A Hierarchical Singular Value Decomposition Algorithm for Low Rank Matrices

Vinita Vasudevan  
Department of Electrical Engineering  
Indian Institute of Technology-Madras  
Chennai-600036, India  
vinita@iitm.ac.in  

M.Ramakrishna  
Department of Aerospace Engineering  
Indian Institute of Technology-Madras  
Chennai-600036, India  
krishna@iitm.ac.in

ABSTRACT

Singular value decomposition (SVD) is a widely used technique for dimensionality reduction and computation of basis vectors. In many applications, especially in fluid mechanics and image processing, the matrices are dense, but low-rank matrices. In these cases, a truncated SVD corresponding to the most significant singular values is sufficient. In this paper, we propose a tree-based merge-and-truncate algorithm to obtain an approximate truncated SVD of the matrix. Unlike previous methods, our technique is not limited to “tall and skinny” or “short and fat” matrices and it can be used for matrices of arbitrary size. The matrix is partitioned into blocks and the truncated SVDs of blocks are merged to obtain the final SVD. If the matrices are low rank, this algorithm gives significant speedup over finding the truncated SVD, even when run on a single core. The error is typically less than 3%.

1. INTRODUCTION

Singular Value Decomposition (SVD) is used to obtain basis vectors in a variety of data-driven modelling techniques. It is a key step in principal component analysis (PCA) (also known as proper orthogonal decomposition (POD)), where the mean-centered data is arranged as a matrix. This is followed by an SVD of the matrix to obtain the basis vectors, which are called the POD modes or eigenfeatures. Besides, dimensionality reduction is a key step in many data-driven algorithms such as facial recognition, latent semantic indexing, collaborative filtering etc., which are used in the evolving data-driven design and modelling algorithms.

In many of these cases, the matrices are large and very often dense, but inherently low rank matrices. Computing the SVD of an \( m \times n \) matrix has complexity \( O(mn \min(n,m)) \). Since this is super-linear in the size of the data, it becomes computationally expensive for large data sets. However, if we have a low rank matrix, we would need only \( k \) basis vectors, where \( k << m, n \). One way of computing the rank \( k \) approximation is to compute the SVD of the full matrix and retain only the \( k \) largest singular values and vectors. It can be shown that this is the best rank \( k \) approximation with respect to any unitarily invariant norm. The cost of computing this approximation using an SVD followed by truncation turns out to be expensive, especially if the matrices are nearer square matrices. Moreover, in this “Bigdata” era, it is entirely possible that the dataset resides on physically different servers and bandwidth and memory constraints on each machine make it impossible to transfer all the data to a single machine to do the analysis.

Ideally, what is required is a truly distributed algorithm, where all the computation is done in-situ with minimal data transfer and the results of the computation could also reside on several machines. This has been attempted in \([2, 10]\). These algorithms assume a “tall and skinny” data matrix, which is a good assumption for many problems. They partition the matrix row-wise, and each partition containing a small subset of the rows. If the matrix has \( n \) columns, they show that an approximate PCA/SVD can be computed with \( O(n^2) \) communication cost. A drawback of the method proposed in \([2]\) is that it requires the reconstruction of the low rank approximation of each block of data, followed by accumulation of all these matrices and an SVD of an \( n \times n \) matrix. In \([3]\), they partition the matrix row-wise and perform a hierarchical QR decomposition by doing a tree-based merge of the \( R \) matrices. The SVD of the resultant small \( R \) matrix is used to compute the SVD of the full matrix. In \([10]\), they once again partition the matrix row-wise and find the SVD of each partition. This is following by a stacking of the truncated \( \Sigma V^T \) of each partition on top of each other and then doing a global SVD. They also do a randomised SVD of each block to reduce the cost of the block SVDs. Doing the global SVD can still be quite expensive. Instead of doing a global SVD, a tree-based merging algorithm using truncated SVDs has been proposed in \([9]\) to find the SVD of “short and fat” matrices. Here, the partitioning is done column-wise rather than row-wise.

Methods for incremental SVDs have been proposed in \([5, 6, 7, 8, 3]\). These algorithms incrementally compute the SVD of a matrix when new row/columns are added to the matrix. They use a combination of QR and the SVD of a smaller matrix to get the new SVD. The algorithms proposed are essentially sequential algorithms, meant for streaming data.

There are also a number of randomised algorithms, that obtain an approximate truncated SVD in linear time. A comparison of the performance and accuracy of these algorithms is included in \([4]\).

In this paper, we propose a hierarchical block based SVD algorithm to obtain a low rank approximation. It combines the advantages of the methods proposed in \([2, 10]\) and is suitable for low rank matrices of arbitrary size. Unlike \([2, 10]\), our algorithm is not limited to tall and skinny/short and fat matrices and it is possible to partition the matrix into blocks, both row-wise and column-wise. The existing algorithms get a runtime improvement when run parallelly using several cores. We demonstrate that it is possible to get speedup even when run on a single core, if partitioned appropriately. We do tree-based merge of the truncated SVDs
The matrix is partitioned row-wise, with each partition of the distributed data-sets which reside on several machines and based on the algorithm proposed in [2]. It is targeted to reduce the error in the approximation. The distributed SVD algorithms proposed in [1, 10] are based on the algorithm proposed in [2]. It is targeted to performing a principal component analysis (PCA) of massive distributed data-sets which reside on several machines and computation is not possible on a single server. The aim is to minimise communication costs. The assumption here is that the \( m \times n \) matrix \( X \), is tall and skinny with \( m \gg n \). The matrix is partitioned row-wise, with each partition \( (X_i) \) containing a subset of rows. The steps involved are:

1. Perform an approximate PCA of \( X \) locally in each machine. Let \( S_i = X_i^T X_i \approx V_i \Sigma_i^2 V_i^T \). This is an \( n \times n \) matrix.
2. The matrices \( S_i \) are transferred to the central server and summed i.e., \( S = \sum_{i=1}^p S_i \).
3. Perform a PCA of \( S \) to get an approximate truncated SVD.

The algorithm proposed in [3], performs a QR decomposition of each partition instead of an approximate SVD. The resultant “R” matrices from each partition are combined in a tree-based structure to obtain the “R” matrix corresponding to the full matrix \( X \). The SVD of the final “R” gives the correct \( \Sigma V^T \) of \( X \).

### 2.2 Subspace tracking algorithm

FAST, proposed by [3], is an incremental SVD algorithm targeted to subspace tracking. Let \( X = [X_1 \ X_2 \ \cdots \ X_n] = U \Sigma V^T \) be an \( m \times n \) matrix. If a new column \( X_{n+1} \) is added to \( X \) and \( X_1 \) is removed, the goal is to find the new SVD incrementally, rather than by re-doing the entire computation. The idea behind this and similar algorithms is to find the component of \( X_{n+1} \) that is orthogonal to the subspace \( U \). This is done by subtracting out the projection of \( X_{n+1} \) onto \( U \) to obtain the orthogonal component \( X_0 \) as follows.

\[
X_0 = X_{n+1} - U U^T X_{n+1}
\]

\[
q = \frac{X_0}{||X_0||}
\]

If \( X_t = [X_2 \ X_3 \ \cdots \ X_n] \),

\[
X_{new} = [X_t \ X_{n+1}]
\]

\[
= [U \ q] \begin{bmatrix} U^T X_t & U^T X_{n+1} \end{bmatrix}
\]

\[
= [U \ q] E
\]

\[ E \]

is an \((n+1) \times n\) matrix and its SVD is inexpensive. If \( E = U_E \Sigma_E V_E^T \), the SVD of \( X_{new} \) can be written as

\[
X_{new} = [U \ q] U_E \Sigma_E V_E^T
\]

\[
= U_N \Sigma_N V_N^T
\]

where \( \Sigma_N = \Sigma_E \) and \( U_N = [U \ q] U_E \) and \( V_N = V_E \).

### 2.3 Online incremental Algorithm

A generalisation of this algorithm is proposed in [6]. Given \( X = UV^T \), the author uses a similar technique to find the SVD of \( Y = X + AB^T \). Here \( A \) and \( B \) can have an arbitrary number of columns and rows respectively. The entries in \( A \) and \( B \) reflect additions/changes to \( X \). Let \( Q_A R_A = (I - UU^T)A \) and \( Q_B R_B = (I - VV^T)B \) be the QR decomposition of the component of \( A \) orthogonal to \( U \) and the component of \( B \) orthogonal to \( V \). This implies

\[
[U \ A] = [U \ Q_A] \begin{bmatrix} I & U^T A \\ 0 & R_A \end{bmatrix}
\]

\[
[V \ B] = [V \ Q_B] \begin{bmatrix} I & V^T B \\ 0 & R_B \end{bmatrix}
\]

Substituting this in \( Y \), we get

\[
Y = [U \ Q_A] \begin{bmatrix} \Sigma & 0 \\ 0 & \Sigma \end{bmatrix} \begin{bmatrix} U^T A \\ R_A \end{bmatrix} + [V \ Q_B] \begin{bmatrix} \Sigma & 0 \\ 0 & \Sigma \end{bmatrix} \begin{bmatrix} V^T B \\ R_B \end{bmatrix}
\]

As in the previous case, the new SVD can be computed using the SVD of the smaller matrix \( E \).

Often only a low rank approximation to the subspace is required. \( U \) is then an \( m \times k \) matrix, where \( k << n, m \). In general, if \( p \) additional columns are added, the complexity of the computation is \( O(2mkp) + O(2mp^2) + O(k + p)^3 \) corresponding to computation of the orthogonal component, QR decomposition of the orthogonal component and SVD of \( E \).

### 3. PROPOSED IMPLEMENTATION

We first start with a simple proof for computing the SVD using either the row or column-wise split, instead of the covariance matrix based proof in [2, 9, 10]. This proof also extends in a straightforward manner to having simultaneous row and column splits that are needed for large square matrices.

Assume the matrix \( X \) is an \( m \times n \) matrix and is split row-wise into sub-matrices \( X_1 \) and \( X_2 \), with sizes \( m_1 \times n \) and \( m_2 \times n \) respectively. Let \( X_1 = U_1 \Sigma_1 V_1^T \) and \( X_2 = U_2 \Sigma_2 V_2^T \).

The SVD of \( X = [X_1 \ X_2] \) can be written as

\[
\begin{bmatrix} X_1 \ X_2 \end{bmatrix} = [U_1 \ 0] \begin{bmatrix} \Sigma_1 V_1^T \\ 0 \Sigma_2 V_2^T \end{bmatrix} = [U_1 \ 0] [U_2 \ E]$


If $E = \bar{U}\Sigma V^T$, we get

$$
\begin{bmatrix}
X_1 \\
X_2
\end{bmatrix} = \begin{bmatrix} U_1 & 0 \\
0 & U_2
\end{bmatrix} \bar{U}\Sigma V^T = U\Sigma V^T
$$

where $U = \begin{bmatrix} U_1 & 0 \\
0 & U_2
\end{bmatrix}$. If partitioning is correct, we can then use the SVD of the matrix $\tilde{U}\Sigma_1 V_1^T$.

The algorithm can therefore be a merge-and-truncate (MAT) algorithm, and this in turn is a simple merge.

If $m_1, m_2 < n$, $V_1$ and $V_2$ have dimensions $m_1 \times n$ and $m_2 \times n$. Therefore, the combined matrix $\begin{bmatrix} \Sigma_1 V_1^T \\
\Sigma_2 V_2^T
\end{bmatrix}$ is an $m \times n$ matrix. By splitting it up and doing three SVDs, we end up actually increasing the computational complexity! However, if partitioned properly, this process results in a reduction in the computational complexity as will be seen in the next section.

When there are several partitions, the MAT operations can be done pairwise using a tree-based algorithm as indicated in Figure 1. Note that the “U” (left singular-vectors) matrix is not required for the merge and it need not be propagated. This is useful since the size of this matrix increases with each merge.

The algorithm can also be split column-wise as

$$
\begin{bmatrix}
X_1 \\
X_2
\end{bmatrix} \approx \begin{bmatrix} U_{1x} \Sigma_{1x} & U_{2x} \Sigma_{2x} \\
U_{1y} \Sigma_{1y} & U_{2y} \Sigma_{2y}
\end{bmatrix}
$$

In this case, merging can be done as follows.

$$
\begin{bmatrix}
X_1 \\
X_2
\end{bmatrix} \approx \begin{bmatrix} U_{1x} \Sigma_{1x} & U_{2x} \Sigma_{2x} \\
U_{1y} \Sigma_{1y} & U_{2y} \Sigma_{2y}
\end{bmatrix} \begin{bmatrix} V_{T}^1 & 0 \\
0 & V_{T}^2
\end{bmatrix} = U\Sigma V^T
$$

Once again, the SVDs of the two blocks are truncated before the merge and the final SVD is also truncated to get a low rank approximation. Also in this case, the right singular vectors $V$ are not required for the merge and hence are not propagated through the tree structure.

If the matrix is split both row and column-wise, it is easy to see that the blocks can be merged row-wise and column-wise. Let the matrix $X$ be partitioned as $X_{1x} X_{2x} X_{3x} X_{4x}$. A column-wise merge of $X_{1x} X_{2x}$ and $X_{3x} X_{4x}$ is followed by a computation of the corresponding $V$ matrices. Finally, the two blocks of rows can be merged using $V^T$ of each block. This is illustrated in Figure 3 for a more general case of a column-wise split into $c$ blocks and a row-wise split of $d$ blocks. Here, the MAT algorithm is used to first merge column-wise for each set of rows ($X_i$) to obtain $U_i \Sigma_i$. This is followed by computation of the corresponding $V_i$, which can be obtained by performing an SVD of $U_i V_i$. The MAT algorithm can then be used to merge $U_i V_i$ using a tree structure to give the approximate singular values and right singular vectors, $\Sigma_i$ and $V_i$.

It is possible to make the merging process more efficient. The MAT algorithm merge requires finding the SVD of matrices of the form $\begin{bmatrix} \Sigma_1 \Sigma_2 \\
\Sigma_2 \Sigma_1
\end{bmatrix}$ and $\begin{bmatrix} U_{1x} \Sigma_{1x} & U_{2x} \Sigma_{2x}
\end{bmatrix}$, which, depending on the block size, could become expensive. This can be made more efficient if the orthogonal complement is merged, which can be done using a combination of QR decomposition and an SVD of a smaller matrix using a method similar to [7]. If $X_1 = U_1 \Sigma_1 V^T_1$ and $X_2 = U_2 \Sigma_2 V^T_2$ are rank $k$ and $l$ respectively, we can find the product of $U_2$ orthogonal to $U_1$ as $Q = U_2 - U_1 R$. If $Q = U_o R$,

$$
\begin{bmatrix}
X_1 \\
X_2
\end{bmatrix} \approx \begin{bmatrix} U_1 & U_o \\
0 & U_o
\end{bmatrix} \begin{bmatrix} \Sigma_1 \begin{bmatrix} U_{1x} \Sigma_{1x} & U_{2x} \Sigma_{2x}
\end{bmatrix} & 0 \\
0 & \Sigma_2 R
\end{bmatrix} = \begin{bmatrix} U_1 & U_o \\
0 & U_o
\end{bmatrix} E \begin{bmatrix} V_{T}^1 & 0 \\
0 & V_{T}^2
\end{bmatrix}
$$

Now $E$ is a much smaller $(k + l) \times (k + l)$ matrix. If $E = \begin{bmatrix} V_{E} & 0 \\
0 & V_{E}
\end{bmatrix}$, we get

$$
\begin{bmatrix}
X_1 \\
X_2
\end{bmatrix} \approx \begin{bmatrix} U_1 & U_o \\
0 & U_o
\end{bmatrix} \begin{bmatrix} \Sigma_1 \begin{bmatrix} U_{1x} \Sigma_{1x} & U_{2x} \Sigma_{2x}
\end{bmatrix} & 0 \\
0 & \Sigma_2 R
\end{bmatrix} \begin{bmatrix} V_{T}^1 & 0 \\
0 & V_{T}^2
\end{bmatrix}
$$

where $U = \begin{bmatrix} U_1 & U_o \\
0 & U_o
\end{bmatrix}$. This is advantageous since we now have to perform an SVD of a much smaller matrix. Although it requires an additional QR decomposition, the total number of operations required is lower for QR than for SVD [11, 13].

Depending on the order of the two sets of MAT operations, we get the singular values and either the left or right singular vectors. Assume that after all the MAT operations are over, we have the right singular vectors and we need to

---

Figure 1: Row based partitioning followed by merge of the individual SVDs

Figure 2: Block partitioning consisting of two sets of MAT steps
compute left singular vectors $U_r$. Clearly propagation and multiplication of the matrices is not an option. Another way to do it is to compute the left singular vectors using the final $\Sigma_r V_r^T$ as $U_r = XV_r \Sigma_r^{-1}$. However, the vectors obtained need not be orthogonal, since $\Sigma_r V_r^T$ is approximate due to the truncation at various levels. Instead, we propose the following. We know that $V_r$ is an $r \times m$ orthogonal matrix (assuming a rank $r$ approximation of $X$). Let $X_p = XV_r V_r^T$ be the projection of $X$ onto the $r$ dimensional subspace of the row space. If $Y = XV_r = U_r \Sigma_r V_r^T$, then $X_p = U_r \Sigma_r V_r^T$ where $U_p = U_r$, $\Sigma_p = \Sigma_r$ and $V_p = V_r V_y$. This is the exact SVD of the projection of $X$ onto the $r$ dimensional subspace spanned by $V_y$ and an approximation to the best rank-$r$ truncated SVD of $X$.

The steps involved in the algorithm are indicated in Algorithm 1. The matrix is first partitioned row-wise and each slice is passed to the function $\text{DoSVDofColSlices}$. Here, the slice is partitioned column-wise and SVD of each partition is computed. The $U$, $\Sigma$ of each partition are merged using the function $\text{DoMergeOfSlices}$, which uses the BlockMerge routine. $\text{DoSVDofColSlices}$ returns the result of the merger as $U_j$, $\Sigma_j$ for the $j^{th}$ row slice. This is followed by computation of the corresponding $V_j$ and $\Sigma_j$, as explained. After the $V_j$ and $\Sigma_j$ of each row $j$ is calculated, they are merged using the same merge algorithm to obtain $V$ and $\Sigma$.

Once this is complete, we can follow it up with an iteration to improve accuracy. Algorithm 2 details the steps. It is essentially equivalent to a power iteration. In practice, we have found that in all the cases we have tested, two-three iterations proved to be sufficient.

3.1 Complexity

In the literature, typically “tall and skinny” matrices are partitioned row-wise and “short and fat” matrices are partitioned column-wise [10, 9]. If this is the case, a runtime speedup can only be obtained when the SVDs of the individual blocks are computed in parallel fashion with multiple cores. For “tall and skinny” matrices, the runtime is $O(mn^2)$. Therefore, if partitioned column-wise, a runtime improvement can be obtained even on a single machine.

To illustrate this, we do a simplified analysis with all blocks containing the same number of rows and look at the number of floating point operations (flops) when an $m \times n$ matrix is partitioned column-wise into $P$ blocks, each containing $s = n/P$ columns. The MAT algorithm is used to obtain the low rank approximation. Also assume that $m \gg n$, the number of flops required for the SVD of the full matrix is approximately $6mn^2 + 16n^3$ [12, 13].

The first step is an SVD of each of the $P$ blocks, for which the number of flops is $P(6ms^2 + 16s^3)$. Instead of having a truncation based on the magnitude of the singular values, assume that each SVD is truncated to get a rank $k$ matrix. Therefore, at each level of the binary tree, the merge cost includes finding the orthogonal complement $(2mk^2)$, QR decomposition $(8mk^2)$, SVD of a $2k \times 2k$ matrix $(176k^2)$, and matrix multiplication to get $U$ is $4mk^2$. This is done $P - 1$ times. The total number of flops is $P [6ms^2 + 16s^3] + (P - 1) [14mk^2 + 176k^2]$. Since $k \leq s$, the total number of flops is $< 20ms^2 + 192s^3$. Therefore, we can easily get a speedup.

The analysis is similar if the matrix is split into rows and is “short and fat”. If we have a row and column split, splitting

\begin{algorithm}
1: $X_{m \times n}$: Input Matrix, $(d, c)$: Block size
2: $\gamma$: Truncate parameter used in BlockMerge for MAT.
3: \begin{algorithmic}
4: \Function{DoSVDofBlocks}{$X_{m \times n}, d, c$}
5: \State $Nd = \text{round}(m/d + 0.5)$
6: \State $lX = \text{list}()$, $lW = \text{list}()$, $lSigma = \text{list}()$
7: \For{$i$ in range($Nd$)}
8: \State $U_j$, $\Sigma_j = \text{SVD}(U_j^T X)$
9: \State $V_j$, $\Sigma_j = \text{SVD}(U_j^T V_r)$
10: \State $lW_i += V_j$, $lSigma_i += \Sigma_j$
11: \EndFor
12: $\Sigma = \text{DoMergeOfSlices}(lSigma, lSigma)$
13: \Return $U$, $\Sigma$
\EndFunction
14: \Function{DoMergeOfSlices}{$U_i$, $\Sigma_i$}
15: \State $Nl$ is odd
16: \State $lSigma_1 = \text{SVD}(X(l))$;
17: \State $lSigma_2 = \text{SVD}(X(l))$
18: \State $U_i = \Sigma_i$; $\Sigma = \text{BlockMerge}(U_i, \Sigma, \Sigma)$
19: \State $lSigma = \Sigma$
20: \State $lSigma = \text{DoMergeOfSlices}(lSigma, lSigma)$
21: \State $\Sigma = \Sigma$
22: \EndFunction
\end{algorithmic}
\end{algorithm}

\begin{algorithm}
1: \Function{Algorithm 2 for Iterative Improvement}{$U_1, \Sigma_1, U_2, \Sigma_2$}
2: \State $U_2, \Sigma_2, V_r^T = \text{SVD}(XV_r)$
3: \State $\Sigma = \Sigma$
4: \State $\text{Error} = ||\Sigma - \Sigma||_2/||\Sigma||_2$
5: \State \If{$\text{Error} > \epsilon$}
6: \State $\Sigma = \Sigma$
7: \EndIf
8: \Return $U_1, \Sigma, V$\end{algorithm}
Also note that this speedup is possible even without parallelization. Since the first level SVDs and MAT operations at each level of the binary tree can be run independently of each other, there is significant scope for further improvement in the run-time, when run in parallel.

4. RESULTS

We have carried out experiments on matrices containing density and velocity data obtained using CFD simulations as well as the FACES dataset \[13\]. All the matrices are dense and low rank. The singular values of the density dataset as well as the FACES dataset decay more gradually, while the decay is sharp for the velocity data. For all matrices, we investigated the speedup obtained over performing a full SVD and then discarding the appropriate number of singular values. The error due to the approximation was measured as \[\|X_k - X_k^\cap\|_F/\|X_k\|_F\], where \(X_k\) is the rank-k approximation obtained using the full SVD followed by truncation and \(X_k^\cap\) is the rank-k approximation obtained using various algorithms. The code was written in Python and the SVD routine in LAPACK (available in Scipy), along with the multi-threaded openBLAS library, was used for algorithm.

We are not presenting results for the parallel version of our code. The code was run on a core i7 (4 core, 8 threads) machine running Linux. In all cases, the results reported are the average run times over five runs.

Table 1: Run time (in seconds) of SVD(X), SVD(X^T) and SVD(X^T X). \(X\) is a 132,098 \(\times\) 1024 matrix containing velocity data obtained using CFD simulations. The times reported are the average of 5 runs.

| Run time(s) | SVD(X) | SVD(X^T) | SVD(X^T X) |
|-------------|--------|----------|-------------|
| 21          | 39.8   | 4.2      |

Table 2: Speedup with respect to the SVD(X) as a function of the number of rows in each slice using various methods for a 132,098 \(\times\) 1024 matrix. TSQR is the method proposed in \[1\]. The number in brackets is the percentage error.

| No. of rows | TSQR | Algorithm in \[9\] |
|-------------|------|------------------|
| 8           | 0.3  | 1.12 (2.14)      |
| 16          | 0.32 | 0.94 (2.14)      |
| 128         | 0.37 | 0.47 (2.14)      |
| 512         | 0.43 | 0.2 (2.14)       |
| 2048        | 0.8  | 0.12 (2.03)      |
| 4096        | 0.22 | (2)              |
| 8192        | 0.4  | 0.38 (1.74)      |
| 16364       | 1.19 | 0.57 (1.57)      |
| 32768       | 1    | 0.7 (1.53)       |

Table 3: Variation with the merge parameter \(\gamma\). The table contains the maximum speedup, the block size at which this obtained and the corresponding error and the rank for the velocity matrix.

| \(\gamma\) | Max. Speedup | Block size | Error (%) | Rank |
|-----------|--------------|------------|-----------|------|
| 0.01      | 9.5          | (132,098 \(\times\) 8) | 0.005      | 1    |
| 0.05      | 5.2          | (132,098 \(\times\) 8) | 0.03       | 2    |
| 0.02      | 3.8          | (132,098 \(\times\) 8) | 0.58       | 4    |
| 0.01      | 2.8          | (16,364 \(\times\) 16) | 1.1        | 26   |
| 0.005     | 2.33         | (116,364 \(\times\) 64) | 0.87       | 53   |

Table 3 contains maximum speedup, error and rank of the matrix approximation for various values of the merge parameter \(\gamma\). As expected the speedup decreases as the rank of the approximate matrix increases. In all cases, the block size for which the maximum speedup was obtained had many more rows than columns. However, the sensitivity to block size is not very significant, as long as the number of rows is much larger than the number of columns. For example, with \(\gamma = 0.02\), the maximum speedup of 3.8 with a block size of 132 \(\times\) 8. A block size of 16,364 \(\times\) 16, the speedup obtained is 3.4 with an error of 0.65% and a rank of 11. It is also seen from the table that larger speedups are obtained when the number of columns in each block is slightly larger than the final number of singular vectors (rank). As \(\gamma\) increases, the rank of the approximated matrix decreases, as expected.

The results for the speedup and error for the density matrix are contained in Figures \[3\] and \[4\]. Here, the matrix size is 66049 \(\times\) 1024 and the singular values decay more gradually than the velocity matrix. As mentioned, the speedup is the ratio of the run time of our algorithm and the run time proposed in \[9\]. The matrix was split up row-wise and the \(R\) matrices in TSQR/ \(\Sigma^T\) matrices in the algorithm proposed in \[9\] were merged. In most cases, we got almost no speedup. Note that, in TSQR, the focus was to reduce communication costs when the matrix is stored in a distributed fashion in several computers. Also, it gets all the 1024 singular values unlike the algorithm proposed in \[9\]. Partitioning a “tall and skinny” matrix row-wise is not expected to give a speedup unless the SVDs of individual blocks are computed in parallel. Since the algorithm in \[9\] gives a low rank approximation, the percentage error is shown in brackets. It is seen to be quite small.

Next, we tried a combined row and column split and used the proposed MAT algorithm for the 132,098 \(\times\) 1024 matrix containing velocity data. Figures \[3\] and \[4\] show the speedup and error for the velocity matrix. Without iterative improvement, the algorithm runs about four times faster than doing a full SVD followed by truncation. With iterative improvement, the speedup drops, but it is still above two in most cases. Generally, it is seen that the speedup is larger when the blocks are “tall and skinny”. The average error is between 1-2%. As expected, the error drops if iterative improvement is included. It is also apparent that the error as well as the number of singular values obtained and consequently rank of the approximate matrix is also relatively independent of block size used. Also significant is the fact that the number of columns in each block can be much lower than the final number of singular values obtained, so that blocks that have 8 or 16 columns also yield 25 singular vectors. Figure \[5\] shows the singular values obtained for various block sizes for the velocity data as well as the actual singular values of the matrix. It is seen that they match closely, independent of the block size.
of doing a full SVD and then truncating. It is seen that a speedup is obtained in most cases and the largest speedup of about two is obtained when the block size is 8192 × 64. The speedup obtained is less than for the velocity data, as the singular values decay more gradually. Therefore, for the same value of γ, a larger (65 as opposed to about 25) number of singular values are obtained.

From the results for the density and velocity matrix, it seems like the optimum block size for maximum speedup is when the number of columns is around the number of singular vectors desired and the number of rows in each block is much larger.

Figures 5 and 6 contain the speedup and error with respect to SVD($X^T X$). Here, the matrix $X^T X$ was first computed and then split into blocks of various sizes. γ was set to $10^{-4}$ to allow for comparison with results in Figures 3 and 4. The same value of ε was used. The speedup obtained is significantly larger, as each block is now much smaller. The error is also significantly lower. We think this is because the rank of the approximated matrix is larger (between 33-35). As a result, the large singular values, which typically dominate the error, are approximated better.

Figures 10 and 11 show the effect of iterative improvement on the singular values and the angle between the actual and approximate left-singular vectors, for a block size of 16,364 × 16. It is seen that most of the error is in the last few singular vectors and singular values. The first 19 singular values and vectors match very closely even without iterative improvement.

We have also done experiments with the ORL database of FACES [14]. Here, the dimensions of the matrix is 10,304 × 400. The singular values decay more gradually as shown in Figure 12. As seen in the figure, the singular values are approximated well independent of the block size. Figures 13 and 14 contain the speedup and percentage error respectively. The speedup is lower, as it is a smaller matrix to start with. Typically, most of the error arises due to a poorer approximation of the last few singular values. Since the decay of singular values is more gradual, the error in these singular values is a larger percentage of the total error. Therefore, the error in this case is larger than for the CFD datasets. In fact, the error with a block size of 10,304 × 100 is about 5% and it is almost entirely due to the slightly poorer approximation of the last two singular values.

5. CONCLUSIONS

In this paper, we have presented a block-based hierarchical merge-and-truncate algorithm to compute a low rank SVD of a matrix. It is suitable for use in reduced order modelling where the matrices are inherently low rank, but can be quite large and dense. Unlike previous algorithms, it allows for a simultaneous row and column split. We get significant
Figure 6: Speedup for various block sizes for a density dataset obtained from CFD simulations. Merge parameter $\gamma = 10^{-2}$, Iterative improvement convergence criterion $\epsilon = 10^{-3}$. The rank of the approximation obtained was 65-67.

Figure 7: Percentage error for various block sizes for a density dataset obtained from CFD simulations. Merge parameter $\gamma = 10^{-2}$, Iterative improvement convergence criterion $\epsilon = 10^{-3}$. The rank of the approximation obtained was 65-67.

Figure 8: Speedup for various block sizes for a velocity dataset with respect to SVD($X^T X$). Merge parameter $\gamma = 10^{-2}$, Iterative improvement convergence criterion $\epsilon = 10^{-3}$. The rank of the approximation obtained was 32-34.

Figure 9: Speedup for various block sizes for a velocity dataset with respect to SVD($X^T X$). Merge parameter $\gamma = 10^{-2}$, Iterative improvement convergence criterion $\epsilon = 10^{-3}$. The rank of the approximation obtained was 32-34.
percentage error is marginal. The algorithm is very easy to parallelise and can give considerable improvement in the run-time.

Some more work is needed to get error bounds as well as optimal block sizes for various matrices. We have used the SVD routine in LAPACK to obtain the SVD of each block. However, it is possible to use any of the randomised algorithms to obtain an approximate SVD of each block.

6. REFERENCES
[1] Z. Bai, R. Chan and F. Luk, “Principal Component Analysis for distributed data Sets with Updating”, J. Cao, W. Nejdl, and M. Xu (Eds.): Advanced Parallel processing Technologies 2005, LNCS 3756, pp.471-483, 2005.
[2] Y. M. Qu, G. Ostrouchov, N. Samatova, and A. Geist, Principal Component Analysis for Dimension Reduction in Massive Distributed Data Sets, Proceedings to the Second SIAM International Conference on Data Mining, April 2002.
[3] C.G.Baker, K.A.Gallivan and P.Van Doreen,”Low-rank incremental methods for computing dominant singular subspaces”, Linear Algebra and its Applications, 436, pp 2860-2888, 2012.
[4] A.Menon and Charles Elkan, “Fast algorithms for approximating singular value decomposition”, ACM Transactions on Knowledge Discovery from Data, Vol. 5, No. 2, Article 13, Publication date: February 2011.
[5] D. W. Tufts, E. C. Real, and J. Cooley, “Fast approximate subspace tracking (FAST),” in Proceedings, IEEE Int. Conf. Acoust., Speech, Signal Processing; vol. 1, 1997.
[6] A. Levy, M. Lindenbaum, Sequential Karhunen-Loeve basis extraction and its application to images, IEEE Trans. Image Process. vol. 9, no.8, pp 1371-1374, 2000.
[7] M. Brand, “Fast online SVD revisions for lightweight recommender systems,” in Proceedings, SIAM International Conference on Data Mining, 2003, pp. 37-46.
[8] M.Brand, “Fast low-rank modifications of the thin singular value decomposition”, Linear Algebra and its Applications 415, pp 20-30, 2006.
[9] M.A.Iwen and B.W.Ong, “A distributed and incremental SVD algorithm for agglomerative data analysis on large networks”, SIAM J.Matrix.Anal., vol.37, pp 1699-1718, 2016.
[10] Y. Liang, M. Balcan, V. Kanchanapally and D. Woodruff, “Improved Distributed Principal Component Analysis”, Advances in Neural Information Processing Systems 27, pp 3113-3121, 2014.
[11] T.F.Chan, “An Improved Algorithm for Computing the Singular Value Decomposition. ACM Trans. Math. Softw. vol. 8, no. 1, pp 84-88, Mar. 1982.
[12] Ake Björck, “Numerical Methods in Matrix Computations”, Springer, 2015.
[13] G. Golub and Van Loan, “Matrix Computations”, Third edition, Hindustan Book Agency.
[14] AT&T laboratories Cambridge 2002, “The database of faces”, https://www.cl.cam.ac.uk/research/dtg/attarchive/facedatabase.html