FameSVD: Fast and Memory-efficient Singular Value Decomposition

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Abstract

We propose a novel algorithm to perform the Singular Value Decomposition (SVD) by leveraging the internal property of SVD. Due to the derivation being explored deterministically rather than stochastically, the convergence is guaranteed. Complexity analysis is also conducted. Our proposed SVD method outperforms classic algorithms with significant margin both in runtime and memory usage. Furthermore, we discuss the relationship between SVD and Principal Component Analysis (PCA). For those SVD or PCA algorithms that do not acquire all eigenvalues or cannot get them precisely, we utilize the matrix analysis knowledge to get the sum of all eigenvalues in order that cumulative explained variance criterion could be used in not-all-eigenvalues-are-known cases.

1 Introduction

Dimensionality reduction has always been a trendy topic in machine learning. Linear subspace method for reduction, e.g., Principal Component Analysis and its variation have been widely studied[21, 16, 23], and some pieces of literature introduce probability and randomness to realize PCA[18, 12, 11, 14, 20]. However, linear subspace is not applicable when the data lies in a non-linear manifold[2, 15]. Due to the direct connection with PCA, Singular Value Decomposition (SVD) is one of the most well-known algorithms for low-rank approximation[19, 9], and it has been widely used throughout the machine learning and statistics community. Some implementations of SVD are solving least squares[10, 22], latent semantic analysis[7, 19], genetic analysis, matrix completion[17, 15, 14, 4], data mining[6, 1] etc. However, when it comes to a large scale matrix, the runtime of traditional SVD is intolerable and the memory usage could be enormously consuming.

Notations: we have a matrix $A$ with size $m \times n$, usually $m \gg n$. Our goal is to find the Principal Components (PCs) given the cumulative explained variance threshold $t$. 

Assumptions: In this paper, every entry of matrix $A$ is real-valued; W.l.o.g., assume $m \gg n$ and $A$ has zero mean over each feature.

For your information, either each column or row of $A$ could represent an example, and the definition will be specified when necessary.

In the traditional approach of PCA, we need to compute the covariance matrix $S$, then perform the eigen-decomposition on $S$. By selecting the top $K$ largest eigenvalues and corresponding eigenvectors, we get our Principal Components (PCs). Nevertheless, if each column of $A$ is an example and the row size of $A$ is tremendously large, saving even larger covariance matrix into memory is expensive, let alone the eigen-decomposition process.

In this work, we proposed an effective and efficient SVD algorithm and could implement on PCA by discovering the relations between them.

2 Preliminary knowledge

2.1 Singular Value Decomposition (SVD)

Any real or complex matrix can be approximated over the summation of a series of rank-1 matrix. In SVD, we have

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

where

$$U = [u_1 \cdots u_n] \in \mathbb{R}^{m \times n}$$

$$\Sigma = diag(\sigma_1 \cdots \sigma_n) \in \mathbb{R}^{n \times n}$$

$$V = [v_1 \cdots v_n] \in \mathbb{R}^{n \times n}$$

Here $U$ and $V$ are orthogonal matrices, i.e.

$$U^TU = I_n$$

$$UU^T = I_m$$

$$V^TV = VV^T = I_n$$

We could also rewrite SVD as following

$$Av_i = \sigma_i u_i, i = 1 \cdots n$$

(1)

Geometrically speaking, the matrix $A$ rotates the unit vector $v_i$ to $u_i$ and then stretches the Euclidean norm of $u_i$ with a factor of $\sigma_i$.

The orthogonal matrices $U$ and $V$ can be obtained by eigen-decomposition of matrix $AA^T$ and $A^TA$, and the singular values $\sigma_i's$ are the square root of the eigenvalues of $AA^T$ or $A^TA$.

Proof:

$$AA^T = U\Sigma V^T V\Sigma^T U^T = U\Sigma^2 U^T$$

(2)

$$A^TA = V\Sigma^T U^T U\Sigma V^T = V\Sigma^2 V^T$$

(3)

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Set $\Lambda = \Sigma^2 = \text{diag}(\sigma_1^2 \cdots \sigma_n^2)$, i.e.

$$\lambda_i = \sigma_i^2$$ \hspace{1cm} (4)

We could rewrite Eq. (2) and Eq. (3) as

$$AA^T u_i = \lambda_i u_i$$ \hspace{1cm} (5)

$$A^T A v_i = \lambda_i v_i$$ \hspace{1cm} (6)

Therefore, the column vectors of $U$ and $V$ are the eigenvectors (with the unit norm) of $AA^T$ and $A^T A$, respectively. Moreover, the eigenvalues $\lambda_i$ are square of singular values $\sigma_i$, as in Eq. (4). In other words, the square root of eigenvalues are singular values.

### 2.2 Relations with PCA

If each column of $A$ represents an example or data point, set $Y = U^T A$ to our transformed data points, where $U$ is the left singular matrix in SVD. The covariance matrix of $Y$ is

$$\text{cov}(Y) = YY^T = U^T A A^T U = U^T U \Sigma^2 U^T U = \Sigma^2$$ \hspace{1cm} (7)

If each row of $A$ represents an example or data point, set $Y = AV$ to our transformed data points, where $V$ is the right singular matrix in SVD. The covariance matrix of $Y$ is

$$\text{cov}(Y) = Y^T Y = V^T A^T A V = V^T V \Sigma^2 V^T V = \Sigma^2$$ \hspace{1cm} (8)

It means the transformed data $Y$ are uncorrelated. Therefore, the column vectors of orthogonal matrix $U$ in SVD are the projection bases for Principal Components.

### 3 Our contributions: FameSVD and PCA Evaluation

#### 3.1 FameSVD

Although the derivation of SVD is clear theoretically, practically speaking, however, it is unwise to do eigen-decomposition on matrix $AA^T$, as it has a tremendous size of $m \times m$, which will deplete memory and cost a great amount of time. On the contrary, the matrix $A^T A$ only has a size of $n \times n$, thus it is plausible that we compute orthogonal matrix $V$ first. Then we can plug the Eq. (1) into Eq. (4) and get

$$u_i = \frac{Av_i}{\sqrt{\lambda_i}}, \quad i = 1 \cdots n$$ \hspace{1cm} (9)
This equation is the key to improving time and space efficiency because we do not perform eigen-decomposition on huge matrix $AA^T \in \mathbb{R}^{m \times m}$, which takes $O(m^3)$ time and $O(m^2)$ space.

Then we column-wisely combine $u_i$ to get $U$, and the same for $v_i$ to form $V$. For $\Sigma$, it is $\text{diag}(\sqrt{\sigma_1} \cdots \sqrt{\sigma_n})$.

### 3.2 PCA Evaluation with some eigenvalues unknown

In Section 2, we have proved that the column vectors of orthogonal matrix $U$ or $V$ in SVD are the projection bases for PCA. In the literature of PCA, there are many criteria for evaluating the residual error, e.g., Frobenius norm and induced $L_2$ norm of the difference matrix (original matrix minus approximated matrix), explained variance and cumulative explained variance.

In this work, we use the cumulative explained variance criterion for evaluation.

**cumulative explained variance criterion:** Given the threshold $t$, find the minimal integer $K$ such that

$$\sum_{i=1}^{K} \lambda_i \geq t$$

where each $\lambda_i$ is the eigenvalue of matrix $A^T A$ or $AA^T$. Every $\lambda_i = \sigma_i^2$ indicates the variance in principal axis, this is why the criterion is named cumulative explained variance.

For those SVD or PCA algorithms who do not obtain all the eigenvalues or can not get accurate them accurately, it seems that the denominator term $\sum_{i=1}^{n} \lambda_i$ can not be calculated. Actually, the sum of all eigenvalues can be done by

$$\sum_{i=1}^{n} \lambda_i = tr(A^T A) = tr(AA^T) = \|A\|_F^2 = \sum_{i,j} a_{ij}^2$$

Therefore, we do not need to implement eigen-decomposition on either large matrix $AA^T \in \mathbb{R}^{m \times m}$ or small matrix $A^T A \in \mathbb{R}^{n \times n}$. Eq. (11) saves us $O(n^3)$ time and $O(n^2)$ space.

### 4 Complexity Analysis

In this section, we compare the time complexity and space complexity of Krylov method, Randomized PCA and FameSVD. Due to the copyrights issue, the mechanisms of MatLab and Python built-in econSVD are not available, whose complexity analysis will not be conducted.

To restate again, our matrix $A$ has size $m \times n$ and $m > n$.

#### 4.1 Time Complexity

For time complexity, we use the number of FLoating-point OPerations (FLOP) as a quantification metric.
For matrix $A \in \mathbb{R}^{m \times n}$ and $B \in \mathbb{R}^{n \times l}$, the time complexity of matrix multiplication $AB$ takes $mnl$ FLOP of products and $ml(n - 1)$ FLOP of summations. Therefore, the multiplication of two matrices takes $O(mnl + ml(n - 1)) = O(2mnl - ml) = O(mnl)$ FLOP. We could ignore the coefficient here for it will not bring bias to our analysis.

For your information, the coefficient of time complexity in Big-O notation will not be ignored when comparing different SVD algorithms as it is of importance in our analysis.

4.1.1 Krylov method

For the Krylov method, we discuss the time complexity of each step.

1. Forming standard normal distribution matrix $G$ of size $n \times l$ takes $O(nl)$ FLOP, where in practice $l = 0.5n$.
2. Forming matrix $H^{(0)} = AG \in \mathbb{R}^{m \times l}$ takes $O(mnl)$ FLOP.
3. Forming matrix $H^{(i)} = A(A^T H^{(i-1)}) \in \mathbb{R}^{m \times l}$ takes $O(2imnl)$ FLOP, as the matrix multiplication in bracket $A^T H^{(i-1)}$ takes $O(nml)$ FLOP, then multiplying by $A$ takes $O(mnl)$ FLOP. In total, it takes $O(2imnl)$ FLOP to generate $i$ matrices.
4. Forming matrix $H = \begin{pmatrix} H^{(0)} & | & H^{(1)} & | & \ldots & | & H^{(i)} \end{pmatrix} \in \mathbb{R}^{m \times (i+1)l}$ by concatenating each $H^{(i)}$ takes $O(1)$ FLOP.
5. Performing QR decomposition on $H$ takes $O(2m[(i+1)l] - 2[(i+1)l]^{3/3})$ FLOP.
6. Forming $T = A^T Q \in \mathbb{R}^{n \times (i+1)l}$ takes $O((i+1)mnl)$ FLOP.
7. Performing SVD on $T = \tilde{V} \tilde{\Sigma} W^T$ takes $O(n[(i+1)l]^2)$ FLOP.
8. Forming $\tilde{U} = QW$ takes $O(m[(i+1)l]^2)$ FLOP.

In total, the time complexity of Krylov method is

$$O(nl + (3i + 2)mnl + (i + 1)^2l^2(m^2 + n^2 + 2m - \frac{2}{3}(i + 1)l))$$ FLOP \hspace{1cm} (12)

In practice, $l = 0.5n$, $i = 1$, then the time complexity will be

$$O(\frac{n^2}{2} + \frac{5}{2}mn^2 + 4(m^2n^2 + 2mn^2 + n^4 - \frac{2}{3}n^3))$$ FLOP \hspace{1cm} (13)

4.1.2 Randomized PCA

For Randomized PCA, we discuss the time complexity of each step. It is very similar to the Krylov method.

1. Forming standard normal distribution matrix $G$ of size $n \times l$ takes $O(nl)$ FLOP, where in practice $l = 0.5n$. 

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2. Forming matrix $H^{(0)} = AG \in \mathbb{R}^{m \times l}$ takes $O(ml)$ FLOP.

3. Forming matrix $H^{(i)} = A(A^T H^{(i-1)}) \in \mathbb{R}^{m \times l}$ takes $O(2imnl)$ FLOP, as the matrix multiplication in bracket $A^T H^{(i-1)}$ takes $O(nml)$ FLOP, then multiplying by $A$ takes $O(mnl)$ FLOP. In total, it takes $O(2imnl)$ FLOP.

4. Performing QR decomposition on $H$ takes $O(2imnl^2 - 2l^3/3)$ FLOP.

5. Forming $T = A^T Q \in \mathbb{R}^{n \times l}$ takes $O(mnl)$ FLOP.

6. Performing SVD on $T = \tilde{V} \tilde{\Sigma} W^T$ takes $O(nl^2)$ FLOP.

7. Forming $\tilde{U} = QW$ takes $O(ml^2)$ FLOP.

In total, the time complexity of Randomized PCA is

$$O(nl + (2i + 2)mnl + l^2(3m + n - \frac{2}{3}l)) \text{ FLOP}$$  \hspace{1cm} (14)

In practice, $l = 0.5n$, $i = 1$, then the time complexity will be

$$O\left(\frac{n^2}{2} + \frac{11}{4}mn^2 + \frac{n^3}{6}\right) \text{ FLOP}$$  \hspace{1cm} (15)

**4.1.3 FameSVD**

We discuss the time complexity of FameSVD for each step.

1. Forming matrix $A^T A \in \mathbb{R}^{n \times n}$ takes $O(mn^2)$ FLOP.

2. Performing eigen-decomposition on $A^T A \in \mathbb{R}^{n \times n}$ takes $O(n^3)$ FLOP.

3. Taking the square root of each eigenvalue of $A^T A$ takes $O(n)$ FLOP.

4. Forming $u_i = \frac{Av_i}{\sigma_i}$ takes $O(n(mn + m))$ FLOP, as $Av_i$ takes $O(mn)$ FLOP while divided by $\sigma_i$ takes $O(m)$ FLOP. In total, we have $n$ equations like this, thus it takes $O(n(mn + m))$ FLOP.

In total, the time complexity of FameSVD is

$$O(2mn^2 + n^3 + n + mn)$$  \hspace{1cm} (16)

**4.2 Space Complexity**

We evaluate the space complexity by the number of matrix entries. For a matrix $A \in \mathbb{R}^{m \times n}$, its space complexity is $O(mn)$. In MatLab or Python programming language, each entry takes 8 bytes memory.
4.2.1 Krylov method

1. Forming standard normal distribution matrix $G$ of size $n \times l$ takes $O(nl)$, where in practice $l = 0.5n$.

2. Forming matrix $H^{(0)} = AG \in \mathbb{R}^{m \times l}$ takes $O(ml)$.

3. Forming matrix $H^{(i)} = A(A^T H^{(i-1)}) \in \mathbb{R}^{m \times l}$ takes $O(ml)$.

4. Forming matrix $H = \begin{pmatrix} H^{(0)} \\ H^{(1)} \\ \vdots \\ H^{(i)} \end{pmatrix} \in \mathbb{R}^{m \times (i+1)l}$ by concatenating each $H^{(i)}$ takes $O((i+1)ml)$.

5. Performing QR decomposition on $H$ takes $O((i+1)ml)$. Note that we discard matrix $R$, only $Q$ is saved.

6. Forming $T = A^T Q \in \mathbb{R}^{n \times (i+1)l}$ takes $O((i+1)nl)$.

7. Performing SVD on $T = \tilde{V} \tilde{\Sigma} W^T$ takes $O((i+1)nl + 2[(i+1)l]^2)$, for matrix $\tilde{V} \in \mathbb{R}^{n \times (i+1)l}$ takes $O((i+1)nl)$ and $\tilde{\Sigma} \in \mathbb{R}^{(i+1)l \times (i+1)l}$ takes $O([(i+1)l]^2)$, and $W \in \mathbb{R}^{(i+1)l \times (i+1)l}$ takes $O([(i+1)l]^2)$. In total, it takes $O((i+1)nl + 2[(i+1)l]^2)$.

8. Forming $\tilde{U} = QW$ takes $O((i+1)ml)$.

In total with $A$ taking $O(mn)$, the space complexity of Krylov method is

$$O(mn + (3i + 4)ml + (2i + 3)nl + 2[(i+1)l]^2)$$

In practice, $l = 0.5n, i = 1$, then the space complexity of Krylov method will be

$$O\left(\frac{9}{2}mn + \frac{9}{2}n^2\right)$$

(18)

4.2.2 Randomized PCA

1. Forming standard normal distribution matrix $G$ of size $n \times l$ takes $O(nl)$, where in practice $l = 0.5n$.

2. Forming matrix $H^{(0)} = AG \in \mathbb{R}^{m \times l}$ takes $O(ml)$.

3. Forming matrix $H^{(i)} = A(A^T H^{(i-1)}) \in \mathbb{R}^{m \times l}$ takes $O(ml)$.

4. Performing QR decomposition on $H$ takes $O(ml)$. Note that we discard matrix $R$, only $Q$ is saved.

5. Forming $T = A^T Q \in \mathbb{R}^{n \times l}$ takes $O(nl)$.

6. Performing SVD on $T = \tilde{V} \tilde{\Sigma} W^T$ takes $O(nl + 2l^2)$, for matrix $\tilde{V} \in \mathbb{R}^{n \times l}$ takes $O(nl)$ and $\tilde{\Sigma} \in \mathbb{R}^{l \times l}$ takes $O(l^2)$, and $W \in \mathbb{R}^{l \times l}$ takes $O(l^2)$. In total, it takes $O(nl + 2l^2)$.  

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7. Forming \( \tilde{U} = QW \) takes \( O(ml) \).

In total with \( A \) taking \( O(mn) \), the space complexity of Randomized PCA is

\[
O(mn + 3ml + 3nl + 2l^2)
\]  \hspace{1cm} (19)

In practice, \( l = 0.5n \), \( i = 1 \), then the space complexity of Randomized PCA will be

\[
O\left(\frac{9}{2}mn + 3n^2\right)
\]  \hspace{1cm} (20)

### 4.2.3 FameSVD

We discuss the space complexity of FameSVD for each step.

1. Forming matrix \( A^T A \in \mathbb{R}^{n \times n} \) takes \( O(n^2) \).
2. Performing eigen-decomposition on \( A^T A \) takes \( O(n^2 + n) \).
3. Taking the square root of each eigenvalue of \( A^T A \) takes \( O(n) \).
4. Forming \( u_i = \frac{A v_i}{\sigma_i} \) takes \( O(mn) \), as each \( u_i \) takes \( O(m) \) and we have \( n \) equations like this, thus in total it takes \( O(mn) \).
5. Forming \( V \) takes \( O(n^2) \).
6. Storing \( n \) singular values takes \( O(n) \).

In total with \( A \) taking \( O(mn) \), the space complexity of FameSVD is

\[
O(3n^2 + 3n + 2mn)
\]  \hspace{1cm} (21)

### 4.3 Summary of Complexity Analysis

| Method        | Time complexity                                           | Space complexity             |
|---------------|----------------------------------------------------------|------------------------------|
| Krylov method | \( O\left(\frac{n^2}{2} + \frac{5}{2}mn^2 + 4m^2n^2 + 2mn^2 + n^4 - \frac{2}{3}n^3\right)\) \hspace{1cm} | \( O\left(\frac{9}{2}mn + \frac{9}{2}n^2\right)\) | |
| Randomized PCA | \( O\left(\frac{n^2}{2} + \frac{11}{4}mn^2 + \frac{n^3}{6}\right)\) \hspace{1cm} | \( O\left(\frac{9}{2}mn + 3n^2\right)\) | |
| FameSVD       | \( O(2mn^2 + n^3 + n + mn)\) \hspace{1cm} | \( O(3n^2 + 3n + 2mn)\) | |

We summarized the time complexity and space complexity in Table 1. Under the assumptions that \( m \gg n \), for time complexity, by keeping the highest order term and its coefficient, we could see that for Krylov method, it
Figure 1: Runtime comparisons between 4 methods of SVD. The matrix column size is fixed at 2000, but row size varies. Our proposed FameSVD method outperforms the rest.

\[ O(4m^2n^2) \text{ FLOP} \] while Randomized PCA takes \( O\left(\frac{11}{4}mn^2\right) \text{ FLOP} \) and our proposed FameSVD only takes \( O(2mn^2) \) FLOP. Therefore, FameSVD is the fastest SVD algorithm among the aforementioned. Furthermore, our proposed FameSVD keeps all the eigenpairs rather than only first \( k \) pairs as Krylov method and Randomized PCA do.

For space complexity, we could see that FameSVD needs the least memory usage as \( O(3n^2 + 3n + 2mn) \) and Krylov method needs the most memory space as \( O\left(\frac{9}{2}mn + \frac{9}{2}n^2\right) \). Randomized PCA holds the space complexity in between.

5 Experiments

We generate a matrix \( A \) whose entry obeys standard normal distribution, i.e., \( a_{ij} \sim \mathcal{N}(0, 1) \), with 5 row sizes in list \([2000, 4000, 6000, 8000, 10000]\) and 12 column sizes in \([100, 200, 300, 400, 500, 600, 800, 900, 1000, 1200, 1500, 2000]\), 60 matrices of \( A \) in total. The experiment is repeated 10 times to get an average runtime. On evaluating the residual error, the rate of Frobenius norm is used

\[
\delta = \frac{\|A - U\Sigma V^T\|_F}{\|A\|_F}
\]

(22)

In Fig. 1 we compare the runtime of 4 SVD methods: FameSVD (Our method), Krylov method, Randomized PCA, econ SVD (MatLab built-in economic SVD). The matrix column size is fixed at 2000, and we increase the row size gradually. We could observe that all 4 methods follow a linear runtime pattern when row size increases. Of these 4 methods, our proposed FameSVD method outperforms the other 3 approaches.
Figure 2: Runtime comparisons between 4 methods of SVD. The matrix row size is fixed at 10000, but column size varies. Our proposed FameSVD method outperforms the rest.

In Fig. 2 we fix the row size of matrix at 10000, and we increase the column size gradually. We could observe that all 4 methods behave as non-linear runtime pattern when row size increases. Out of all 4 methods, our proposed FameSVD method takes the least runtime in every scenario.

Figure 3: Memory usage between 3 methods of SVD. The matrix row size is fixed at 10000, but column size varies. Our proposed FameSVD needs the least memory.

In Fig. 3 the row size of matrix is fixed at 10000, but column size varies. We could see that our proposed FameSVD uses the minimal amount of memory while Randomized PCA needs the most.

We also evaluate our algorithm on handwritten digit dataset MNIST[8]. We form our matrix $A$ with size $60000 \times 784$ by concatenating 60000 of vectorized
Figure 4: Left to right: Original image, Randomized PCA, Krylov method and FameSVD. The first 392 (784/2) principal components are reserved.

$28 \times 28$ intensity image. For runtime, it takes 4.54 s and 10.79 s for Randomized PCA and Krylov method respectively to obtain the first 392 (784/2) principal components. However, it only takes FameSVD 3.12 s to get all the 784 eigenvalues and eigenvectors; For memory usage, 1629.1 MB for Randomized PCA and 1636.1 MB for Krylov method. In the meanwhile, only 731.9 MB is used for FameSVD.

Our experiments are conducted on MatLab R2013a and Python 3.7 with NumPy 1.15.4, with Intel(R) Core(TM) i7-6700 CPU @ 3.40GHz 3.40GHz, 8.00 GB RAM, and Windows 7. The proposed method is faster than the built-in economic SVD of both MatLab and NumPy.

6 Conclusion

In this paper, we propose a fast and memory-efficient algorithm to do Singular Value Decomposition on a large scale matrix. We conduct time and space complexity analysis which proves that our algorithm has better performance both in time and space usage. Moreover, the experiment matches our complexity analysis.

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