Approximate Euclidean lengths and distances beyond Johnson-Lindenstrauss

Aleksandros Sobczyk  
IBM Research and ETH Zürich  
Zürich, Switzerland  
obc@zurich.ibm.com  

Mathieu Luisier  
ETH Zürich  
Zürich, Switzerland  
mluisier@iis.ee.ethz.ch

Abstract

A classical result of Johnson and Lindenstrauss states that a set of $n$ high dimensional data points can be projected down to $O(\log n/\epsilon^2)$ dimensions such that the square of their pairwise distances is preserved up to a small distortion $\epsilon \in (0, 1)$. It has been proved that the JL lemma is optimal for the general case, therefore, improvements can only be explored for special cases. This work aims to improve the $\epsilon^{-2}$ dependency based on techniques inspired by the Hutch++ Algorithm [34], which reduces $\epsilon^{-2}$ to $\epsilon^{-1}$ for the related problem of implicit matrix trace estimation.

We first present an algorithm to estimate the Euclidean lengths of the rows of a matrix. We prove for it element-wise probabilistic bounds that are at least as good as standard JL approximations in the worst-case, but are asymptotically better for matrices with decaying spectrum. Moreover, for any matrix, regardless of its spectrum, the algorithm achieves $\epsilon$-accuracy for the total, Frobenius norm-wise relative error using only $O(\epsilon^{-1})$ queries. This is a quadratic improvement over the norm-wise error of standard JL approximations. We also show how these results can be extended to estimate (i) the Euclidean distances between data points and (ii) the statistical leverage scores of tall-and-skinny data matrices, which are ubiquitous for many applications, with analogous theoretical improvements. Proof-of-concept numerical experiments are presented to validate the theoretical analysis.

1 Introduction

The Johnson-Lindenstrauss (JL) lemma [29] is a fundamental concept in dimensionality reduction and data science. Given a set of $n$ high dimensional data points $X = \{x_1, ..., x_n\}$, where each $x_i \in \mathbb{R}^d$, the goal is to find a projection $f : \mathbb{R}^d \rightarrow \mathbb{R}^k$ that maps the vectors to a much smaller dimension $k \ll d$ such that the geometry of the original set is approximately preserved. Specifically, the projection should preserve the pairwise distances up to a small distortion $\epsilon \in (0, 1)$, that is

$$(1 - \epsilon)\|x_i - x_j\|^2 \leq \|f(x_i) - f(x_j)\|^2 \leq (1 + \epsilon)\|x_i - x_j\|^2,$$

for all $i, j \in [n]$. If $f$ satisfies this property, then it is called an $\epsilon$-isometry. Johnson and Lindenstrauss proved that, given $\epsilon$, such an $f$ can be found in randomized polynomial time and that the projected dimension is no larger than $O(\log n/\epsilon^2)$. In the last decades the JL lemma has made an impact in many areas, including Graph Algorithms [6, 42], Machine Learning [5, 11, 16, 24], Numerical Linear Algebra [14, 33, 40, 44] and Optimization [20, 22, 38].

In the existing literature, a common approach to approximate the metric is to first find a map that preserves Euclidean lengths instead of distances. The approximate isometry property is then achieved by applying this map to all the pairwise difference vectors, since the Euclidean distance between $x$ and $y$ is equal to the length of $x - y$; cf. [18, 29]. In this work we follow the same methodology. We first study the problem of approximating the Euclidean lengths of the rows of an
For a set $A$ while the 2-norm is assumed for both matrices and vectors when the norm subscript is omitted. There is therefore no advantage in taking an approximate solution over computing the true solution.

Vectors with small letters, and scalars with Greek letters.

It is known that Gaussian matrices can provide JLTs; c.f. [5, 29].

When the input matrix is explicitly available, satisfying the complex analysis, some constant $i$ the transpose of $A^*$ is the identity matrix of size $N$ of $A$.

By default, the Householder notation is used, denoting matrices with capital letters, vectors with small letters, and scalars with Greek letters. $[n]$ is the set \{1, 2, ..., $n$\}, where $n \in \mathbb{N}$. $I_n$ is the identity matrix of size $n \times n$ and $e_i$ its $i$-th column. $A_{i,j}$ is the element of $A$ in row $i$ and column $j$. $A_k$ denotes the best rank-$k$ approximation of $A$ in the 2-norm. $\|A\|_F$ is the Frobenius norm of $A$, while the 2-norm is assumed for both matrices and vectors when the norm subscript is omitted. $A^\dagger$ is the transpose of $A$ and $A^\dagger$ is the pseudoinverse. $\mathbb{P}[\alpha] \in [0, 1]$ denotes the probability of an event $\alpha$ to occur. $\mathcal{N}(\mu, \sigma)$ is the normal distribution with mean value $\mu$ and standard deviation $\sigma$. $\sigma_i(A)$ denotes the $i$-th largest singular value of $A$. $\text{nnz}(A)$ is the number of nonzeros $A$. $\tilde{O}(k) := O(k \log^c(k))$ for some constant $c$. We refer to matrices with i.i.d. elements from $\mathcal{N}(0, 1)$ as Gaussian matrices. In the complexity analysis, $\omega$ denotes the fast matrix multiplication exponent, where $2 \leq \omega < 2.37286$ [4].

**Why Gaussians?** In this work we focus on Gaussian random projections. Other constructions satisfying the $(\epsilon, \delta, n)$-JLT definition exist in the literature, such as randomized Fourier/Hadamard [2, 3, 43] or sparse [1, 15, 17, 30, 32, 35] transforms. When the input matrix is explicitly available,
algorithm is called “Adaptive,” since it needs to make two passes over the input matrix. The main contributions are the following:

1. The proposed algorithms require asymptotically less matrix-vector queries to achieve the same accuracy as standard JL random projections for matrices with decaying spectrum, that is, spectral decay properties are reflected in the approximation bounds. To the best of our knowledge, this is the first work to provably reduce the number of required matrix-vector queries for Euclidean length approximations.

2. For any matrix, regardless of its spectrum, the proposed algorithms require a number of matrix-vector queries that depends on $1/\epsilon$ to achieve $\epsilon$-accuracy for the total, Frobenius norm-wise error, as opposed to $1/\epsilon^2$ for standard JL.

3. For the worst-case inputs, that is, for matrices with flat spectrum, the approximated values are at least as good as standard JL.

4. The techniques can be directly applied to and give similar improvements for the related problems of approximate pairwise Euclidean distances and approximate leverage scores.

Algorithm 1 Adaptive Euclidean Norm Estimation

Input: Matrix $A \in \mathbb{R}^{n \times d}$, $n \geq d$, positive integer $m < d$.
Output: $\tilde{x}_i \approx \|e_i^T A\|^2$.

1. Construct two random matrices $S, G \in \mathbb{R}^{d \times m}$ with i.i.d. elements from $N(0, 1)$.
2. Compute $B = A^T (AS) \quad \triangleright \quad O(dm)$
3. Compute an orthonormal basis $Q \in \mathbb{R}^{d \times m}$ for $\text{range}(B)$ (e.g., via QR).
4. Compute $A = AQ$ and $C = AG.$
5. Compute $\tilde{A} = A(I - QQ^T) G = C - \tilde{A}(Q^T G)$.
6. return $\tilde{x}_i = \|e_i^T \tilde{A}\|^2 + \|e_i^T \Delta\|^2$, for all $i \in [n]$.

In Table 1 we summarize the approximation guarantees of the proposed Algorithms 1, 2, and 3 for the aforementioned problems. We also compare it to the corresponding bounds of existing JL-based approximations to highlight the achieved improvements. For the precise statements we refer to the corresponding sections.
Table 1: Comparison between the approximation bounds that are achieved in this work versus standard JL random projections for the three different problems considered here. In all cases, the number of matrix-vector queries \( m \) that are performed is the same. It is proportional to \( \epsilon^{-2} \) (up to logarithmic factors on \( n, \delta \)), where \( \epsilon \in (0, 1/2) \) is the accuracy and \( \delta \in (0, 1/2) \) the success probability. Here, \( k \) is an integer such that \( m = \Omega(k/\delta) \) and \( A_k = A - A_k \). \( M \) is a matrix such that its rows define pairwise distance vectors between the rows of \( A \). The \( \theta_i \)'s are the leverage scores of the input matrix.

| Element-wise | Frobenius norm-wise |
|--------------|---------------------|
| This work | JL | This work | JL | ref. |
| Row norms | \( \epsilon \|e_i^\top A\| \|e_i^\top A_k\| \) | \( \epsilon \|e_i^\top A\|^2 \) | \( \epsilon^2 \|A\|_F^2 \) | \( \epsilon \|A\|_F^2 \) | Thms. 1 & 2 |
| Distances | \( \epsilon \|e_i^\top M\| \|e_i^\top M_k\| \) | \( \epsilon^2 \|M\|_F^2 \) | \( \epsilon \|M\|_F^2 \) | Thm. 5 |
| Leverage scores | \( \epsilon \theta_i \) | \( \epsilon \theta_i \) | \( \epsilon^2 d \) | \( \epsilon d \) | Thm. 3 |

\( T_{MM}(A, m) = 3 \times T_{MM}(C, m) = O(\text{nnz}(C) m) \). The results are stated for general \( T_{MM}(A, m) \), but they will be specialized, where applicable, for the targeted applications.

**Related work.** A related topic is stochastic matrix trace estimation [7, 27, 28, 34, 37, 39]. Intuitively, a set of data points can be seen as the columns of a matrix. In various applications the trace of such a matrix contains useful information like triangle counts in graphs [6]. Hutchinson [27] proposed a randomized algorithm to rapidly approximate the trace of such a matrix, which uses similar ideas to JL: it projects the rows of the matrix onto a low-dimensional subspace so that the trace can be quickly computed. Avron and Toledo showed that the dimension of that subspace needs to be proportional to \( \epsilon^{-2} \) in order to guarantee a worst-case \( \epsilon \)-approximation for the trace [7]. This dependence on \( \epsilon \) matches the requirements for the \( \epsilon \)-isometry of JL. The \( \epsilon^{-2} \) overhead can be prohibitive when \( \epsilon \) is small, i.e. in applications where high accuracy is needed. Recently, in their seminal work, Meyer, Musco, Musco, and Woodruff [34] proved a remarkable result: their Hutch++ algorithm is the first to obtain \( \epsilon \)-accuracy for stochastic trace estimation while requiring only \( 1/\epsilon \) matrix-vector queries. For the related problem of estimating the diagonal elements of a matrix, which was also recently studied in depth [9, 26], Baston and Nakatsukasa [9] achieved \( \epsilon \)-accuracy for the total, norm-wise error of the entire diagonal using \( O(1/\epsilon) \) matrix-vector queries, but not for each individual diagonal element, which should not be possible due to the optimality of the JL lemma [31]. It is worth noting that the squared row norms of a matrix \( A \) can be found in the diagonal of \( AA^\top \), therefore, our work is closely related. Our results for the total norm-wise error, however (see e.g. Theorem 2), are tighter than simply using [9] on \( AA^\top \), since we are exploiting the special structure of \( AA^\top \). From a Fine-Grained complexity perspective, estimating row norms can be easily reduced to diagonal estimation, but the opposite reduction is not straightforward, therefore, one can argue that diagonal estimation is harder, which justifies our tighter bounds.

**Outline.** The analysis of Algorithm 1 is given in Section 2. In Sections 3 and 4 we show two important applications of the main results, namely for the estimation of the pairwise Euclidean distances between a set of data points and for the estimation of the statistical leverage scores of a tall-and-skinny data matrix. In Section 5 we present indicative experiments to validate the theoretical analysis, before finally giving concluding remarks and future directions in Section 6.

**2 Analysis of Algorithm 1**

In this section we provide the analysis of Algorithm 1. Preliminary results and long proofs which were omitted from the main text and can be found in the Appendix. We state the following general result for the element-wise bounds of Algorithm 1.

**Lemma 2.** *(Proof in the Appendix)* Let \( A \in \mathbb{R}^{n \times d} \). If we use Algorithm 1 with \( m \) matrix-vector queries to estimate the Euclidean lengths of the rows \( e_i^\top A, i \in [n] \), then as long as \( m \geq l \geq 32 \log(4n/\delta) \) it holds that

\[
|\hat{x}_i - \|e_i^\top A\|^2| \leq \epsilon \frac{\log(4n)}{\delta} \|e_i^\top A(I - QQ^\top)\|^2, \text{ for all } i \in [n],
\]

with probability at least \( 1 - \delta \) for all \( i \in [n] \) simultaneously.
Evidently, this result implies that if we can determine a suitable bound for \( \|e_i^T A(I - QQ^T)\|^2 \) then we automatically get a proper bound for the element-wise approximations of Algorithm 1. If \( A \) has a fast decaying spectrum and \( Q \) captures the dominant eigenspace of \( A \) we can expect that our approximations are very accurate, even for small \( l \). For the general case, however, the following Lemma 3 as well as the optimality of the JL lemma \([31]\) already hint that this is not possible (see also Appendix II, Limitations of low-rank projections).

**Lemma 3.** Let \( A \in \mathbb{R}^{n \times d} \). For \( 1 \leq k < d \), it holds that \( \|e_i^T (A - A_k)\|^2 \leq \sigma_{k+1}^2(A) \leq \frac{\|A_k\|^2}{k} \).

**Proof.** Clearly, \( \|e_i^T (A - A_k)\|^2 \leq \max_{\|x\|=1} \|x^T (A - A_k)\|^2 = \sigma_{k+1}^2(A) \). For the second part we have that \( \sigma_{k+1}^2(A) \leq \frac{1}{k} \sum_{i=1}^k \sigma_i^2(A) = \frac{\|A_k\|^2}{k} \).

### 2.1 Projecting rows on randomly chosen subspaces

To proceed further with the analysis, we show some length-preserving properties of the orthogonal projector \( QQ^T \), which is an orthogonal projector on a random subspace as obtained in line 3 of Algorithm 1. Note that Corollary 1 is stated for constant factor approximations. Here we provide a brief proof sketch. For the main result we refer to Lemma 8 in Appendix III.

**Corollary 1** (Projection on rowspace(\(SA^T A\))). *(Proof in the Appendix)* Let \( \delta \in (0, \frac{1}{2}) \), \( A_k = A - A_k \), and \( S \) be such that

(i) \( S \sim D \), where \( D \) is an \((1/3, \delta)\)-OSE for any fixed \( k \)-dimensional subspace;

(ii) \( S \) is a \((1/3, \delta, 2n)\)-JLT.

If \( Q \) is a matrix that forms an orthonormal basis for rowspace(\(SA^T A\)), then, with probability at least \( 1 - 2\delta \), for all \( i \in [n] \) simultaneously, it holds that

\[
\|e_i^T A(I - QQ^T)\|^2 \leq \|e_i^T (\tilde{A}_k)\|^2 \leq \|e_i^T A_k\| + 2 \sum_{\|e_i^T A_k\|} \|e_i^T A_k\| \leq 2\|e_i^T A\| \|e_i^T \tilde{A}_k\|.
\]

**Proof sketch.** To prove the result it suffices to find a projector within rowspace(\(SA^T A\)) with the desired properties. To do this, we consider the matrix \( \Pi_k = V_k(SV_k^2 \Sigma_k^2)SA^T A \), where \( V_k, \Sigma_k \) originate from the SVD of \( A_k = U_k \Sigma_k V_k^T \). Clearly, this \( \Pi_k \) is a rank-\( k \) matrix within rowspace(\(SA^T A\)). After some algebra, the problem reduces to get a bound for the quantities \( \|e_i^T A \Sigma_k^2 V_k^T A \Sigma_k^2 V_k^T A \Sigma_k^2 V_k^T A \| \), for all \( i \in [n] \), where the existence of \( \Sigma^{-1} \) is guaranteed due to the \((1/3, \delta)\)-OSE property of \( S \). For each \( i \), this quantity is the absolute value of the inner product \( \langle S(V_k \Sigma_k^{-1} V_k^T A \Sigma_k^{-1} V_k^T A) e_i, S(V_k \Sigma_k^{-1} V_k^T A \Sigma_k^{-1} V_k^T A) e_i \rangle \), which can be written in a simplified form as \( \langle S \Sigma_k^{-1} S \Sigma_k^{-1} V_k^T A \rangle e_i \). Therefore, we use an \((1/3, \delta, 2n)\)-JLT to bound the inner products between the vectors of the set

\[
V = \{ e_i^T A \Sigma_k^2 V_k^T e_i \mid e_i \in [n] \} \cup \{ e_i^T \Sigma_k^2 V_k^T A \mid e_i \in [n] \}.
\]

Having all pieces in-place, we can finally bound the element-wise approximations of Algorithm 1.

**Theorem 1.** *(Proof in the Appendix)* Let \( A \in \mathbb{R}^{n \times d} \) and \( n \geq d \). If we use Algorithm 1 with \( m \) matrix-vector queries to estimate the Euclidean lengths of the rows of \( A \), then there exists a global constant \( C \) such that, as long as

(i) \( m \geq l \geq O(\log(n/\delta)) \), such that \( G \) satisfies Lemma 1 and \( S \) forms an \((1/3, \delta, 2n)\)-JLT,

(ii) \( m \geq O(k + \log(1/\delta)) \), such that \( S \) forms an \((1/3, \delta)\)-OSE for a \( k \)-dimensional subspace,

then it holds that

\[
\|\tilde{x}_i - \|e_i^T A\|^2 \leq C \sqrt{\frac{\log(\frac{2}{l})}{l}} \|e_i^T (A - A_k)\| \|e_i^T A\| \leq C \sqrt{\frac{\log(\frac{2}{l})}{l}} \|A_k\|_F \|e_i^T A\|,
\]

for all \( i \in [n] \) with probability at least \( 1 - 3\delta \).
**Discussion.** We can investigate the bounds for special matrix cases. We highlight the approximation power of Algorithm 1 for matrices with decaying spectrum. For matrices with a linear decay it suffices to take \( m \gtrsim O(\epsilon^{-1} \sqrt{\log(n/\delta)}) \) queries to achieve an almost \( \epsilon \)-accuracy. For matrices with exponential decay we can use as few as \( m \gtrsim O(\log(1/\epsilon)) \) matrix-vector queries. For matrices with no decay, e.g., for orthogonal projector matrices, Lemma 2 already guarantees that Algorithm 1 provides at least as accurate element-wise approximations as standard JL projections. We recall once more that the JL lemma is optimal in the general case [31], therefore, improvements can only be derived for special cases, like the ones considered here.

### 2.2 Frobenius norm bounds

Due to the tightness of Lemma 3, which is crucial for the element-wise bounds, it is highly unlikely that low-rank projection-based methods can generally achieve better element-wise approximations. However, if we carefully examine the total, Frobenius norm-wise error, we can in fact obtain a true \( \epsilon \)-relative error approximation. This cannot be done by “simply” adding together all element-wise bounds, i.e., we must use a different “collective” approach. This result also makes the element-wise bounds more appealing: even if there remain few outliers that violate the element-wise constraints, the total error is still very small. We note that this is a quadratic improvement over the norm-wise error of standard JL projections.

**Theorem 2.** (Proof in the Appendix) In Algorithm 1, for some absolute constants \( c, C \), if \( l > c \log(1/\delta) \), it holds that

\[
\| \hat{X} - A \|_F^2 \leq C \sqrt{\frac{\log(\omega)}{l \delta} } \| A \|_F^2,
\]

where \( \hat{X} \) is the sum of the returned approximations. For \( l = k = O\left( \frac{\sqrt{\log(\frac{1}{\delta})}}{\epsilon} \right) \), where \( \epsilon \in (0,1/2) \), setting \( m \gtrsim O(k/\delta + \log(\frac{1}{\delta})) \), it follows that

\[
\| \hat{X} - A \|_F^2 \leq \epsilon \| A \|_F^2.
\]

### 2.3 Complexity

The complexity of Algorithm 1 is as follows. In the first step two matrices \( S \) and \( G \) must be generated with \( d \times m \) random elements each. Hence, \( O(dm) \) calls to a random number generator are required. In the second step, the products \( A^\top (AS) \) and \( A^\top (AG) \) can be both computed in \( O(T_{MM}(A,m) + T_{MM}(A^\top,m)) \). Next we need to create an orthonormal basis for \( A^\top AS \) which has size \( d \times m \). This can be done with a standard Householder QR or another orthogonal factorization in \( O(dm^2) \) [25, Chapter 5]. The complexity of this operation can be improved using fast matrix multiplication primitives [19]. The product \( AQ \) costs \( O(T_{MM}(A,m)) \). We then have to compute \( \tilde{A}(Q^\top G) \), which takes \( O(dm^2) \) or \( O(dm \omega^{-1}) \) to first obtain \( Q^\top G \) and then the same cost to get \( \tilde{A}(Q^\top G) \). Finally, for the last step the squared row norms of \( 2n \) vectors, the rows of \( \tilde{A} \), and the rows of \( \tilde{\Delta} \), are needed. For each row of \( A \) and \( \tilde{\Delta} \) the cost of computing the squared Euclidean norm is \( O(m) \), therefore the cost for the last step is \( O(nm) \). Summing up, the total cost of Algorithm 1 is \( O(dm^2 + T_{MM}(A,m) + nm) \).

### 3 Euclidean distances

In many applications it is desired to find an approximate isometry for a set of data points. Let \( A \in \mathbb{R}^{n \times d} \) be a matrix whose rows define these \( d \)-dimensional data points. Assume we are interested to estimate all the \( \binom{d}{2} \) distances between the rows of \( A \). Let \( B \) be a matrix with size \( \binom{n}{2} \times n \) and each row of \( B \) is equal to the vector \( (e_i - e_j)^\top \) for some \( i, j \in [n] \). Each row \( (e_i - e_j)^\top \) of \( B \), when multiplied with \( A \), gives the difference vector \( e_i^\top A - e_j^\top A \). Therefore, to estimate the Euclidean distances between the rows of \( A \), it is sufficient to estimate the Euclidean lengths of the rows of the matrix \( BA \). In Algorithm 2 we describe this procedure for a general “incidence matrix” \( B \), e.g., when one wants to estimate only a subset of the pairwise distances. Since \( B \) has in general more rows than \( A \), the matrix multiplications must be computed in the correct order to minimize their complexity.

\footnote{Note that \( B \) is nothing more than the edge incidence matrix of a complete graph.}
We next consider the problem of approximating the leverage scores of a tall-and-skinny matrix. The algorithm is as follows. O(dm) operations are needed to generate $G$ and $S$. The product $\tilde{S} = A^T B^T BAS$ is evaluated in three steps. We first compute $AS$ in $O(T_{MM}(A, m))$, then $B(AS)$ and $B^T(BAS)$ in $O(nm)$, and finally $A^T(B^T BAS)$ in $O(T_{MM}(A^T, m))$. The intermediate products can be calculated in batches to save memory. The QR factorization of $\tilde{S}$ requires $O(dm^2)$. The products $\tilde{A} = AQ$ and $C = AG$ both require $O(T_{MM}(A, m))$, whereas the product $Q^T G$ can be performed in $O(dm^2)$. Accordingly, the product $\tilde{A}(Q^T G)$ needs $O(tm^2)$ and $C - \tilde{A}(Q^T G)$ $O(tm^2)$. In the last step each row norm costs $O(m)$ operations, resulting in $O(nm)^2$. The total complexity of Algorithm 2 is therefore

$$O\left(T_{MM}(A, m) + T_{MM}(A^T, m) + nm + dm^2 + tdm\right).$$

4 Statistical leverage scores

We next consider the problem of approximating the leverage scores of a tall-and-skinny matrix. The leverage scores of the rows of $A$ can be found in the diagonal of the orthogonal projector matrix $P = AA^T = UU^T$, where $U$ is any orthonormal basis for $\text{range}(A)$. Specifically, the leverage score $\theta_i$ of the $i$-th row of $A$ is equal to all the following quantities

$$\theta_i = \|e_i^T AA^T\|^2 = e_i^T AA^T e_i = e_i^T U^T U e_i = \|e_i^T U\|^2.$$

It is known that the leverage scores of a $n \times d$ matrix $A$ with $\text{rank}(A) = r \leq d$ sum to $r$: $\sum_{i=1}^n \theta_i = r$. Leverage scores are important in outlier detection, graph sparsification, and numerical linear algebra. We consider the general case where $U$ is not explicitly available, and we only have access to $A$.

To simplify the analysis, we assume that the matrix $A$ has full column rank. The true rank $r$ of $A$ (or the numerical rank, if $A$ is approximately low-rank) as well as a corresponding set of $r$ linearly independent columns of $A$ can be computed in $O(\text{nnz}(A) + d^3/(\epsilon^2 \delta))$, with provable approximation guarantees for the leverage scores of the selected column subset. See sections 4 and 5 of [41] for details and [8, 12, 13] for related algorithms and lower bounds.

To use Algorithm 1 to estimate leverage scores, we first need a linear operator that computes $AA^Tv$, for an arbitrary vector $v$. Since evaluating $(A^T A)$ in order to compute its pseudoinverse and ultimately the orthogonal projector $AA^T = A(A^T A)^{-1} A^T$ is expensive, we opt for a fast approximate operator. For this we can use standard techniques from the literature. One of the first approximation algorithms for tall-and-skinny leverage scores was proposed in [21]. In [41] it was shown that this algorithm is only efficient for dense matrices, or more specifically for matrices with at least $\omega(\log n)$ nonzeros per row. Given $\tilde{A} \in \mathbb{R}^{n \times d}$ with $n \gg d$ and $\omega(\log n)$ nonzeros per row, the idea consists of approximating the leverage scores of the rows of $A$ with the squared Euclidean row norms of the matrix

$$A(\Pi_1 A)^\dagger \Pi_2.$$
Here, \( \Pi_1 \) is a subspace embedding for \( \text{range}(A) \) and \( \Pi_2 \) is an \( \epsilon \)-JLT. It can be proved that \((\Pi_1 A)^\dagger\) is in fact an approximate “orthogonalizer” for \( A \), a property that we can leverage in our algorithm. Specifically, we apply Algorithm 1 to approximate the Euclidean row norms of \( \tilde{A}(\Pi_1 A)^\dagger \), instead of multiplying with \( \Pi_2 \). This procedure is described in Algorithm 3.

**Algorithm 3.** Adaptive Leverage Scores Estimation

```
\textbf{Input:} A \in \mathbb{R}^{n \times d}, with n \gg d and \omega(\log n) nonzeros per row, positive integer m < d.
\textbf{Output:} Approximate leverage scores \( \hat{\theta}_i \approx \|e_i^T A A^\dagger\|^2, i \in [n] \).

# Step 1: Construct approximate pseudoinverse operator
1: Construct \( \Pi_1 \), an \((\epsilon_1, \delta)-\text{OSE}\) for \( \text{range}(A) \).
2: Compute \( R \) from a QR factorization of \( \Pi_1 A \), i.e., \( \Pi_1 A = QR \) and use \( R^{-1} \) as a substitute for \((\Pi_1 A)^\dagger\).

# Step 2: Low-rank approximation
3: Construct two random matrices \( S, G \in \mathbb{R}^{d \times m} \) with i.i.d. elements from \( N(0, 1) \). \( \triangleright O(dm) \)
4: Compute the product \( \tilde{S} = R^{-T}(A^\dagger (A R^{-1} S))) \). \( \triangleright O(T_{MM}(A, m)) \)
5: Compute an orthonormal basis \( Q \in \mathbb{R}^{d \times m} \) for \( \text{range}(\tilde{S}) \) (e.g., via QR). \( \triangleright O(dm^2) \)

# Step 3: Project and compute row norms
6: Compute \( \tilde{A} = A R^{-1} Q \) and \( C = A R^{-1} G \). \( \triangleright O(T_{MM}(A, m)) \)
7: Compute \( \Delta = A (I - Q G^\top) G = C - A (Q G^\top) \). \( \triangleright O(dm^2) \)
8: return Alg3\((A, i) = \hat{\theta}_i = \| (e_i^T \tilde{A}) \|^2 + \| (e_i^T \tilde{B}) \Delta \|^2 \), for all \( i \in [n] \). \( \triangleright O(nm) \)
```

The following theorem gives approximation bounds for the leverage scores returned by Algorithm 3.

**Theorem 3.** Let \( A \in \mathbb{R}^{n \times d} \), \( \theta_i = \|e_i^T A A^\dagger\|^2 \) and \( \hat{\theta}_i \) the values returned by Algorithm 3. The following hold:

\[
|\hat{\theta}_i - \theta_i| \leq (\epsilon_1 + \sqrt{\epsilon_2})\theta_i, \quad \text{and} \quad \left| \sum_{i=1}^n \hat{\theta}_i - d \right| \leq (\epsilon_1 + \epsilon_2)d.
\]

**Proof.** Let \( \hat{\theta}_i = \|e_i^T A (\Pi_1 A)^\dagger\|^2 \), so that

\[
|\hat{\theta}_i - \theta_i| = |\hat{\theta}_i - \hat{\theta}_i + \hat{\theta}_i - \theta_i| \leq |\hat{\theta}_i - \hat{\theta}_i| + |\hat{\theta}_i - \theta_i|.
\]

From [21, Lemma 9] it follows that \( |\hat{\theta}_i - \theta_i| \leq \frac{\epsilon_1}{1 - \epsilon_1} \theta_i \). Subsequently, \( \hat{\theta}_i \leq (1 + \epsilon_1) \theta_i = \frac{1}{1 - \epsilon_1} \theta_i \).

From Theorem 1 we recall that for appropriate \( m, l, k \),

\[
|\hat{\theta}_i - \theta_i| \leq \sqrt{\epsilon_2} \hat{\theta}_i \leq \frac{\sqrt{\epsilon_2}}{1 - \epsilon_1} \theta_i.
\]

Combining all these observations we find that

\[
|\hat{\theta}_i - \theta_i| \leq |\hat{\theta}_i - \hat{\theta}_i| + |\hat{\theta}_i - \theta_i| \leq \frac{\epsilon_1 + \sqrt{\epsilon_2}}{1 - \epsilon_1} \theta_i \leq 2(\epsilon_1 + \sqrt{\epsilon_2}) \theta_i.
\]

Rescaling \( \epsilon_1 \) and \( \epsilon_2 \) gives the element-wise bounds. For the Frobenius norm bounds we can use similar arguments in combination with Theorem 2. \( \square \)

**Complexity and choice of \( \epsilon_1, \epsilon_2 \).** The complexity of Algorithm 3 can be split into two parts: (i) the complexity of obtaining an \( \epsilon_1 \)-approximate orthonormal basis for \( A \), and (ii) the complexity of estimating the row norms of this basis. The complexity of the former has been heavily studied in the literature and depends on the choice of the subspace embedding. For very tall-and-skinny matrices, an efficient construction is to use a combination of a CountSketch [15, 35], a Subsampled Randomized Hadamard Transform (SRHT) [43] and a Gaussian subspace embedding; see e.g. [15]. This provides a sketch \( \Pi_1 A \) with dimension \( O(d/\epsilon^2) \times d \) in \( T(\Pi_1 A) \) time. Computing the QR factorization of the sketch requires \( O(d^3/\epsilon^2) \) to obtain \( R \). Since \( R \) is upper triangular, the computation of \( R^{-1} G \) and \( R^{-1} Q \) both take \( O(d^2 m) \). The products \( A R^{-1} Q \) and \( A R^{-1} G \) cost \( O(T_{MM}(A, m)) \) each. The last step takes \( O(nm) \). The total complexity is

\[
O(T(\Pi_1 A) + dm^2/\epsilon^2 + T_{MM}(A, m) + nm).
\]
We proposed an adaptive algorithm to estimate the Euclidean row norms of a matrix $A$. We finally constructed the symmetric matrix $Q = \Lambda S G$, which are based on results from [14], or the Nyström++ of [37].

As future work, several directions can be envisioned. Most prominently, it would be interesting to determine whether the studied techniques can be used to improve Oblivious Subspace Embeddings [40, 44]. Such improvements would have an immediate impact in many problems in NLA, e.g. least squares regression, low-rank approximations and column subset selection. Two other relevant topics concern (a) the possibility to derive lower bounds similar to [34] for Euclidean row norms estimation and (b) to make the algorithms non-adaptive, like the non-adaptive versions of Hutch++ [28, 34] which are based on results from [14], or the Nyström++ of [37].

5 Numerical experiments

Algorithm 1 was implemented in Python using NumPy. We conducted experiments to verify the approximation guarantees and the convergence improvements against standard Gaussian random projections. Following [34], we generated synthetic matrices with decay in the spectrum. Specifically, $d \times d$ matrices $A$, with $d = 5000$, were created as follows. We drew a random orthogonal $d \times d$ matrix $Q$. We then fixed a diagonal $d \times d$ matrix $\Lambda$ which defines the eigenvalues of the matrix. Each element $\Lambda_{ii}$, $i \in [d]$ is set to $i^{-c}$ for a given $c \geq 0$. The larger the $c$, the faster the spectral decay.

We finally constructed the symmetric $A = QAQ^T$ which were used in the numerical experiments. Following [34], we applied four different decay factors, specifically $c = \{0.5, 1, 1.5, 2\}$.

The approximation errors of standard JL projections versus Algorithm 1 are compared in Figure 1. We plot the approximation errors of both methods as the number of samples increases. We plot two types of errors, the maximum element-wise and the Frobenius norm-wise errors

$$\max_i |\tilde{x}_i - \|e_i^\top A\|^2| \quad \text{and} \quad \frac{\|\tilde{X} - \|A\|^2_F\|}{\|A\|^2_F},$$

where $\tilde{x}_i$ are the approximated row norms and $\tilde{X}$ is their sum returned by either Algorithm 1 or standard JL projections. The exact same number of matrix vector queries is used in both methods. Standard JL projections involve only one random matrix $G$, which is multiplies $A$ from the right. $G$ has size $d \times m$, $m$ being the number of samples. In Algorithm 1, on the other hand, $A$ is multiplied four times with a matrix from the right. Therefore, we set $G$, $S$, and $Q$ in Algorithm 1 to have size $d \times m/4$, so that both algorithms are tested with the same number of matrix-vector products. In each plot we illustrate the mean error over 10 independent runs and the standard deviation. Standard JL approximations perform marginally better than Algorithm 1 only for the element-wise errors and only for the matrix with very slow decay. In all other cases, Algorithm 1 performs significantly better.

6 Conclusion

We proposed an adaptive algorithm to estimate the Euclidean row norms of a matrix $A$. This algorithm improves standard Johnson-Lindenstrauss estimators in the following aspects: (i) Quadratically less matrix-vector queries are required to achieve the same Frobenius norm-wise accuracy for all matrices; (ii) Asymptotically less matrix-vector queries are needed to achieve the same element-wise accuracy for matrices with decaying spectrum; (iii) At least as accurate element-wise approximations as standard JL are achieved for worst-case input matrices, that is, for matrices with flat spectrum. We also showed how these results can be applied to other important problems, specifically to estimate Euclidean distances between data points, which is related to the fundamental concept of approximate isometries that has many applications in data science, as well as for statistical leverage scores estimations, which are ubiquitous quantities not only in data science and statistics, but also in numerical linear algebra and spectral graph theory.

As future work, several directions can be envisioned. Most prominently, it would be interesting to determine whether the studied techniques can be used to improve Oblivious Subspace Embeddings [40, 44]. Such improvements would have an immediate impact in many problems in NLA, e.g. least squares regression, low-rank approximations and column subset selection. Two other relevant topics concern (a) the possibility to derive lower bounds similar to [34] for Euclidean row norms estimation and (b) to make the algorithms non-adaptive, like the non-adaptive versions of Hutch++ [28, 34] which are based on results from [14], or the Nyström++ of [37].
(a) Very slow eigenvalue decay \((c = 0.5)\)

(b) Slow eigenvalue decay \((c = 1.0)\)

(c) Moderate eigenvalue decay \((c = 1.5)\)

(d) Fast eigenvalue decay \((c = 2.0)\)

Figure 1: Comparison between the element-wise (dashed curves with “x” marker) and norm-wise (solid curves with “star” marker) relative errors of Algorithm 1 (blue) and standard Gaussian random projections (red) versus number of matrix-vector multiplication queries (x-axis) ran on random matrices with power law spectra. The mean relative error of the approximation averaged over 10 independent runs is plotted. The upper and lower bounds around each curve represent the standard deviation. As expected, for matrices with a very slow decay standard JL projections perform marginally better with respect to the element-wise errors, but Algorithm 1 performs significantly better for all other cases.

Acknowledgements

The authors would like to thank Cameron Musco for helpful comments.

References

[1] Dimitris Achlioptas. Database-friendly random projections: Johnson-Lindenstrauss with binary coins. *Journal of computer and System Sciences*, 66(4):671–687, 2003.

[2] Nir Ailon and Bernard Chazelle. The fast Johnson-Lindenstrauss transform and approximate nearest neighbors. *SIAM J. Comput.*, 39(1):302–322, 2009.

[3] Nir Ailon and Edo Liberty. Fast dimension reduction using rademacher series on dual bch codes. *Discrete & Computational Geometry*, 42(4):615–630, 2009.

[4] Josh Alman and Virginia Vassilevska Williams. A refined laser method and faster matrix multiplication. In Proc. 2021 ACM-SIAM Symposium on Discrete Algorithms, pages 522–539. SIAM, 2021.

[5] Rosa I Arriaga and Santosh Vempala. An algorithmic theory of learning: Robust concepts and random projection. *Machine learning*, 63(2):161–182, 2006.
[6] Haim Avron. Counting triangles in large graphs using randomized matrix trace estimation. In *Workshop on Large-scale Data Mining: Theory and Applications*, volume 10, pages 10–9, 2010.

[7] Haim Avron and Sivan Toledo. Randomized algorithms for estimating the trace of an implicit symmetric positive semi-definite matrix. *JACM*, 58(2):1–34, 2011.

[8] Maria-Florina Balcan, Yi Li, David P Woodruff, and Hongyang Zhang. Testing matrix rank, optimally. In *Proc. 30th ACM-SIAM Symposium on Discrete Algorithms*, pages 727–746. SIAM, 2019.

[9] Robert A Baston and Yuji Nakatsukasa. Stochastic diagonal estimation: probabilistic bounds and an improved algorithm. *arXiv preprint arXiv:2201.10684*, 2022.

[10] Kai Bergermann and Martin Stoll. Fast computation of matrix function-based centrality measures for layer-coupled multiplex networks. *Physical Review E*, 105(3):034305, 2022.

[11] Christos Boutsidis, Anastasios Zouzias, and Petros Drineas. Random projections for k-means clustering. *Advances in Neural Information Processing Systems*, 23, 2010.

[12] Nadiia Chepurko, Kenneth L Clarkson, Praneeth Kacham, and David P Woodruff. Near-optimal algorithms for linear algebra in the current matrix multiplication time. In *Proc. 2022 ACM-SIAM Symposium on Discrete Algorithms*, pages 3043–3068. SIAM, 2022.

[13] Ho Yee Cheung, Tsz Chiu Kwok, and Lap Chi Lau. Fast matrix rank algorithms and applications. *JACM*, 60(5):1–25, 2013.

[14] Kenneth L Clarkson and David P Woodruff. Numerical linear algebra in the streaming model. In *Proc. 41st ACM Symposium on Theory of Computing*, pages 205–214, 2009.

[15] Kenneth L Clarkson and David P Woodruff. Low-rank approximation and regression in input sparsity time. *JACM*, 63(6):1–45, 2017.

[16] Ernesto Estrada and Naomichi Hatano. Communicability in complex networks. *Physical Review E*, 77(3):036111, 2008.

[17] Alex Gittens and Michael W Mahoney. Revisiting the Nyström method for improved large-scale machine learning. *JMLR*, 17(1):3977–4041, 2016.

[18] G.H. Golub and C.F. Van Loan. *Matrix Computations*. Johns Hopkins Studies in the Mathematical Sciences. Johns Hopkins University Press, 2013.
[26] Eric Hallman, Ilse CF Ipsen, and Arvind Saibaba. Monte Carlo methods for estimating the diagonal of a real symmetric matrix. *arXiv preprint arXiv:2202.02887*, 2022.

[27] Michael F Hutchinson. A stochastic estimator of the trace of the influence matrix for laplacian smoothing splines. *Communications in Statistics-Simulation and Computation*, 18(3):1059–1076, 1989.

[28] Shuli Jiang, Hai Pham, David Woodruff, and Richard Zhang. Optimal sketching for trace estimation. *Advances in Neural Information Processing Systems*, 34, 2021.

[29] William B Johnson and Joram Lindenstrauss. Extensions of Lipschitz mappings into a Hilbert space. *Contemp. Math.*, 26(1):189–206, 1984.

[30] Daniel M. Kane and Jelani Nelson. Sparsifying Johnson-Lindenstrauss Transforms. *JACM*, 61(1):1–23, January 2014.

[31] Kasper Green Larsen and Jelani Nelson. Optimality of the Johnson-Lindenstrauss lemma. In *58th IEEE Symposium on Foundations of Computer Science*, pages 633–638. IEEE, 2017.

[32] Ping Li, Trevor J Hastie, and Kenneth W Church. Very sparse random projections. In *Proc. 12th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*, pages 287–296, 2006.

[33] Michael W. Mahoney. Randomized algorithms for matrices and data. *Foundations and Trends® in Machine Learning*, 3(2):123–224, 2011.

[34] Raphael A. Meyer, Cameron Musco, Christopher Musco, and David P. Woodruff. Hutch++: Optimal stochastic trace estimation. In *Symposium on Simplicity in Algorithms*, pages 142–155. SIAM, January 2021.

[35] Jelani Nelson and Huy L Nguyên. Osnap: Faster numerical linear algebra algorithms via sparser subspace embeddings. In *54th IEEE Symposium on Foundations of Computer Science*, pages 117–126. IEEE, 2013.

[36] Mark EJ Newman. A measure of betweenness centrality based on random walks. *Social networks*, 27(1):39–54, 2005.

[37] David Persson, Alice Cortinovis, and Daniel Kressner. Improved variants of the Hutch++ algorithm for trace estimation. *SIAM J. Matrix Anal. Appl.*, 43(3):1162–1185, 2022.

[38] Mert Pilanci and Martin J Wainwright. Newton sketch: A near linear-time optimization algorithm with linear-quadratic convergence. *SIAM J. Optim.*, 27(1):205–245, 2017.

[39] Farbod Roosta-Khorasani and Uri Ascher. Improved bounds on sample size for implicit matrix trace estimators. *Foundations of Computational Mathematics*, 15(5):1187–1212, 2015.

[40] Tamas Sarlos. Improved approximation algorithms for large matrices via random projections. In *47th IEEE Symposium on Foundations of Computer Science*, pages 143–152. IEEE, 2006.

[41] Aleksandros Sobczyk and Efstratios Gallopoulos. Estimating leverage scores via rank revealing methods and randomization. *SIAM J. Matrix Anal. Appl.*, 42(3):1199–1228, 2021.

[42] Daniel A Spielman and Nikhil Srivastava. Graph sparsification by effective resistances. *SIAM J. Comput.*, 40(6):1913–1926, 2011.

[43] Joel A Tropp. Improved analysis of the subsampled randomized hadamard transform. *Advances in Adaptive Data Analysis*, 3(01n02):115–126, 2011.

[44] David P. Woodruff. Sketching as a tool for numerical linear algebra. *Foundations and Trends® in Theoretical Computer Science*, 10(1–2):1–157, 2014.
Checklist

1. For all authors...
   (a) Do the main claims made in the abstract and introduction accurately reflect the paper’s contributions and scope? [Yes]
   (b) Did you describe the limitations of your work? [Yes] See for example Section II in the Appendix (which is also mentioned in the main text), where we describe why our methods cannot achieve true element-wise $\epsilon$-approximations.
   (c) Did you discuss any potential negative societal impacts of your work? [N/A] This work is more related to the mathematical foundations of AI.
   (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]

2. If you are including theoretical results...
   (a) Did you state the full set of assumptions of all theoretical results? [Yes] We always state what the inputs of our algorithms are expected to be, what sizes or properties should the matrices have, etc.
   (b) Did you include complete proofs of all theoretical results? [Yes] Short proofs were left in the main text. Longer proofs were placed in the Appendix. All new Lemmas, Theorems and Corollaries have been rigorously proved. All imported theoretical results have been clearly cited.

3. If you ran experiments...
   (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [No] No because the code is proprietary.
   (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [N/A] We do not perform training.
   (c) Did you report error bars (e.g., with respect to the random seed after running experiments multiple times)? [Yes] See Section 5
   (d) Did you include the total amount of compute and the type of resources used (e.g., type of GPUs, internal cluster, or cloud provider)? [No] Our small scale indicative experiments were ran on a small laptop.

4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets...
   (a) If your work uses existing assets, did you cite the creators? [N/A] We did not use any external assets.
   (b) Did you mention the license of the assets? [N/A] We did not use any external assets.
   (c) Did you include any new assets either in the supplemental material or as a URL? [N/A] We did not use any external assets.
   (d) Did you discuss whether and how consent was obtained from people whose data you’re using/curating? [N/A] We did not use any external assets.
   (e) Did you discuss whether the data you are using/curating contains personally identifiable information or offensive content? [N/A] We did not use any external assets.

5. If you used crowdsourcing or conducted research with human subjects...
   (a) Did you include the full text of instructions given to participants and screenshots, if applicable? [N/A] We did not use crowdsourcing or conducted research with human subjects.
   (b) Did you describe any potential participant risks, with links to Institutional Review Board (IRB) approvals, if applicable? [N/A] We did not use crowdsourcing or conducted research with human subjects.
   (c) Did you include the estimated hourly wage paid to participants and the total amount spent on participant compensation? [N/A] We did not use crowdsourcing or conducted research with human subjects.