It is worthwhile mentioning that in practice we do not form the matrix

$$
\begin{bmatrix}
R & 0 \\
0 & I_s
\end{bmatrix}
$$

by splitting $\tilde{R}$ into $\begin{bmatrix}
\tilde{R}_1 \\
\tilde{R}_2
\end{bmatrix}$, and then $R$ is updated by $\begin{bmatrix}
R \tilde{R}_1 \\
\tilde{R}_2
\end{bmatrix}$. The total computational cost to update the matrix $R$ is $O(nr^3)$. Since $r \ll m, n$, then the cost can be neglected. However, it is worthwhile mentioning that the technique in [4] can be applied to update the right singular space by computing $r$ pseudo-inverse of a small matrix, and then the computational cost can be reduced to $O(nr^2)$. 

15
Once completed the SVD of $U_{\ell+s}$, we then update the SVD of $U_{\ell+s+1}$. To better describe the algorithm. We assume that $Q\Sigma R^\top$ is the core SVD of $U_\ell$ and $\tilde{Q}\tilde{\Sigma}\tilde{R}^\top$ is the core SVD of $U_{\ell+s}$, then

$$\tilde{Q} = Q\tilde{Q}, \quad \tilde{R} = \begin{bmatrix} R & 0 \\ 0 & I_s \end{bmatrix} \tilde{R},$$

(4.16)

where $\tilde{Q}$ and $\tilde{R}$ are the left and right singular matrix of (4.14), respectively.

By our assumption, the residual of $u_{\ell+s+1}$ is larger than tol when project it onto the space spanned by the columns of $Q$. To keep the same accuracy, we should follow Brand’s idea to compute the residual of $u_{\ell+s+1}$ that project it onto the space spanned by the columns of $\tilde{Q}$.

In other words, for those columns, we have to compute their residual twice. Hence the computational cost of those repetitions can be high. Next, we show that this cost can be avoided.

To this end, we follow the idea of Brand to construct the SVD of $[U_{\ell+s} \mid u_{\ell+s+1}]$ by

1. letting $e = u_{\ell+s+1} - \tilde{Q}Q^\top Wu_{\ell+s+1}$ and let $p = \|e\|_W$ and $\bar{e} = e/p$,
2. finding the full SVD of $\bar{Y} = \begin{bmatrix} \tilde{\Sigma} & \tilde{Q}^\top u_{\ell+s+1} \\ 0 & p \end{bmatrix}$, and let $\bar{Q}\bar{\Sigma}\bar{R}^\top$ be the SVD of $\bar{Y}$, then
3. updating the SVD of $[U_{\ell+s} \mid u_{\ell+s+1}]$ by

$$[U_{\ell+s} \mid u_{\ell+s+1}] = \left( \begin{bmatrix} \tilde{Q} \\ \bar{e} \end{bmatrix} \right) \Sigma \left( \begin{bmatrix} \tilde{R} & 0 \\ 0 & 1 \end{bmatrix} \right)^\top.$$

(4.17)

Next, we discuss the above three steps. First, the computation in step (1) is not needed due to Lemma 2. Second, we do need to compute $\tilde{Q}^\top u_{\ell+s+1}$ in step (2). However, since $\tilde{Q}^\top u_{\ell+s+1} = Q^\top Q u_{\ell+s+1}$ and we have already computed $Q^\top u_{\ell+s+1},$ then the update of $\tilde{Q}^\top Q^\top u_{\ell+s+1}$ is almost nothing. For the step (3), by using (4.16) we have

$$[U_{\ell+s} \mid u_{\ell+s+1}] = \left( \begin{bmatrix} Q\tilde{Q} \\ \bar{e} \end{bmatrix} \right) \Sigma \left( \begin{bmatrix} \tilde{R} & 0 \\ 0 & 1 \end{bmatrix} \right)^\top = \left( \begin{bmatrix} Q \\ \bar{e} \end{bmatrix} \right) \left( \begin{bmatrix} Q \tilde{Q} \\ 0 \ 0 \ 1 \end{bmatrix} \right) \Sigma \left( \begin{bmatrix} \tilde{R} & 0 \\ 0 & 1 \end{bmatrix} \right)^\top.$$

(4.18)

This suggest to update the left singular matrix $Q$ by adding the vector $\bar{e}$, compute $\tilde{Q}$ and then store it, the computational cost is $O(r^2)$. For the right singular matrix, we directly compute it and the time complexity is $O(nr^2)$. The step (3) will be executed $r$ times, then the whole CPU time for this step is $O(nr^3)$. We note that if we use the technique in [4], the computational cost can be reduced to $O(nr^2)$ by computing $r$ pseudo-inverse of a matrix.

### 4.2 Reorthogonalization

As we claimed in Section 2, small numerical errors in practice can cause a loss of orthogonality. A reorthogonalization to the matrix $([\tilde{Q} \mid \bar{e}]Q$ in [7, 13] is needed and the computational cost is high due to the two for loops in Algorithm 3.

Observing the identity (4.18), we note that the orthogonal matrices $Q$ and $\tilde{Q}$ are small and only $r$ of them multiplied together, they can keep the orthogonality in a reasonable numerical precision.
An answer to an open question in the incremental SVD

Hence we do not need to perform reorthogonalizations to these small orthonormal matrices. This answers the question which was asked by Brand in [4].

Based on our numerical experiment in Example 2. The matrix \([Q \, \bar{e}]\) could lose its orthogonality very quickly. Therefore, we consider reorthogonalizations to the matrix \([Q \, \bar{e}]\). We note that this is necessary and was not included in Brand’s original algorithm.

By the construction of \([Q \, \bar{e}]\), we can reorthogonalize it recursively: only apply the \(W\)-weighted Gram-Schmidt to the new adding vector \(\bar{e}\) since the matrix \(Q\) has already been reorthogonalized in previous steps if the weighted inner product between \(\bar{e}\) and the first column of \(Q\) is larger than some tolerance. Furthermore, if \(\bar{e} = 0\), then the last column will be truncated. In other words, we do not need to perform the reorthogonalization in the truncation part (\(\|p\|_W < \text{tol}\)); see Algorithm 7 for more details.

Algorithm 7 (Incremental SVD (III))

\[
\begin{align*}
\textbf{Input:} & \quad Q \in \mathbb{R}^{m \times k}, \Sigma \in \mathbb{R}^{k \times k}, R \in \mathbb{R}^{\ell \times k}, u_{\ell + 1} \in \mathbb{R}^m, W \in \mathbb{R}^{m \times m}, \text{tol}, V, Q_0, q \\
1: & \quad \text{Set } d = Q^\top (Wu_{\ell + 1}); e = u_{\ell + 1} - Qd; p = (e^\top We)^{1/2}; \\
2: & \quad \text{if } p < \text{tol} \text{ then} \\
3: & \quad \quad q = q + 1; \\
4: & \quad \quad \text{Set } V\{q\} = Q_0^\dagger d; \\
5: & \quad \text{else} \\
6: & \quad \quad \text{if } q > 0 \text{ then} \\
7: & \quad \quad \quad \text{Set } Y = \begin{bmatrix} \Sigma | \text{cell2mat}(V) \end{bmatrix}; \\
8: & \quad \quad \quad [Q_Y, \Sigma_Y, R_Y] = \text{svd}(Y, \text{‘econ’}); \\
9: & \quad \quad \quad \text{Set } Q_0 = Q_0Q_Y, \Sigma = \Sigma_Y, R_1 = R_Y(1: k, 1 : \text{end}-1), R_2 = R_Y(k + 1, 1 : \text{end}-1), \\
10: & \quad \quad \quad R = \begin{bmatrix} \, R_1 \, \, R_2 \, \end{bmatrix}; \\
11: & \quad \quad \quad \text{Set } d = Q_Yd \\
12: & \quad \quad \text{end if} \\
13: & \quad \quad \text{Set } e = e/p; \\
14: & \quad \quad \text{if } |e^\top WQ(:, 1)| > \text{tol} \text{ then} \\
15: & \quad \quad \quad e = e - Q(Q^\top (We)); p_1 = (e^\top We)^{1/2}; e = e/p_1; \\
16: & \quad \quad \text{end if} \\
17: & \quad \quad \text{Set } Y = \begin{bmatrix} \Sigma \, d \, \, 0 \, p \end{bmatrix}; \\
18: & \quad \quad [Q_Y, \Sigma_Y, R_Y] = \text{svd}(Y); \\
19: & \quad \quad \text{Set } Q_0 = \begin{bmatrix} Q_0 \, 0 \, 0 \\ 0 \, 0 \, 1 \end{bmatrix} Q_Y, \quad Q = [Q \, e], \quad \Sigma = \Sigma_Y, \quad R = \begin{bmatrix} R \, 0 \, 0 \\ 0 \, 0 \, 1 \end{bmatrix} R_Y. \\
20: & \quad \quad \text{Set } V = []; q = 0; \\
21: & \quad \text{end if} \\
22: & \quad \text{return } Q, \Sigma, R, V, Q_0, q \\
\end{align*}
\]

4.3 The complexity of Algorithm 7

We restrict ourselves the case \(W = I\) to discuss the Algorithm 7. Recall that \(U \in \mathbb{R}^{m \times n}\) with low rank \(r\).

1. Line 1: this is exactly the same with Algorithm 5 the complexity is \(O(mnr)\).

2. Lines 3-4: the vector \(d \in \mathbb{R}^k \) with \(k \leq r\), hence this step is almost nothing for both CPU time and memory storage. Brand’s method does not have this step.
3. Lines 7-11: the main cost is the update of $R$ and the CPU time is less than $(nr^3)$. As we mentioned before, the cost can be reduced to $O(nr^2)$. We leave it here since $r \ll m$.

4. Lines 14-16: the CPU time of the reorthogonalization is $O(mr)$ each time and this part will be executed $O(r)$ times, hence the whole complexity is $O(mr^2)$. This part was not concluded in Algorithm 5 and it is necessary for some data sets.

5. Lines 17-20: the whole complexity is less than $O(nr^3)$. Again, this can be reduced to $O(nr^3)$ by using the technique in [4].

By our assumption, $r \ll m,n$, hence the CPU time of Algorithm 7 is $O(mnr)$.

We note that the output of Algorithm 7, $V$, may be not empty. This implies that the output of Algorithm 7 is not the SVD of $U$. Hence we have to update the SVD for the vectors in $V$. We give the implementation of this step in Algorithm 8, and the complexity is $O(mr^2)$. Finally, we complete the full implementation in Algorithm 9.

Algorithm 8 (Incremental SVD (III) final check)

| Input: $Q \in \mathbb{R}^{m \times k}$, $\Sigma \in \mathbb{R}^{k \times k}$, $R \in \mathbb{R}^{\ell \times k}$, $V$, $Q_0$, $q$
| 1: if $q > 0$ then
| 2: Set $Y = \left[ \Sigma \mid \text{cell2mat}(V) \right]$;
| 3: $[Q_Y, \Sigma_Y, R_Y] = \text{svd}(Y, 'econ')$;
| 4: Set $Q = Q(Q_0Q_Y)$, $\Sigma = \Sigma_Y$, $\Sigma = \Sigma_Y$, $R_1 = R_Y(1:k, 1:end-1)$,
| 5: $R_2 = R_Y(k+1, 1:end-1)$, $R = \begin{bmatrix} RR_1 \\ R_2 \end{bmatrix}$;
| 6: else
| 7: Set $Q = QQ_0$;
| 8: end if
| 9: return $Q$, $\Sigma$, $R$.

Algorithm 9 (Fully incremental SVD (III))

| Input: $W \in \mathbb{R}^{m \times m}$, tol
| 1: Get $u_1$;
| 2: $[Q, \Sigma, R] = \text{InitializeISVD}(u_1, W)$; % Algorithm 1
| 3: Set $V = []$; $Q_0 = 1$; $q = 0$;
| 4: for $\ell = 2, \ldots, n$ do
| 5: Get $u_\ell$
| 6: $[q, V, Q_0, Q, \Sigma, R] = \text{UpdateISVD3}(q, V, Q_0, Q, \Sigma, R, u_\ell, W, \text{tol})$; % Algorithm 10
| 7: end for
| 8: $[Q, \Sigma, R] = \text{UpdateISVD3check}(q, V, Q_0, Q, \Sigma, R)$; % Algorithm 12
| 9: return $Q$, $\Sigma$, $R$

Example 3. In this example, we revisit Example 1 to test the efficiency and accuracy of Algorithm 9. We show the orthogonality of the left singular vector matrix in Figure 4 where

$$E_W(Q) = \|I - Q^TWQ\|, \quad E_I(\tilde{Q}) = \|I - \tilde{Q}^T\tilde{Q}\|.$$ 

We see that our Algorithm 9 keeps a good orthogonality.
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Figure 4: Example 3: Top: the orthogonality of $\tilde{Q}$ and $Q$ with $W = I$. Bottom: the orthogonality of $\tilde{Q}$ and $Q$ with $W = M$.

Next, we show the CPU time (seconds) of the main part of the Algorithm 7 in Table 2. The whole simulations take about 34 and 118 seconds for $W = I$ and $W = M$, respectively. Comparing with Table 1, the CPU times is reduced greatly, especially with a weighted norm setting ($W \neq I$). Furthermore, the projection part (line 1 in Algorithm 7) takes about 99% of the whole simulation time, this implies there is litter space to improve the efficiency of Algorithm 9.

| Line(s) in Algorithm 7 | 1 | 3-4 | 7-11 | 14-16 | 17-20 |
|------------------------|---|-----|------|-------|-------|
| $W = I$                | 33.457 | 0.2416 | 0.0327 | 0.1251 | 0.2882 |
| $W = M$                | 116.41 | 0.1870 | 0.0650 | 0.6526 | 0.7120 |

Table 2: Example 3. The CPU time (seconds) for two different weighted norms by using Algorithm 9.
5 Another truncation

For many data sets, they may have a large number of nonzero singular values but most of them are very small. Without truncating those small singular values, the incremental SVD algorithm maybe keep computing them and hence the computational cost is huge. Following [7, Algorithm 4], we set another truncation if the last few singular values are less than a tolerance.

Next, we show that it is only necessary to check the last singular value. Let $U_{\ell+1} = [Q_1 ... Q_{\ell+1}]$, $e = u_{\ell+1} - QQ^\top u_{\ell+1}$ and $p = \|e\|_W > \text{tol}$, then

$$Y = \begin{bmatrix} \sigma_1 & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \cdots & \sigma_k & 0 \\ 0 & \cdots & 0 & \sigma_{k+1} \end{bmatrix},$$

where $\sigma_1 \geq \cdots \geq \sigma_{k+1}$ are the singular values of $Y$. Then we have

$$\sigma_{k+1} \leq p.$$  \hfill (5.1a)

$$\sigma_{k+1} \leq \sigma_k \leq \sigma_{k-1} \leq \cdots \leq \sigma_1 \leq \mu_1.$$  \hfill (5.1b)

Proof. First, we consider $Y^\top Y$,

$$Y^\top Y = \begin{bmatrix} \sum_1^2 WQΣ & \sum_1^2 WQΣ \\ u_{\ell+1}^\top WQΣ & p^2 + u_{\ell+1}^\top WQΣ WQ \sigma_{k+1} \end{bmatrix}.$$ 

By using the Cauchy interlace theorem [9, Theorem 1] we have

$$\sigma_{k+1} \leq \sigma_k \leq \sigma_{k-1} \leq \cdots \leq \sigma_1 \leq \mu_1.$$ 

Next, we take $e = [0, 0, \ldots, 1]$ to obtain

$$p^2 = eYY^\top e \geq \min_{\|x\| = 1} xYY^\top x = \lambda_{\min}(YY^\top) = \mu_{k+1}^2.$$ 

Inequality (5.1a) implies that the last singular value of $Y$ can possibly be very small, no matter how large of $p$. That is to say the tolerance we set for $p$ can not avoid the algorithm keeping compute very small singular values. Hence, another truncation is needed if the data has a large number of very small singular values. Inequality (5.1b) guarantees us that only the last singular value of $Y$ can possibly less than the tolerance. Hence, we only need to check the last one.

(i) If $\Sigma_Y(k+1, k+1) \geq \text{tol}$, then

$$Q \leftarrow [Q_1 ... Q_{\ell+1}] \quad \Sigma \leftarrow \Sigma_Y \quad R \leftarrow \begin{bmatrix} R_1 \\ 0 \\ 1 \end{bmatrix} R_Y.$$  \hfill (5.2)

(ii) If $\Sigma_Y(k+1, k+1) < \text{tol}$, then

$$Q \leftarrow [Q_1 ... Q_{\ell+1}] \quad \Sigma \leftarrow \Sigma_Y(1 : k, 1 : k) \quad R \leftarrow \begin{bmatrix} R_1 \\ 0 \\ 1 \end{bmatrix} R_Y(1 : 1 : k).$$  \hfill (5.3)
As we discussed in Section 4, we can avoid time complexity $O(m^2r)$ in (5.2) by only updating the small matrix $Q_Y$ and storing $Q_Y$ and $[Q \mid  \tilde{c}]$ separately. Unfortunately, to truncate the very small singular values, it seems very difficult that we can find two orthonormal matrices $\hat{Q} \in \mathbb{R}^{m \times k}$ and $\tilde{Q} \in \mathbb{R}^{k \times k}$ in $O(r^2)$ time such that

$$[Q \mid \tilde{c}] Q_Y(:,1:k) = \hat{Q}\tilde{Q}.$$ 

Hence, we directly use (5.2) and (5.3) to update the matrix $Q$ and $R$. Assume the data has $d$ nonzero singular values, then this new truncation needs $O((m+n)r^2d)$ time, here $r$ is the number of singular values which are larger than the tolerance.

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**Algorithm 10 (Incremental SVD (IV))**

**Input:** $Q \in \mathbb{R}^{m \times k}$, $\Sigma \in \mathbb{R}^{k \times k}$, $R \in \mathbb{R}^{l \times k}$, $u_{t+1} \in \mathbb{R}^m$, $W \in \mathbb{R}^{m \times m}$, $tol$, $V$, $Q_0$, $q$

1. Set $d = Q^T(Wu_{t+1})$; $e = u_{t+1} - Qd$; $p = (e^TWe)^{1/2}$;

2. if $p < tol$ then
3. \hspace{1em} $q = q + 1$;
4. \hspace{1em} Set $V\{q\} = d$;
5. else
6. \hspace{1em} if $q > 0$ then
7. \hspace{2em} Set $Y = [\Sigma \mid \text{cell2mat}(V)]$;
8. \hspace{2em} $[Q_Y, \Sigma_Y, R_Y] = \text{svd}(Y, 'econ')$;
9. \hspace{2em} Set $Q_0 = Q_0Q_Y$, $\Sigma = \Sigma_Y$, $R_1 = R_Y(1:k,1:end-1)$,
10. \hspace{2em} $R_2 = R_Y(k+1,1:end-1)$, $R = \begin{bmatrix} RR_1 \\ R_2 \end{bmatrix}$;
11. \hspace{1em} Set $d = Q_Y^Td$
12. end if
13. Set $e = e/p$;
14. if $|e^TWQ(:,1)| > tol$ then
15. \hspace{1em} $e = e - Q(Q^T(We))$; $p_1 = (e^TWe)^{1/2}$; $e = e/p_1$;
16. end if
17. Set $Y = \begin{bmatrix} \Sigma & d \\ 0 & p \end{bmatrix}$;
18. $[Q_Y, \Sigma_Y, R_Y] = \text{svd}(Y)$;
19. if $\Sigma(k+1,k+1) > tol$ then
20. \hspace{1em} Set $Q_0 = \begin{bmatrix} Q_0 & 0 \\ 0 & 1 \end{bmatrix} Q_Y$, $Q = [Q \mid e]Q_0$, $\Sigma = \Sigma_Y$, $R_1 = R_Y(1:k,1:end-1)$,
21. \hspace{1em} $R_2 = R_Y(k+1,1:end-1)$, $R = \begin{bmatrix} RR_1 \\ R_2 \end{bmatrix}$, $Q_0 = I_{k+1}$;
22. else
23. \hspace{1em} Set $Q_0 = \begin{bmatrix} Q_0 & 0 \\ 0 & 1 \end{bmatrix} Q_Y$, $Q = [Q \mid e]Q_0(:,1:k)$,
24. \hspace{1em} $\Sigma = \Sigma_Y(1:k,1:k)$, $R = \begin{bmatrix} R & 0 \\ 0 & 1 \end{bmatrix} R_Y(:,1:k)$, $Q_0 = I_k$
25. end if
26. $V = []$; $q = 1$;
27. end if
28. return $Q$, $\Sigma$, $R$, $V$, $Q_0$, $q$

Next, we complete the full implementation in Algorithms 11 and 12.
Algorithm 11 (Incremental SVD (IV) final check)

Input: $Q \in \mathbb{R}^{m \times k}$, $\Sigma \in \mathbb{R}^{k \times k}$, $R \in \mathbb{R}^{l \times k}$, $V$, $q$

1: if $q > 0$ then
2: Set $Y = [\Sigma \mid \text{cell2mat}(V)]$;
3: $[Q_Y, \Sigma_Y, R_Y] = \text{svd}(Y, 'econ')$;
4: Set $Q = QQ_Y$, $\Sigma = \Sigma_Y$, $R_1 = R_Y(1:k, 1:end-1)$,
5: $R_2 = R_Y(k+1, 1:end-1)$, $R = \begin{bmatrix} RR_1 \\ R_2 \end{bmatrix}$;
6: end if
7: return $Q$, $\Sigma$, $R$.

Algorithm 12 (Fully incremental SVD (IV))

Input: $W \in \mathbb{R}^{m \times m}$, $\text{tol}$

1: Get $u_1$;
2: $[Q, \Sigma, R] = \text{InitializeISVD}(u_1, W)$; \hfill \% Algorithm 1
3: Set $V = []$; $Q_0 = 1$; $q = 1$;
4: for $\ell = 2, \ldots, n$ do
5: Get $u_\ell$
6: $[q, V, Q_0, Q, \Sigma, R] = \text{UpdateISVD4}(q, V, Q_0, Q, \Sigma, R, u_\ell, W, \text{tol})$; \hfill \% Algorithm 10
7: end for
8: $[Q, \Sigma, R] = \text{UpdateISVD4check}(q, V, Q_0, Q, \Sigma, R)$; \hfill \% Algorithm 11
9: return $Q$, $\Sigma$, $R$

6 Conclusion

In this paper, we answered the open question which was asked by Brand in [4]. We prove that the output of our new algorithm is the same with Brand’s original algorithm. Numerical experiments showed that our new algorithm not only saves the CPU, but also keeps a very good orthogonality for the left singular vector matrix. In the future, we will compare our new algorithm with many other incremental SVD algorithms in [1]. Besides this, we will apply this new algorithm for many different problems, such as model order reduction and fractional PDEs.

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