

PROBABILISTIC ALGORITHMS FOR FINDING MATRIX DECOMPOSITIONS

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ABSTRACT. This paper is a sample prepared to illustrate the use of the American Mathematical Society's L^AT_EX document class `amsart` and publication-specific variants of that class for AMS-L^AT_EX version 2.

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

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

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 $\mathbf{\Omega}$ and the right and left singular values of \mathbf{A} . ²
- (2) Estimate the error using the distribution of the random matrix. We provide both expectation and probability tail bounds for the error.

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

$$(0.1) \quad \mathbf{A} = \mathbf{U} \begin{bmatrix} k & n-k \\ \mathbf{\Sigma}_1 & \mathbf{\Sigma}_2 \end{bmatrix} \begin{bmatrix} n \\ \mathbf{V}_1^* \\ \mathbf{V}_2^* \end{bmatrix} \begin{bmatrix} k \\ n-k \end{bmatrix}$$

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

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

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

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

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

²Note that we do not deal with randomness yet.

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

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

$$(0.2) \quad \|(\mathbf{I} - \mathbf{P}_Y)\mathbf{A}\|^2 \leq \|\Sigma_2\|^2 + \|\Sigma_2\Omega_2\Omega_1^\dagger\|^2,$$

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

Remark 0.2. Note that Σ_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 \mathbf{A} amplified by Σ_2 .

We would also like to be able to analyze the power scheme described in REF, i.e., $\mathbf{B} = (\mathbf{A}\mathbf{A}^*)\mathbf{A} = \mathbf{U}\Sigma^{2q+1}\mathbf{V}^*$. The rationale behind the power scheme was that the random approximation of the k -dimensional gross action of \mathbf{A} can be improved if we amplify $\Sigma_1 - \Sigma_2$ by power iteration. This can be easily verified by this simple theorem 0.4.

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

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

Remark 0.5. Let's consider the operator norm, i.e., $\|\Sigma_1\| = \sigma_{k+1}$. Then

$$\|(\mathbf{I} - \mathbf{P}_Z)\mathbf{A}\| \leq \|(\mathbf{I} - \mathbf{P}_Z)\mathbf{B}\|^{1/(2q+1)} \leq \left(1 + \|\Omega_2\Omega_1^\dagger\|^2\right)^{1/(4q+2)} \sigma_{k+1}$$

so the power scheme shrinks the suboptimality exponentially fast.

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

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

$$\|\mathbf{A} - \hat{\mathbf{A}}_{(k)}\| \leq \sigma_{k+1} + \|(\mathbf{I} - \mathbf{P}_Z)\mathbf{A}\|.$$

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.

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

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

$$(0.3) \quad \left(\mathbb{E} \|\mathbf{SGT}\|_{\text{F}}^2\right)^{1/2} = \|\mathbf{S}\|_{\text{F}} \|\mathbf{T}\|_{\text{F}} \quad \text{and} \quad \mathbb{E} \|\mathbf{SGT}\| \leq \|\mathbf{S}\| \|\mathbf{T}\|_{\text{F}} + \|\mathbf{S}\|_{\text{F}} \|\mathbf{T}\|.$$

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

$$(0.4) \quad \left(\mathbb{E} \|\mathbf{G}^\dagger\|_{\text{F}}^2\right)^{1/2} = \sqrt{\frac{k}{p-1}} \quad \text{and} \quad \mathbb{E} \|\mathbf{G}^\dagger\| \leq \frac{e\sqrt{k+p}}{p}.$$

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

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

Draw a standard Gaussian matrix \mathbf{G} . Then

$$\mathbb{P}\{h(\mathbf{G}) \geq \mathbb{E} h(\mathbf{G}) + Lt\} \leq e^{-t^2/2}.$$

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 corresponding bounds on the tails of the distribution.

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

(1)

$$\mathbb{E} \|(\mathbf{I} - \mathbf{P}_{\mathbf{Y}})\mathbf{A}\|_{\text{F}} \leq \left(1 + \frac{k}{p-1}\right)^{1/2} \left(\sum_{j>k} \sigma_j^2\right)^{1/2}.$$

(2)

$$\mathbb{E} \|(\mathbf{I} - \mathbf{P}_{\mathbf{Y}})\mathbf{A}\| \leq \left(1 + \sqrt{\frac{k}{p-1}}\right) \sigma_{k+1} + \frac{e\sqrt{k+p}}{p} \left(\sum_{j>k} \sigma_j^2\right)^{1/2}.$$

Proof. Hölder's inequality and theorem 0.1 give

$$\mathbb{E} \|(\mathbf{I} - \mathbf{P}_{\mathbf{Y}})\mathbf{A}\|_{\text{F}} \leq \left(\mathbb{E} \|(\mathbf{I} - \mathbf{P}_{\mathbf{Y}})\mathbf{A}\|_{\text{F}}^2\right)^{1/2} \leq \left(\|\Sigma_2\|_{\text{F}}^2 + \mathbb{E} \|\Sigma_2 \Omega_2 \Omega_1^\dagger\|_{\text{F}}^2\right)^{1/2}.$$

Then, we condition on Ω_1 and use proposition 0.8 and first part of proposition 0.9

$$\begin{aligned} \mathbb{E} \|\Sigma_2 \Omega_2 \Omega_1^\dagger\|_{\text{F}}^2 &= \mathbb{E} \left(\mathbb{E} \left[\|\Sigma_2 \Omega_2 \Omega_1^\dagger\|_{\text{F}}^2 \mid \Omega_1 \right] \right) = \mathbb{E} \left(\|\Sigma_2\|_{\text{F}}^2 \|\Omega_1^\dagger\|_{\text{F}}^2 \right) \\ &= \|\Sigma_2\|_{\text{F}}^2 \cdot \mathbb{E} \|\Omega_1^\dagger\|_{\text{F}}^2 = \frac{k}{p-1} \cdot \|\Sigma_2\|_{\text{F}}^2, \end{aligned}$$

Putting everything together

$$\mathbb{E} \|(\mathbf{I} - \mathbf{P}_{\mathbf{Y}})\mathbf{A}\|_{\text{F}} \leq \left(1 + \frac{k}{p-1}\right)^{1/2} \|\Sigma_2\|_{\text{F}}.$$

and the first part is proved.

The bound on the operator norm is very similar, theorem 0.1 implies that

$$\mathbb{E} \|(\mathbf{I} - \mathbf{P}_{\mathbf{Y}})\mathbf{A}\| \leq \mathbb{E} \left(\|\Sigma_2\|^2 + \|\Sigma_2 \Omega_2 \Omega_1^\dagger\|^2 \right)^{1/2} \leq \|\Sigma_2\| + \mathbb{E} \|\Sigma_2 \Omega_2 \Omega_1^\dagger\|.$$

Conditioning again on Ω_1 , we can bound the expectation w.r.t Ω_2

$$\begin{aligned} \mathbb{E} \|\Sigma_2 \Omega_2 \Omega_1^\dagger\| &\leq \mathbb{E} \left(\|\Sigma_2\| \|\Omega_1^\dagger\|_{\text{F}} + \|\Sigma_2\|_{\text{F}} \|\Omega_1^\dagger\| \right) \\ &\leq \|\Sigma_2\| \left(\mathbb{E} \|\Omega_1^\dagger\|_{\text{F}}^2 \right)^{1/2} + \|\Sigma_2\|_{\text{F}} \cdot \mathbb{E} \|\Omega_1^\dagger\|. \end{aligned}$$

Finally applying proposition 0.9, we get to the final result

$$\mathbb{E} \|\Sigma_2 \Omega_2 \Omega_1^\dagger\| \leq \sqrt{\frac{k}{p-1}} \|\Sigma_2\| + \frac{e\sqrt{k+p}}{p} \|\Sigma_2\|_{\text{F}}.$$

□

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 $u, t \geq 1$,*

$$\|(\mathbf{I} - \mathbf{P}_Y)\mathbf{A}\|_F \leq \left(1 + t \cdot \sqrt{12k/p}\right) \left(\sum_{j>k} \sigma_j^2\right)^{1/2} + ut \cdot \frac{e\sqrt{k+p}}{p+1} \cdot \sigma_{k+1},$$

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

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

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

with failure probability at most $6p^{-p}$. Similar bounds can also be proven Halko, Martinsson, and Tropp, 2011.

ALGORITHMS

1. FIXED RANK PROBLEM

PROTO-ALGORITHM: SOLVING THE FIXED-RANK PROBLEM

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

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

Theorem 1.1. *Suppose that \mathbf{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 \mathbf{Q} with orthonormal columns. Then*

$$(1.1) \quad \mathbb{E} \|\mathbf{A} - \mathbf{Q}\mathbf{Q}^* \mathbf{A}\| \leq \left[1 + \frac{4\sqrt{k+p}}{p-1} \cdot \sqrt{\min\{m, n\}}\right] \sigma_{k+1},$$

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

The probability that the error satisfies

$$(1.2) \quad \|\mathbf{A} - \mathbf{Q}\mathbf{Q}^* \mathbf{A}\| \leq \left[1 + 11\sqrt{k+p} \cdot \sqrt{\min\{m, n\}}\right] \sigma_{k+1}$$

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

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

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

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

PROTOTYPE FOR RANDOMIZED SVD

Given an $m \times n$ matrix \mathbf{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 $\mathbf{U}\mathbf{\Sigma}\mathbf{V}^$, where \mathbf{U} and \mathbf{V} are orthonormal, and $\mathbf{\Sigma}$ is nonnegative and diagonal.*

Stage A:

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

Stage B:

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

Note: The computation of \mathbf{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 \mathbf{A} and \mathbf{A}^* ; see Algorithm ??.

Theorem 2.1. *Suppose that \mathbf{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 $\mathbf{U}\mathbf{\Sigma}\mathbf{V}^*$. Then*

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

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

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

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

REFERENCES

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

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