PROBABILISTIC ALGORITHMS FOR FINDING MATRIX DECOMPOSITIONS

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Abstract. Low-rank matrix approximations are obliquous in many areas ranging from data analysis to scientific computing. From a data science point of view, probably the most important application is due to Principal Component Analysis (PCA), which aims to reveal hidden linear structure in massive datasets through a low-rank matrix decomposition. Consequently, the complexity of the algorithm plays a central role in the applicability of the algorithms to big data. The most common approximative factorization is the so-called truncated singular value decomposition (k-SVD) which can be computed in $\mathcal{O}(mnk)$ floating-point operations, where k is the target rank of the decomposition and m and n are the corresponding dimensions of the matrix. In this review, we introduce to the reader randomized algorithms that can achieve the aforementioned task with numerous advantadges compared to the classical algorithms. These algorithms are based on the fact that the image of a low-rank matrix can be approximated by the action of the matrix to a reasonable amount of random vectors from the input space. Starting from this point, it is possible to develop algorithms that achieve a complexity of $\mathcal{O}(mn \log k)$ for dense-matrices, matches the flop count of classical Krylov subspace methods for sparse matrices with a gain in robustness, and for large matrices that can not be stored in memory (RAM), they achieve a constant number of passes compared to the $\mathcal{O}(k)$ for classical algorithms.

Introduction

Matrix factorization is listed as one of the most influential set of techniques during the 20th century [1], among the Fast Fourier Transform, MCMC sampling methods and others. As Stewart [3] argues, the principle of the decompositional approach aims to construct computational platforms from which a variety of problems can be solved.

Although the decompositional approach to matrix computational remains fundamental, nowadays in the era of big data most of the classical algorithms are inadequate to tackle most of the problems.

$$\underset{m \times n}{\boldsymbol{A}} \approx \underset{m \times k}{\boldsymbol{B}} \quad \underset{k \times n.}{\boldsymbol{C},} \tag{0.1}$$

Theory

0.1. **Analysis of stage A.** This section focuses on assessing the quality of the basis given by ALGO. More precisely, we want to prove rigorous bounds on the approximation error

$$\|\boldsymbol{A} - \boldsymbol{Q}\boldsymbol{Q}^*\boldsymbol{A}\|$$

where $\|\cdot\|$ denotes either the operator norm or Frobenius norm.

We will split the argument into two parts [1]:

(1) Provide a generic error bound that depends on the interaction between the test matrix $\boldsymbol{\Omega}$ and the right and left singular values of $\boldsymbol{A}$. [2]
(2) Estimate the error using the distribution of the random matrix. We provide both expectation and probability tail bounds for the error.

[1] The authors argue that this bipartite proof is common in the literature of randomized linear algebra

[2] Note that we do not deal with randomness yet.

0.1.1. *(1) Error bounds via Linear Algebra.* As we aim to compute a rank-k approximation of $\boldsymbol{A}$, we appropiately partition the exact SVD as

$$\boldsymbol{A} = \boldsymbol{U} \begin{array}{c} \begin{array}{cc} k & n-k \end{array} \\ \begin{bmatrix} \boldsymbol{\Sigma}_1 & \\ & \boldsymbol{\Sigma}_2 \end{bmatrix} \end{array} \begin{array}{c} n \\ \begin{bmatrix} \boldsymbol{V}_1^* \\ \boldsymbol{V}_2^* \end{bmatrix} \end{array} \begin{array}{c} k \\ n-k \end{array} \tag{0.2}$$

Now, let $\boldsymbol{\Omega}_i = \boldsymbol{V}_i \boldsymbol{\Omega}$ for $i = 1, 2$. Express $\boldsymbol{Y} = \boldsymbol{A\Omega}$ as

$$\boldsymbol{Y} = \boldsymbol{A\Omega} = \boldsymbol{U} \begin{array}{c} \ell \\ \begin{bmatrix} \boldsymbol{\Sigma}_1 \boldsymbol{\Omega}_1 \\ \boldsymbol{\Sigma}_2 \boldsymbol{\Omega}_2 \end{bmatrix} \end{array} \begin{array}{c} k \\ n-k \end{array}$$

where $\boldsymbol{\Sigma}_1 \boldsymbol{\Omega}_1$ controls most of the action of $\boldsymbol{Y}$, and $\boldsymbol{\Sigma}_2 \boldsymbol{\Omega}_2$ is a small perturbation.

The ALGO computes an orthogonal basis $\boldsymbol{Q}$ of $\mathrm{Im}(\boldsymbol{Y})$. In other words, we can express the orthogonal projection to $\mathrm{Im}(\boldsymbol{Y})$ as $\boldsymbol{P}_{\boldsymbol{Y}} = \boldsymbol{P}_{\mathrm{Im}(\boldsymbol{Y})} = \boldsymbol{QQ}^*$ [3]. The following theorem 0.1 bounds the squared error provides a deterministic error bound to the squared error.

Theorem 0.1 (Deterministic error bound)**.** *We have that*

$$|||(\mathbf{I} - \boldsymbol{P}_{\boldsymbol{Y}})\boldsymbol{A}|||^2 \leq |||\boldsymbol{\Sigma}_2|||^2 + |||\boldsymbol{\Sigma}_2 \boldsymbol{\Omega}_2 \boldsymbol{\Omega}_1^\dagger|||^2, \tag{0.3}$$

where $|||\cdot|||$ *denotes either the spectral norm or the Frobenius norm.*

Remark 0.2. Note that $\boldsymbol{\Sigma}_1$ does not appear in the error bound. EXPLAIN

Remark 0.3. The first term is a deterministic clean error term; we want to compute a rank-k approximation so the error can not be smaller than this term. The second term is a random term that depends on the interaction of the right singular values of $\boldsymbol{A}$ amplified by $\boldsymbol{\Sigma}_2$.

We would also like to be able to analyze the power scheme described in REF, i.e, $\boldsymbol{B} = (\boldsymbol{AA}^*)\boldsymbol{A} = \boldsymbol{U}\boldsymbol{\Sigma}^{2q+1}\boldsymbol{V}^*$. The rationale behind the power scheme was that the random approximation of the k-dimensional gross action of $\boldsymbol{A}$ can be improved if we amplify $\boldsymbol{\Sigma}_1 - \boldsymbol{\Sigma}_2$ by power iteration. This can be easily verified by this simple theorem 0.4.

Theorem 0.4 (Power scheme)**.** *Let $\boldsymbol{A}$ be an $m \times n$ matrix, and let $\boldsymbol{\Omega}$ be an $n \times \ell$ matrix. Fix a nonnegative integer q, form $\boldsymbol{B} = (\boldsymbol{A}^*\boldsymbol{A})^q \boldsymbol{A}$, and compute the sample matrix $\boldsymbol{Z} = \boldsymbol{B\Omega}$. Then*

$$\|(\mathbf{I} - \boldsymbol{P}_{\boldsymbol{Z}})\boldsymbol{A}\| \leq \|(\mathbf{I} - \boldsymbol{P}_{\boldsymbol{Z}})\boldsymbol{B}\|^{1/(2q+1)}.$$

Remark 0.5. Let's consider the operator norm, i.e, $\|\boldsymbol{\Sigma}_1\| = \sigma_{k+1}$. Then

$$\|(\mathbf{I} - \boldsymbol{P}_{\boldsymbol{Z}})\boldsymbol{A}\| \leq \|(\mathbf{I} - \boldsymbol{P}_{\boldsymbol{Z}})\boldsymbol{B}\|^{1/(2q+1)} \leq \left(1 + \left\|\boldsymbol{\Omega}_2 \boldsymbol{\Omega}_1^\dagger\right\|^2\right)^{1/(4q+2)} \sigma_{k+1}$$

so the power scheme shrinks the suboptimality exponentially fast.

Finally, we can ask what are the consequences of truncating the SVD of $\boldsymbol{P}_{\boldsymbol{Z}}\boldsymbol{A}$, i.e, compute its best rank-k approximation.

Theorem 0.6 (Analysis of Truncated SVD)**.** *Let $\boldsymbol{A}$ be an $m \times n$ matrix with singular values $\sigma_1 \geq \sigma_2 \geq \sigma_3 \geq \dots$, and let $\boldsymbol{Z}$ be an $m \times \ell$ matrix, where $\ell \geq k$. Suppose that $\widehat{\boldsymbol{A}}_{(k)}$ is a best rank-k approximation of $\boldsymbol{P}_{\boldsymbol{Z}}\boldsymbol{A}$ with respect to the spectral norm. Then*

$$\left\|\boldsymbol{A} - \widehat{\boldsymbol{A}}_{(k)}\right\| \leq \sigma_{k+1} + \|(\mathbf{I} - \boldsymbol{P}_{\boldsymbol{Z}})\boldsymbol{A}\|.$$

Remark 0.7. The result of theorem 0.6 is quite pessimistic, and in practice we observe that truncating the SVD is not that damaging in the randomized setting.

[3]We simplify the notation of the orthogonal projectoin to $\boldsymbol{P}_{\boldsymbol{Y}}$

0.1.2. *(2) Bounds on the gaussian setting.* First we start by providing a bunch of results on gaussian matrices that will are key to prove the bounds on expectation and probability tails.

Proposition 0.8 (Expected norm of a scaled Gaussian matrix)**.** *Fix matrices $\boldsymbol{S}, \boldsymbol{T}$, and draw a standard Gaussian matrix $\boldsymbol{G}$. Then*

$$\left(\mathbb{E}\left\|\boldsymbol{SGT}\right\|_{\mathrm{F}}^{2}\right)^{1/2} = \|\boldsymbol{S}\|_{\mathrm{F}}\|\boldsymbol{T}\|_{\mathrm{F}} \quad \text{and} \quad \mathbb{E}\left\|\boldsymbol{SGT}\right\| \leq \|\boldsymbol{S}\|\,\|\boldsymbol{T}\|_{\mathrm{F}} + \|\boldsymbol{S}\|_{\mathrm{F}}\|\boldsymbol{T}\|. \tag{0.4}$$

Proposition 0.9 (Expected norm of a pseudo-inverted Gaussian matrix)**.** *Draw a $k \times (k+p)$ standard Gaussian matrix $\boldsymbol{G}$ with $k \geq 2$ and $p \geq 2$. Then*

$$\left(\mathbb{E}\left\|\boldsymbol{G}^{\dagger}\right\|_{\mathrm{F}}^{2}\right)^{1/2} = \sqrt{\frac{k}{p-1}} \quad \text{and} \quad \mathbb{E}\left\|\boldsymbol{G}^{\dagger}\right\| \leq \frac{\mathrm{e}\sqrt{k+p}}{p}. \tag{0.5}$$

Proposition 0.10 (Concentration for functions of a Gaussian matrix)**.** *Suppose that h is a Lipschitz function on matrices:*

$$|h(\boldsymbol{X}) - h(\boldsymbol{Y})| \leq L\,\|\boldsymbol{X}-\boldsymbol{Y}\|_{\mathrm{F}} \quad \text{for all } \boldsymbol{X}, \boldsymbol{Y}.$$

Draw a standard Gaussian matrix $\boldsymbol{G}$. Then

$$\mathbb{P}\left\{h(\boldsymbol{G}) \geq \mathbb{E}\,h(\boldsymbol{G}) + Lt\right\} \leq \mathrm{e}^{-t^2/2}.$$

Now, we are ready to state and proof the main theorems in expectations, and afterwards we will confirm that the error does not oscillate too much around the mean by proving the corresponing bounds on the tails of the distribution.

Theorem 0.11 (Average Frobenius error)**.** *The expected approximation error can be bounded as follows*

(1)
$$\mathbb{E}\left\|(\mathbf{I}-\boldsymbol{P_Y})\boldsymbol{A}\right\|_{\mathrm{F}} \leq \left(1+\frac{k}{p-1}\right)^{1/2}\left(\sum\nolimits_{j>k}\sigma_j^2\right)^{1/2}.$$

(2)
$$\mathbb{E}\left\|(\mathbf{I}-\boldsymbol{P_Y})\boldsymbol{A}\right\| \leq \left(1+\sqrt{\frac{k}{p-1}}\right)\sigma_{k+1} + \frac{\mathrm{e}\sqrt{k+p}}{p}\left(\sum\nolimits_{j>k}\sigma_j^2\right)^{1/2}.$$

Proof. Hölder's inequality and theorem 0.1 give

$$\mathbb{E}\left\|(\mathbf{I}-\boldsymbol{P_Y})\boldsymbol{A}\right\|_{\mathrm{F}} \leq \left(\mathbb{E}\left\|(\mathbf{I}-\boldsymbol{P_Y})\boldsymbol{A}\right\|_{\mathrm{F}}^2\right)^{1/2} \leq \left(\left\|\boldsymbol{\Sigma}_2\right\|_{\mathrm{F}}^2 + \mathbb{E}\left\|\boldsymbol{\Sigma}_2\boldsymbol{\Omega}_2\boldsymbol{\Omega}_1^{\dagger}\right\|_{\mathrm{F}}^2\right)^{1/2}.$$

Then, we condition on $\boldsymbol{\Omega}_1$ and use proposition 0.8 and first part of proposition 0.9

$$\mathbb{E}\left\|\boldsymbol{\Sigma}_2\boldsymbol{\Omega}_2\boldsymbol{\Omega}_1^{\dagger}\right\|_{\mathrm{F}}^2 = \mathbb{E}\left(\mathbb{E}\left[\left\|\boldsymbol{\Sigma}_2\boldsymbol{\Omega}_2\boldsymbol{\Omega}_1^{\dagger}\right\|_{\mathrm{F}}^2 \mid \boldsymbol{\Omega}_1\right]\right) = \mathbb{E}\left(\left\|\boldsymbol{\Sigma}_2\right\|_{\mathrm{F}}^2\left\|\boldsymbol{\Omega}_1^{\dagger}\right\|_{\mathrm{F}}^2\right) = \left\|\boldsymbol{\Sigma}_2\right\|_{\mathrm{F}}^2 \cdot \mathbb{E}\left\|\boldsymbol{\Omega}_1^{\dagger}\right\|_{\mathrm{F}}^2 = \frac{k}{p-1}\cdot\left\|\boldsymbol{\Sigma}_2\right\|_{\mathrm{F}}^2,$$

Putting everything together

$$\mathbb{E}\left\|(\mathbf{I}-\boldsymbol{P_Y})\boldsymbol{A}\right\|_{\mathrm{F}} \leq \left(1+\frac{k}{p-1}\right)^{1/2}\left\|\boldsymbol{\Sigma}_2\right\|_{\mathrm{F}}.$$

and the first part if proved.
The bound on the operator norm is very similar, theorem 0.1 implies that

$$\mathbb{E}\left\|(\mathbf{I}-\boldsymbol{P_Y})\boldsymbol{A}\right\| \leq \mathbb{E}\left(\left\|\boldsymbol{\Sigma}_2\right\|^2 + \left\|\boldsymbol{\Sigma}_2\boldsymbol{\Omega}_2\boldsymbol{\Omega}_1^{\dagger}\right\|^2\right)^{1/2} \leq \left\|\boldsymbol{\Sigma}_2\right\| + \mathbb{E}\left\|\boldsymbol{\Sigma}_2\boldsymbol{\Omega}_2\boldsymbol{\Omega}_1^{\dagger}\right\|.$$

Conditioning again on $\boldsymbol{\Omega}_1$, we can bound the expectation w.r.t $\boldsymbol{\Omega}_2$

$$\mathbb{E}\left\|\boldsymbol{\Sigma}_2\boldsymbol{\Omega}_2\boldsymbol{\Omega}_1^{\dagger}\right\| \leq \mathbb{E}\left(\left\|\boldsymbol{\Sigma}_2\right\|\left\|\boldsymbol{\Omega}_1^{\dagger}\right\|_{\mathrm{F}} + \left\|\boldsymbol{\Sigma}_2\right\|_{\mathrm{F}}\left\|\boldsymbol{\Omega}_1^{\dagger}\right\|\right) \leq \left\|\boldsymbol{\Sigma}_2\right\|\left(\mathbb{E}\left\|\boldsymbol{\Omega}_1^{\dagger}\right\|_{\mathrm{F}}^2\right)^{1/2} + \left\|\boldsymbol{\Sigma}_2\right\|_{\mathrm{F}}\cdot\mathbb{E}\left\|\boldsymbol{\Omega}_1^{\dagger}\right\|.$$

Finally applying proposition 0.9, we get to the final result

$$\mathbb{E}\left\|\boldsymbol{\Sigma}_2\boldsymbol{\Omega}_2\boldsymbol{\Omega}_1^{\dagger}\right\| \leq \sqrt{\frac{k}{p-1}}\left\|\boldsymbol{\Sigma}_2\right\| + \frac{\mathrm{e}\sqrt{k+p}}{p}\left\|\boldsymbol{\Sigma}_2\right\|_{\mathrm{F}}.$$

□

Finally, we will state the bounds on the tails that prove that the previously expectation bounds are representative of the random behavior.

Theorem 0.12 (Deviation bounds for the Frobenius error)**.** *Frame the hypotheses of Theorem 0.11. Assume further that $p \geq 4$. For all $u, t \geq 1$,*

$$\|(\mathbf{I} - \boldsymbol{P_Y})\boldsymbol{A}\|_{\mathrm{F}} \leq \left(1 + t \cdot \sqrt{12k/p}\right)\left(\sum\nolimits_{j>k} \sigma_j^2\right)^{1/2} + ut \cdot \frac{\mathrm{e}\sqrt{k+p}}{p+1} \cdot \sigma_{k+1},$$

with failure probability at most $5t^{-p} + 2\mathrm{e}^{-u^2/2}$.

Theorem 0.13 (Deviation bounds for the spectral error)**.** *Frame the hypotheses of Theorem 0.11, and assume further that $p \geq 4$. Then*

$$\|(\mathbf{I} - \boldsymbol{P_Y})\boldsymbol{A}\| \leq \left(1 + 8\sqrt{(k+p) \cdot p \log p}\right)\sigma_{k+1} + 3\sqrt{k+p}\left(\sum\nolimits_{j>k} \sigma_j^2\right)^{1/2},$$

with failure probability at most $6p^{-p}$.

Similar bounds can also be proven for the power scheme [2] that give a high probability guarantee for the bound 0.4.

Algorithms

1. Fixed rank problem

Proto-Algorithm: Solving the Fixed-Rank Problem

Given an $m \times n$ matrix $\boldsymbol{A}$, a target rank k, and an oversampling parameter p, this procedure computes an $m \times (k+p)$ matrix $\boldsymbol{Q}$ whose columns are orthonormal and whose range approximates the range of $\boldsymbol{A}$.

1. Draw a random $n \times (k+p)$ test matrix $\boldsymbol{\Omega}$.
2. Form the matrix product $\boldsymbol{Y} = \boldsymbol{A\Omega}$.
3. Construct a matrix $\boldsymbol{Q}$ whose columns form an orthonormal basis for the range of $\boldsymbol{Y}$.

Theorem 1.1. *Suppose that $\boldsymbol{A}$ is a real $m \times n$ matrix. Select a target rank $k \geq 2$ and an oversampling parameter $p \geq 2$, where $k + p \leq \min\{m, n\}$. Execute the proto-algorithm with a standard Gaussian test matrix to obtain an $m \times (k+p)$ matrix $\boldsymbol{Q}$ with orthonormal columns. Then*

$$\mathbb{E}\,\|\boldsymbol{A} - \boldsymbol{QQ}^*\boldsymbol{A}\| \leq \left[1 + \frac{4\sqrt{k+p}}{p-1} \cdot \sqrt{\min\{m,n\}}\right]\sigma_{k+1}, \tag{1.1}$$

where $\mathbb{E}$ denotes expectation with respect to the random test matrix and σ_{k+1} is the $(k+1)$th singular value of $\boldsymbol{A}$.

The probability that the error satisfies

$$\|\boldsymbol{A} - \boldsymbol{QQ}^*\boldsymbol{A}\| \leq \left[1 + 11\sqrt{k+p} \cdot \sqrt{\min\{m,n\}}\right]\sigma_{k+1} \tag{1.2}$$

is at least $1 - 6 \cdot p^{-p}$ under very mild assumptions on p.

Prototype for Randomized SVD

Given an $m \times n$ matrix $\boldsymbol{A}$, a target number k of singular vectors, and an exponent q (say $q = 1$ or $q = 2$), this procedure computes an approximate rank-$2k$ factorization $\boldsymbol{U\Sigma V}^*$, where $\boldsymbol{U}$ and $\boldsymbol{V}$ are orthonormal, and $\boldsymbol{\Sigma}$ is nonnegative and diagonal.

Stage A:

1 Generate an $n \times 2k$ Gaussian test matrix $\boldsymbol{\Omega}$.
2 Form $\boldsymbol{Y} = (\boldsymbol{AA}^*)^q \boldsymbol{A\Omega}$ by multiplying alternately with $\boldsymbol{A}$ and $\boldsymbol{A}^*$.
3 Construct a matrix $\boldsymbol{Q}$ whose columns form an orthonormal basis for the range of $\boldsymbol{Y}$.

Stage B:

4 Form $\boldsymbol{B} = \boldsymbol{Q}^*\boldsymbol{A}$.
5 Compute an SVD of the small matrix: $\boldsymbol{B} = \widetilde{\boldsymbol{U}}\boldsymbol{\Sigma V}^*$.
6 Set $\boldsymbol{U} = \boldsymbol{Q}\widetilde{\boldsymbol{U}}$.

Note: The computation of $\boldsymbol{Y}$ in Step 2 is vulnerable to round-off errors. When high accuracy is required, we must incorporate an orthonormalization step between each application of $\boldsymbol{A}$ and $\boldsymbol{A}^*$; see Algorithm **??**.

2. Randomized SVD

The Randomized SVD procedure requires only $2(q + 1)$ passes over the matrix, so it is efficient even for matrices stored out-of-core. The flop count satisfies

$$T_{\text{randSVD}} = (2q + 2)\, k\, T_{\text{mult}} + \mathrm{O}(k^2(m + n)),$$

where T_{mult} is the flop count of a matrix–vector multiply with $\boldsymbol{A}$ or $\boldsymbol{A}^*$.

Theorem 2.1. *Suppose that $\boldsymbol{A}$ is a real $m \times n$ matrix. Select an exponent q and a target number k of singular vectors, where $2 \leq k \leq 0.5 \min\{m, n\}$. Execute the Randomized SVD algorithm to obtain a rank-$2k$ factorization $\boldsymbol{U\Sigma V}^*$. Then*

$$\mathbb{E}\,\|\boldsymbol{A} - \boldsymbol{U\Sigma V}^*\| \leq \left[1 + 4\sqrt{\frac{2\min\{m,n\}}{k-1}}\right]^{1/(2q+1)} \sigma_{k+1}, \tag{2.1}$$

where $\mathbb{E}$ denotes expectation with respect to the random test matrix and σ_{k+1} is the $(k + 1)$th singular value of $\boldsymbol{A}$.

In practice, we can truncate the approximate SVD, retaining only the first k singular values and vectors. Equivalently, we replace the diagonal factor $\boldsymbol{\Sigma}$ by the matrix $\boldsymbol{\Sigma}_{(k)}$ formed by zeroing out all but the largest k entries of $\boldsymbol{\Sigma}$. For this truncated SVD, we have the error bound

$$\mathbb{E}\,\left\|\boldsymbol{A} - \boldsymbol{U\Sigma}_{(k)}\boldsymbol{V}^*\right\| \leq \sigma_{k+1} + \left[1 + 4\sqrt{\frac{2\min\{m,n\}}{k-1}}\right]^{1/(2q+1)} \sigma_{k+1}. \tag{2.2}$$

References

[1] Jack Dongarra and Francis Sullivan. "Guest editors introduction: The top 10 algorithms". In: *Computing in Science & Engineering* 2.1 (2000), pp. 22–23.

[2] Nathan Halko, Per-Gunnar Martinsson, and Joel A Tropp. "Finding structure with randomness: Probabilistic algorithms for constructing approximate matrix decompositions". In: *SIAM review* 53.2 (2011), pp. 217–288.

[3] GW Stewart. "The decompositional approach to matrix computation". In: *Computing in Science & Engineering* 2.1 (2000), pp. 50–59.

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