Efficient Anomaly Detection via Matrix Sketching

Vatsal Sharan
Stanford University*
vsharan@stanford.edu

Parikshit Gopalan
VMware Research
pgopalan@vmware.com

Udi Wieder
VMware Research
uwieder@vmware.com

Abstract

We consider the problem of finding anomalies in high-dimensional data using popular PCA based anomaly scores. The naive algorithms for computing these scores explicitly compute the PCA of the covariance matrix which uses space quadratic in the dimensionality of the data. We give the first streaming algorithms that use space that is linear or sublinear in the dimension. We prove general results showing that *any* sketch of a matrix that satisfies a certain operator norm guarantee can be used to approximate these scores. We instantiate these results with powerful matrix sketching techniques such as Frequent Directions and random projections to derive efficient and practical algorithms for these problems, which we validate over real-world data sets. Our main technical contribution is to prove matrix perturbation inequalities for operators arising in the computation of these measures.

1 Introduction

Anomaly detection in high-dimensional numeric data is a ubiquitous problem in machine learning [1, 2]. A typical scenario is where we have a constant stream of measurements (say parameters regarding the health of machines in a data-center), and our goal is to detect any unusual behavior. An algorithm to detect anomalies in such high dimensional settings faces computational challenges: the dimension of the data matrix $\mathbf{A} \in \mathbb{R}^{n \times d}$ may be very large both in terms of the number of data points n and their dimensionality d (in the datacenter example, d could be 10^6 and $n \gg d$). The desiderata for an algorithm to be efficient in such settings are—

1. As n is too large for the data to be stored in memory, the algorithm must work in a streaming fashion where it only gets a constant number of passes over the dataset.
2. As d is also very large, the algorithm should ideally use memory linear or even sublinear in d.

In this work we focus on two popular subspace based anomaly scores: rank-k leverage scores and rank-k projection distance. The key idea behind subspace based anomaly scores is that real-world data often has most of its variance in a low-dimensional rank k subspace, where k is usually much smaller than d. In this section, we assume $k = O(1)$ for simplicity. These scores are based on identifying this principal k subspace using Principal Component Analyis (PCA) and then computing how "normal" the projection of a point on the principal k subspace looks. Rank-k leverage scores compute the normality of the projection of the point *onto* the principal k subspace using Mahalanobis distance, and rank-k projection distance compute the ℓ_2 distance of the point *from* the principal k subspace (see Fig. 1 for an illustration). These scores have found widespread use for detection of anomalies in many applications such as finding outliers in network traffic data [3, 4, 5, 6], detecting anomalous behavior in social networks [7, 8], intrusion detection in computer security [9, 10, 11], in industrial systems for fault detection [12, 13, 14] and for monitoring data-centers [15, 16].

The standard approach to compute principal k subspace based anomaly scores in a streaming setting is by computing $\mathbf{A}^T\mathbf{A}$, the $(d \times d)$ covariance matrix of the data, and then computing the top k
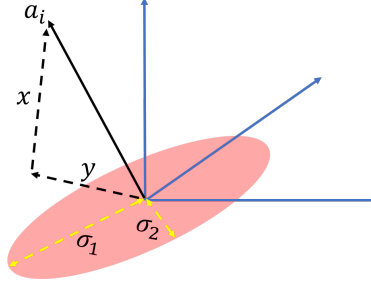

Figure 1: Illustration of subspace based anomaly scores. Here, the data lies mostly in the $k = 2$ dimensional principal subspace shaded in red. For a point $a_{(i)}$ the rank-k projection distance equals $\|x\|_2$, where x is the component of $a_{(i)}$ orthogonal to the principal subspace. The rank-k leverage score measures the *normality* of the projection y onto the principal subspace.

principal components. This takes space $O(d^2)$ and time $O(nd^2)$. The quadratic dependence on d renders this approach inefficient in high dimensions. It raises the natural question of whether better algorithms exist.

1.1 Our Results

In this work, we answer the above question affirmatively, by giving algorithms for computing these anomaly scores that require space linear and even sublinear in d. Our algorithms use popular matrix sketching techniques while their analysis uses new matrix perturbation inequalities that we prove. Briefly, a sketch of a matrix produces a much smaller matrix that preserves some desirable properties of the large matrix (formally, it is close in some suitable norm). Sketching techniques have found numerous applications to numerical linear algebra. Several efficient sketching algorithms are known in the streaming setting [17].

Pointwise guarantees with linear space: We show that any sketch $\tilde{\mathbf{A}}$ of $\mathbf{A}$ with the property that $\|\mathbf{A}^T\mathbf{A} - \tilde{\mathbf{A}}^T\tilde{\mathbf{A}}\|$ is small, can be used to additively approximate the rank-k leverage scores and rank-k projection distances for each row. By instantiating this with suitable sketches such as the Frequent Directions sketch [18], row-sampling [19] or a random projection of the columns of the input, we get a streaming algorithm that uses $O(d)$ memory and $O(nd)$ time.

A matching lower bound: Can we get such an additive approximation using memory only $o(d)$?[2] The answer is no, we show a lower bound saying that any algorithm that computes such an approximation to the rank-k leverage scores or the rank-k projection distances for all the rows of a matrix must use $\Omega(d)$ working space, using techniques from communication complexity. Hence our algorithm has near-optimal dependence on d for the task of approximating the outlier scores for every data point.

Average-case guarantees with logarithmic space: Perhaps surprisingly, we show that it is actually possible to circumvent the lower bound by relaxing the requirement that the outlier scores be preserved for each and every point to only preserving the outlier scores on average. For this we require sketches where $\|\mathbf{A}\mathbf{A}^T - \tilde{\mathbf{A}}\tilde{\mathbf{A}}^T\|$ is small: this can be achieved via random projection of the rows of the input matrix or column subsampling [19]. Using any such sketch, we give a streaming algorithm that can preserve the outlier scores for the rows up to small additive error on average, and hence preserve most outliers. The space required by this algorithm is only $\text{poly}(k)\log(d)$, and hence we get significant space savings in this setting (recall that we assume $k = O(1)$).

Technical contributions. A sketch of a matrix $\mathbf{A}$ is a significantly smaller matrix $\tilde{\mathbf{A}}$ which approximates it well in some norm, say for instance $\|\mathbf{A}^T\mathbf{A} - \tilde{\mathbf{A}}^T\tilde{\mathbf{A}}\|$ is small. We can think of such a sketch as a noisy approximation of the true matrix. In order to use such sketches for anomaly

---

[2]Note that even though each row is d dimensional an algorithm need not store the entire row in memory, and could instead perform computations as each coordinate of the row streams in.

detection, we need to understand how the noise affects the anomaly scores of the rows of the matrix. Matrix perturbation theory studies the effect of adding noise to the spectral properties of a matrix, which makes it the natural tool for us. The basic results here include Weyl's inequality [20] and Wedin's theorem [21], which respectively give such bounds for eigenvalues and eigenvectors. We use these results to derive perturbation bounds on more complex projection operators that arise while computing outlier scores, these operators involve projecting onto the top-k principal subspace, and rescaling each co-ordinate by some function of the corresponding singular values. We believe these results could be of independent interest.

Experimental results. Our results have a parameter ℓ that controls the size and the accuracy of the sketch. While our theorems imply that ℓ can be chosen independent of d, they depend polynomially on k, the desired accuracy and other parameters, and are probably pessimistic. We validate both our algorithms on real world data. In our experiments, we found that choosing ℓ to be a small multiple of k was sufficient to get good results. Our results show that one can get outcomes comparable to running full-blown SVD using sketches which are significantly smaller in memory footprint, faster to compute and easy to implement (literally a few lines of Python code).

This contributes to a line of work that aims to make SVD/PCA scale to massive datasets [22]. We give simple and practical algorithms for anomaly score computation, that give SVD-like guarantees at a significantly lower cost in terms of memory, computation and communication.

2 Notation and Setup

Given a matrix $\mathbf{A} \in \mathbb{R}^{n \times d}$, we let $a_{(i)} \in \mathbb{R}^d$ denote its ith row and $a^{(i)} \in \mathbb{R}^n$ denote its ith column. Let $\mathbf{U\Sigma V}^T$ be the SVD of $\mathbf{A}$ where $\mathbf{\Sigma} = \mathrm{diag}(\sigma_1, \dots, \sigma_d)$, for $\sigma_1 \geq \dots \geq \sigma_d > 0$. Let κ_k be the condition number of the top k subspace of $\mathbf{A}$, defined as $\kappa_k = \sigma_1^2/\sigma_k^2$. We consider all vectors as column vectors (that includes $a_{(i)}$). We denote by $\|\mathbf{A}\|_F$ the Frobenius norm of the matrix, and by $\|\mathbf{A}\|$ the operator norm (which is equal to the largest singular value). Subspace based measures of anomalies have their origins in a classical metric in statistics known as Mahalanobis distance, denoted by $L(i)$ and defined as,

$$L(i) = \sum_{j=1}^{d} (a_{(i)}^T v^{(j)})^2 / \sigma_j^2, \tag{1}$$

where $a_{(i)}$ and $v^{(i)}$ are the ith row of $\mathbf{A}$ and i^{th} column of $\mathbf{V}$ respectively. $L(i)$ is also known as the *leverage score* [23, 24]. If the data is drawn from a multivariate Gaussian distribution, then $L(i)$ is proportional to the negative log likelihood of the data point, and hence is the right anomaly metric in this case. Note that the higher leverage scores correspond to outliers in the data.

However, $L(i)$ depends on the entire spectrum of singular values and is highly sensitive to smaller singular values, whereas real world data sets often have most of their signal in the top singular values. Therefore the above sum is often limited to only the k largest singular values (for some appropriately chosen $k \ll d$) [1, 25]. This measure is called the rank k leverage score $L^k(i)$, where

$$L^k(i) = \sum_{j=1}^{k} (a_{(i)}^T v^{(j)})^2 / \sigma_j^2.$$

The rank k leverage score is concerned with the mass which lies within the principal space, but to catch anomalies that are far from the principal subspace a second measure of anomaly is the rank k *projection distance* $T^k(i)$, which is simply the distance of the data point $a_{(i)}$ to the rank k principal subspace—

$$T^k(i) = \sum_{j=k+1}^{d} (a_{(i)}^T v^{(j)})^2.$$

Assumptions. We now discuss assumptions needed for our anomaly scores to be meaningful.

(1) Separation assumption. If there is degeneracy in the spectrum of the matrix, namely that $\sigma_k^2 = \sigma_{k+1}^2$ then the k-dimensional principal subspace is not unique, and then the quantities L^k and T^k are not well defined, since their value will depend on the choice of principal subspace. This

3

suggests that we are using the *wrong* value of k, since the choice of k ought to be such that the directions orthogonal to the principal subspace have markedly less variance than those in the principal subspace. Hence we require that k is such that there is a gap in the spectrum at k.

Assumption 1. *We define a matrix* $\mathbf{A}$ *as being* (k, Δ)*-separated if* $\sigma_k^2 - \sigma_{k+1}^2 \geq \Delta \sigma_1^2$*. Our results assume that the data are* (k, Δ)*-separated for* $\Delta > 0$*.*

This assumptions manifests itself as an inverse polynomial dependence on Δ in our bounds. This dependence is probably pessimistic: in our experiments, we have found our algorithms do well on datasets which are not degenerate, but where the separation Δ is not particularly large.

(2) Approximate low-rank assumption. We assume that the top-k principal subspace captures a constant fraction (at least 0.1) of the total variance in the data, formalized as follows.

Assumption 2. *We assume the matrix* $\mathbf{A}$ *is approximately rank-k, i.e.,* $\sum_{i=1}^k \sigma_i^2 \geq (1/10) \sum_{i=1}^d \sigma_i^2$*.*

From a technical standpoint, this assumption is not strictly needed: if Assumption 2 is not true, our results still hold, but in this case they depend on the stable rank $\mathrm{sr}(\mathbf{A})$ of $\mathbf{A}$, defined as $\mathrm{sr}(\mathbf{A}) = \sum_{i=1}^d \sigma_i^2 / \sigma_1^2$ (we state these general forms of our results in the appendix).

From a practical standpoint though, this assumption captures the setting where the scores L^k and T^k, and our guarantees are most meaningful. Indeed, our experiments suggest that our algorithms work best on data sets where relatively few principal components explain most of the variance.

Setup. We work in the row-streaming model, where rows appear one after the other in time. Note that the leverage score of a row depends on the entire matrix, and hence computing the anomaly scores in the streaming model requires care, since if the rows are seen in streaming order, when row i arrives we cannot compute its leverage score without seeing the rest of the input. Indeed, 1-pass algorithms are not possible (unless they output the entire matrix of scores at the end of the pass, which clearly requires a lot of memory). Hence we will aim for 2-pass algorithms.

Note that there is a simple 2-pass algorithm which uses $O(d^2)$ memory to compute the covariance matrix in one pass, then computes its SVD, and using this computes $L^k(i)$ and $T^k(i)$ in a second pass using memory $O(dk)$. This requires $O(d^2)$ memory and $O(nd^2)$ time, and our goal would be to reduce this to linear or sublinear in d.

Another reasonable way to define leverage scores and projection distances in the streaming model is to define them with respect to only the input seen so far. We refer to this as the online scenario, and refer to these scores as the online scores. Our result for sketches which preserve row spaces also hold in this online scenario. We defer more discussion of this online scenario to the appendix, and focus here only on the scores defined with respect to the entire matrix for simplicity.

3   Guarantees for anomaly detection via sketching

Our main results say that given $\mu > 0$ and a (k, Δ)-separated matrix $\mathbf{A} \in \mathbb{R}^{n \times d}$ with top singular value σ_1, any sketch $\tilde{\mathbf{A}} \in \mathbb{R}^{\ell \times d}$ satisfying

$$\|\mathbf{A}^T \mathbf{A} - \tilde{\mathbf{A}}^T \tilde{\mathbf{A}}\| \leq \mu \sigma_1^2, \tag{2}$$

or a sketch $\tilde{\mathbf{A}} \in \mathbb{R}^{n \times \ell}$ satisfying

$$\|\mathbf{A}\mathbf{A}^T - \tilde{\mathbf{A}}\tilde{\mathbf{A}}^T\| \leq \mu \sigma_1^2, \tag{3}$$

can be used to approximate rank k leverage scores and the projection distance from the principal k-dimensional subspace. The quality of the approximation depends on μ, the separation Δ, k and the condition number κ_k of the top k subspace.[3] In order for the sketches to be useful, we also need them to be efficiently computable in a streaming fashion. We show how to use such sketches to design efficient algorithms for finding anomalies in a streaming fashion using small space and with fast running time. The actual guarantees (and the proofs) for the two cases are different and incomparable. This is to be expected as the sketch guarantees are very different in the two cases: Equation (2) can be viewed as an approximation to the covariance matrix of the row vectors, whereas Equation (3)

---

[3]The dependence on κ_k only appears for showing guarantees for rank-k leverage scores L^k in Theorem 1.

gives an approximation for the covariance matrix of the column vectors. Since the corresponding sketches can be viewed as preserving the row/column space of $\mathbf{A}$ respectively, we will refer to them as row/column space approximations.

Pointwise guarantees from row space approximations. Sketches which satisfy Equation (2) can be computed in the row streaming model using random projections of the columns, subsampling the rows of the matrix proportional to their squared lengths [19] or deterministically by using the Frequent Directions algorithm [26]. Our streaming algorithm is stated as Algorithm 1, and is very simple. In Algorithm 1, any other sketch such as subsampling the rows of the matrix or using a random projection can also be used instead of Frequent Directions.

Algorithm 1: Algorithm to approximate anomaly scores using Frequent Directions

Input: Choice of k, sketch size ℓ for Frequent Directions [26]
First Pass:
  Use Frequent Directions to compute a sketch $\tilde{\mathbf{A}} \in \mathbb{R}^{\ell \times d}$
SVD:
  Compute the top k right singular vectors of $\tilde{\mathbf{A}}^T \tilde{\mathbf{A}}$
Second Pass: *As each row $a_{(i)}$ streams in,*
  Use estimated right singular vectors to compute leverage scores and projection distances

---

We state our results here, see Section B for precise statements and general results for any sketches which satisfy the guarantee in Eq. (2). All our proofs are deferred to the appendix in the supplementary material.

Theorem 1. *Assume that $\mathbf{A}$ is (k, Δ)-separated. There exists $\ell = k^2 \cdot \mathrm{poly}(\varepsilon^{-1}, \kappa_k, \Delta)$, such that the above algorithm computes estimates $\tilde{T}^k(i)$ and $\tilde{L}^k(i)$ where*

$$|T^k(i) - \tilde{T}^k(i)| \leq \varepsilon \|a_{(i)}\|_2^2,$$

$$|L^k(i) - \tilde{L}^k(i)| \leq \varepsilon k \frac{\|a_{(i)}\|_2^2}{\|\mathbf{A}\|_F^2}.$$

The algorithm uses memory $O(d\ell)$ and has running time $O(nd\ell)$.

The key is that while ℓ depends on k and other parameters, it is independent of d. In the setting where all these parameters are constants independent of d, our memory requirement is $O(d)$, improving on the trivial $O(d^2)$ bound.

Our approximations are additive rather than multiplicative. But for anomaly detection, the candidate anomalies are ones where $L^k(i)$ or $T^k(i)$ is large, and in this regime, we argue below that our additive bounds also translate to good multiplicative approximations. The additive error in computing $L^k(i)$ is about $\varepsilon k/n$ when all the rows have roughly equal norm. Note that the average rank-k leverage score of all the rows of any matrix with n rows is k/n, hence a reasonable threshold on $L^k(i)$ to regard a point as an anomaly is when $L^k(i) \gg k/n$, so the guarantee for $L^k(i)$ in Theorem 1 preserves anomaly scores up to a small multiplicative error for candidate anomalies, and ensures that points which were not anomalies before are not mistakenly classified as anomalies. For $T^k(i)$, the additive error for row $a_{(i)}$ is $\varepsilon \|a_{(i)}\|_2^2$. Again, for points that are anomalies, $T^k(i)$ is a constant fraction of $\|a_{(i)}\|_2^2$, so this guarantee is meaningful.

Next we show that substantial savings are unlikely for any algorithm with strong pointwise guarantees: there is an $\Omega(d)$ lower bound for any approximation that lets you distinguish $L^k(i) = 1$ from $L^k(i) = \varepsilon$ for any constant ε.

Theorem 2. *Any streaming algorithm which takes a constant number of passes over the data and can compute a 0.1 error additive approximation to the rank-k leverage scores or the rank-k projection distances for all the rows of a matrix must use $\Omega(d)$ working space.*

Average-case guarantees from columns space approximations. We derive smaller space algorithms, albeit with weaker guarantees using sketches that give columns space approximations that satisfy Equation (3). Even though the sketch gives column space approximations our goal is still to

compute the row anomaly scores, so it not just a matter of working with the transpose. Many sketches are known which approximate $\mathbf{A}\mathbf{A}^T$ and satisfy Equation (3), for instance, a low-dimensional projection by a random matrix $\mathbf{R} \in \mathbb{R}^{d \times \ell}$ (e.g., each entry of $\mathbf{R}$ could be a scaled i.i.d. uniform $\{\pm 1\}$ random variable) satisfies Equation (3) for $\ell = O(k/\mu^2)$ [27].

On first glance it is unclear how such a sketch should be useful: the matrix $\tilde{\mathbf{A}}\tilde{\mathbf{A}}^T$ is an $n \times n$ matrix, and since $n \gg d$ this matrix is too expensive to store. Our streaming algorithm avoids this problem by only computing $\tilde{\mathbf{A}}^T\tilde{\mathbf{A}}$, which is an $\ell \times \ell$ matrix, and the larger matrix $\tilde{\mathbf{A}}\tilde{\mathbf{A}}^T$ is only used for the analysis. Instantiated with the sketch above, the resulting algorithm is simple to describe (although the analysis is subtle): we pick a random matrix in $\mathbf{R} \in \mathbb{R}^{d \times \ell}$ as above and return the anomaly scores for the sketch $\tilde{\mathbf{A}} = \mathbf{A}\mathbf{R}$ instead. Doing this in a streaming fashion using even the naive algorithm requires computing the small covariance matrix $\tilde{\mathbf{A}}^T\tilde{\mathbf{A}}$, which is only $O(\ell^2)$ space.

But notice that we have not accounted for the space needed to store the $(d \times \ell)$ matrix $\mathbf{R}$. This is a subtle (but mainly theoretical) concern, which can be addressed by using powerful results from the theory of pseudorandomness [28]. Constructions of pseudorandom Johnson-Lindenstrauss matrices [29, 30] imply that the matrix $\mathbf{R}$ can be pseudorandom, meaning that it has a succinct description using only $O(\log(d))$ bits, from which each entry can be efficiently computed on the fly.

Algorithm 2: Algorithm to approximate anomaly scores using random projection

Input: Choice of k, random projection matrix $\mathbf{R} \in \mathbb{R}^{d \times \ell}$
Initialization
  | Set covariance $\tilde{\mathbf{A}}^T\tilde{\mathbf{A}} \leftarrow 0$
First Pass: *As each row $a_{(i)}$ streams in,*
  | Project by $\mathbf{R}$ to get $\mathbf{R}^T a_{(i)}$
  | Update covariance $\tilde{\mathbf{A}}^T\tilde{\mathbf{A}} \leftarrow \tilde{\mathbf{A}}^T\tilde{\mathbf{A}} + (\mathbf{R}^T a_{(i)})(\mathbf{R}^T a_{(i)})^T$
SVD:
  | Compute the top k right singular vectors of $\tilde{\mathbf{A}}^T\tilde{\mathbf{A}}$
Second Pass: *As each row $a_{(i)}$ streams in,*
  | Project by $\mathbf{R}$ to get $\mathbf{R}^T a_{(i)}$
  | For each projected row, use the estimated right singular vectors to compute the leverage scores and projection distances

---

Theorem 3. *For ε sufficiently small, there exists $\ell = k^3 \cdot \mathrm{poly}(\varepsilon^{-1}, \Delta)$ such that the algorithm above produces estimates $\tilde{L}^k(i)$ and $\tilde{T}^k(i)$ in the second pass, such that with high probabilty,*

$$\sum_{i=1}^{n} |T^k(i) - \tilde{T}^k(i)| \leq \varepsilon \|\mathbf{A}\|_{\mathrm{F}}^2,$$

$$\sum_{i=1}^{n} |L^k(i) - \tilde{L}^k(i)| \leq \varepsilon \sum_{i=1}^{n} L^k(i).$$

The algorithm uses space $O(\ell^2 + \log(d)\log(k))$ and has running time $O(nd\ell)$.

This gives an average case guarantee. We note that Theorem 3 shows a new property of random projections—that on average they can preserve leverage scores and distances from the principal subspace, with the projection dimension ℓ being only $\mathrm{poly}(k, \varepsilon^{-1}, \Delta)$, independent of both n and d.

We can obtain similar guarantees as in Theorem 3 for other sketches which preserve the column space, such as sampling the columns proportional to their squared lengths [19, 31], at the price of one extra pass. Again the resulting algorithm is very simple: it maintains a carefully chosen $\ell \times \ell$ submatrix of the full $d \times d$ covariance matrix $\mathbf{A}^T\mathbf{A}$ where $\ell = O(k^3)$. We state the full algorithm in Section C.3.

4 Experimental evaluation

The aim of our experiments is to test whether our algorithms give comparable results to exact anomaly score computation based on full SVD. So in our experiments, we take the results of SVD as the

ground truth and see how close our algorithms get to it. In particular, the goal is to determine how large the parameter ℓ that determines the size of the sketch needs to be to get close to the exact scores. Our results suggest that for high dimensional data sets, it is possible to get good approximations to the exact anomaly scores even for fairly small values of ℓ (a small multiple of k), hence our worst-case theoretical bounds (which involve polynomials in k and other parameters) are on the pessimistic side.

Datasets: We ran experiments on three publicly available datasets: p53 mutants [32], Dorothea [33] and RCV1 [34], all of which are available from the UCI Machine Learning Repository, and are high dimensional ($d > 5000$). The original RCV1 dataset contains 804414 rows, we took every tenth element from it. The sizes of the datasets are listed in Table 1.

Ground Truth: To establish the ground truth, there are two parameters: the dimension k (typically between 10 and 125) and a threshold η (typically between 0.01 and 0.1). We compute the anomaly scores for this k using a full SVD, and then label the η fraction of points with the highest anomaly scores to be outliers. k is chosen by examining the explained variance of the datatset as a function of k, and η by examining the histogram of the anomaly score.

Our Algorithms: We run Algorithm 1 using random column projections in place of Frequent Directions.[4] The relevant parameter here is the projection dimension ℓ, which results in a sketch matrix of size $d \times \ell$. We run Algorithm 2 with random row projections. If the projection dimension is ℓ, the resulting sketch size is $O(\ell^2)$ for the covariance matrix. For a given ℓ, the time complexity of both algorithms is similar, however the size of the sketches are very different: $O(d\ell)$ versus $O(\ell^2)$.

Measuring accuracy: We ran experiments with a range of ℓs, in the range $(2k, 20k)$ for each dataset (hence the curves have different start/end points). The algorithm is given just the points (without labels or η) and computes anomaly scores for them. We then declare the points with the top η' fraction of scores to be anomalies, and then compute the F_1 score (defined as the harmonic mean of the precision and the recall). We choose the value of η' which maximizes the F_1 score. This measures how well the proposed algorithms can approximate the exact outlier scores. Note that in order to get both good precision and recall, η' cannot be too far from η. We report the average F_1 score over 5 runs.

For each dataset, we run both algorithms, approximate both the leverage and projection scores, and try three different values of k. For each of these settings, we run over roughly 10 values for ℓ. The results are plotted in Figs. 2, 3 and 4. Here are some takeaways from our experiments:

- Taking $\ell = Ck$ with a fairly small $C \approx 10$ suffices to get F1 scores > 0.75 in most settings.

- Algorithm 1 generally outperforms Algorithm 2 for a given value of ℓ. This should not be too surprising given that it uses much more memory, and is known to give pointwise rather than average case guarantees. However, Algorithm 2 does surprisingly well for an algorithm whose memory footprint is essentially independent of the input dimension d.

- The separation assumption (Assumption (1)) does hold to the extent that the spectrum is not degenerate, but not with a large gap. The algorithms seem fairly robust to this.

- The approximate low-rank assumption (Assumption (2)) seems to be important in practice. Our best results are for the p53 data set, where the top 10 components explain 87% of the total variance. The worst results are for the RCV1 data set, where the top 100 and 200 components explain only 15% and 25% of the total variance respectively.

Performance.   While the main focus of this work is on the streaming model and memory consumption, our algorithms offer considerable speedups even in the offline/batch setting. Our timing experiments were run using Python/Jupyter notebook on a linux VM with 8 cores and 32 Gb of RAM, the times reported are total CPU times in seconds as measured by the % time function, and are reported in Table 1. We focus on computing projection distances using SVD (the baseline), Random Column Projection (Algorithm 1) and Random Row Projection (Algorithm 2). All SVD computations use the `randomized_svd` function from `scikit.learn`. The baseline computes only the top k singular values and vectors (not the entire SVD). The results show consistent speedups between $2\times$ and $6\times$. Which algorithm is faster depends on which dimension of the input matrix is larger.

---

[4]Since the existing implementation of Frequent Directions [35] does not seem to handle sparse matrices.

Table 1: Running times for computing rank-k projection distance. Speedups between $2\times$ and $6\times$.

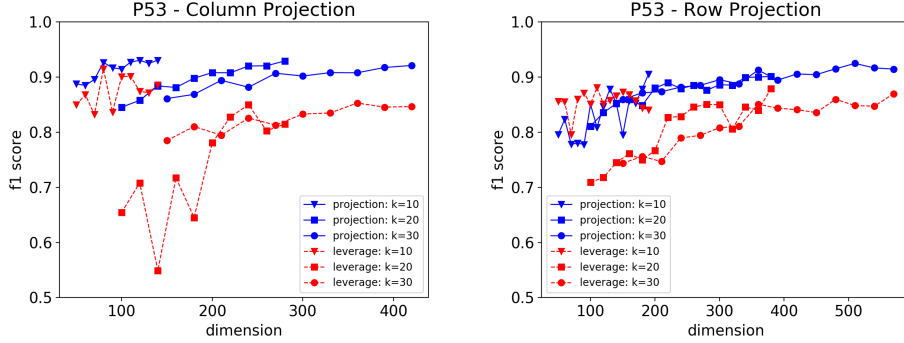| Dataset	Size ($n \times d$)	k	ℓ	SVD	Column Projection	Row Projection
p53 mutants	16772×5409	20	200	29.2s	6.88s	7.5s
Dorothea	1950×100000	20	200	17.7s	9.91s	2.58s
RCV1	80442×47236	50	500	39.6s	17.5s	20.8s

Figure 2: Results for P53 Mutants. We get F_1 score > 0.8 with $> 10\times$ space savings.

5 Related work

In most anomaly detection settings, labels are hard to come by and unsupervised learning methods are preferred: the algorithm needs to learn what the bulk of the data looks like and then detect any deviations from this. Subspace based scores are well-suited to this, but various other anomaly scores have also been proposed such as those based on approximating the density of the data [36, 37] and attribute-wise analysis [38], we refer to surveys on anomaly detection for an overview [1, 2].

Leverage scores have found numerous applications in numerical linear algebra, and hence there has been significant interest in improving the time complexity of computing them. For the problem of approximating the (full) leverage scores ($L(i)$ in Eq. (1), note that we are concerned with the rank-k leverage scores $L^k(i)$), Clarkson and Woodruff [39] and Drineas et al. [40] use sparse subspace embeddings and Fast Johnson Lindenstrauss Transforms (FJLT [41]) to compute the leverage scores using $O(nd)$ time instead of the $O(nd^2)$ time required by the baseline—but these still need $O(d^2)$ memory. With respect to projection distance, the closest work to ours is Huang and Kasiviswanathan [42] which uses Frequent Directions to approximate projection distances in $O(kd)$ space. In contrast to these approaches, our results hold both for rank-k leverage scores and projection distances, for any matrix sketching algorithm—not just FJLT or Frequent Directions—and our space requirement can be as small as $\log(d)$ for average case guarantees. However, Clarkson and Woodruff [39] and Drineas et al. [40] give multiplicative guarantees for approximating leverage scores while our guarantees for rank-k leverage scores are additive, but are nevertheless sufficient for the task of detecting anomalies.

6 Conclusion

We show that techniques from sketching can be used to derive simple and practical algorithms for computing subspace-based anomaly scores which provably approximate the true scores at a significantly lower cost in terms of time and memory. A promising direction of future work is to use them in real-world high-dimensional anomaly detection tasks.
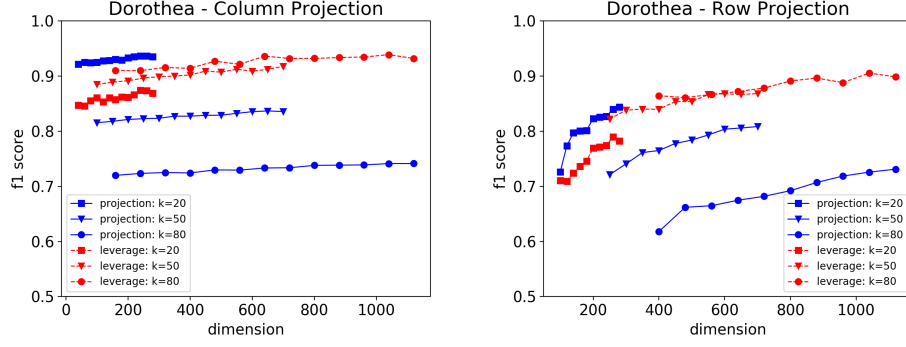
Acknowledgments

Figure 3: Results for the Dorothea dataset. Column projections give more accurate approximations, but they use more space.
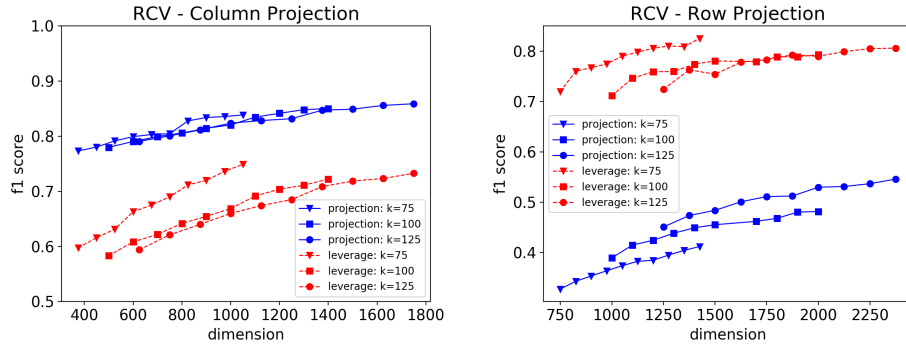

Figure 4: Results for the RCV1 dataset. Our results here are worse than for the other datasets, we hypothesize this is due to this data having less pronounced low-rank structure.

References

[1] Charu C. Aggarwal. *Outlier Analysis*. Springer Publishing Company, Incorporated, 2nd edition, 2013. ISBN 9783319475783.

[2] Varun Chandola, Arindam Banerjee, and Vipin Kumar. Anomaly detection: A survey. *ACM Comput. Surv.*, 41(3):15:1–15:58, 2009.

[3] Anukool Lakhina, Mark Crovella, and Christophe Diot. Diagnosing network-wide traffic anomalies. In *ACM SIGCOMM Computer Communication Review*, volume 34, pages 219–230. ACM, 2004.

[4] Anukool Lakhina, Mark Crovella, and Christophe Diot. Mining anomalies using traffic feature distributions. In *ACM SIGCOMM Computer Communication Review*, volume 35, pages 217–228. ACM, 2005.

[5] Ling Huang, XuanLong Nguyen, Minos Garofalakis, Joseph M Hellerstein, Michael I Jordan, Anthony D Joseph, and Nina Taft. Communication-efficient online detection of network-wide anomalies. In *INFOCOM 2007. 26th IEEE International Conference on Computer Communications. IEEE*, pages 134–142. IEEE, 2007.

[6] Ling Huang, XuanLong Nguyen, Minos Garofalakis, Michael I Jordan, Anthony Joseph, and Nina Taft. In-network pca and anomaly detection. In *Advances in Neural Information Processing Systems*, pages 617–624, 2007.

[7] Bimal Viswanath, Muhammad Ahmad Bashir, Mark Crovella, Saikat Guha, Krishna P Gummadi, Balachander Krishnamurthy, and Alan Mislove. Towards detecting anomalous user behavior in online social networks. In *USENIX Security Symposium*, pages 223–238, 2014.

[8] Rebecca Portnoff. *The Dark Net: De-Anonymization, Classification and Analysis*. PhD thesis, EECS Department, University of California, Berkeley, Mar 2018.

[9] Mei-ling Shyu, Shu-ching Chen, Kanoksri Sarinnapakorn, and Liwu Chang. A novel anomaly detection scheme based on principal component classifier. In *in Proceedings of the IEEE Foundations and New Directions of Data Mining Workshop, in conjunction with the Third IEEE International Conference on Data Mining (ICDM'03*. Citeseer, 2003.

[10] Wei Wang, Xiaohong Guan, and Xiangliang Zhang. A novel intrusion detection method based on principle component analysis in computer security. In *International Symposium on Neural Networks*, pages 657–662. Springer, 2004.

[11] Jonathan J Davis and Andrew J Clark. Data preprocessing for anomaly based network intrusion detection: A review. *Computers & Security*, 30(6-7):353–375, 2011.

[12] Leo H Chiang, Evan L Russell, and Richard D Braatz. *Fault detection and diagnosis in industrial systems*. Springer Science & Business Media, 2000.

[13] Evan L Russell, Leo H Chiang, and Richard D Braatz. Fault detection in industrial processes using canonical variate analysis and dynamic principal component analysis. *Chemometrics and intelligent laboratory systems*, 51(1):81–93, 2000.

[14] S Joe Qin. Statistical process monitoring: basics and beyond. *Journal of chemometrics*, 17(8-9): 480–502, 2003.

[15] Wei Xu, Ling Huang, Armando Fox, David Patterson, and Michael I Jordan. Detecting large-scale system problems by mining console logs. In *Proceedings of the ACM SIGOPS 22nd symposium on Operating systems principles*, pages 117–132. ACM, 2009.

[16] Haibo Mi, Huaimin Wang, Yangfan Zhou, Michael Rung-Tsong Lyu, and Hua Cai. Toward fine-grained, unsupervised, scalable performance diagnosis for production cloud computing systems. *IEEE Transactions on Parallel and Distributed Systems*, 24(6):1245–1255, 2013.

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

[18] Edo Liberty. Simple and deterministic matrix sketching. In *Proceedings of the 19th ACM SIGKDD international conference on Knowledge discovery and data mining*, pages 581–588. ACM, 2013.

[19] Petros Drineas, Ravi Kannan, and Michael W Mahoney. Fast monte carlo algorithms for matrices i: Approximating matrix multiplication. *SIAM Journal on Computing*, 36(1):132–157, 2006.

[20] Roger A Horn and Charles R Johnson. Topics in matrix analysis. corrected reprint of the 1991 original. *Cambridge Univ. Press, Cambridge*, 1:994, 1994.

[21] Per-Åke Wedin. Perturbation bounds in connection with singular value decomposition. *BIT Numerical Mathematics*, 12(1):99–111, Mar 1972.

[22] Nathan Halko, Per-Gunnar Martinsson, and Joel A Tropp. Finding structure with randomness: Probabilistic algorithms for constructing approximate matrix decompositions. *SIAM review*, 53 (2):217–288, 2011.

[23] Petros Drineas, Malik Magdon-Ismail, Michael W. Mahoney, and David P. Woodruff. Fast approximation of matrix coherence and statistical leverage. *J. Mach. Learn. Res.*, 13(1):3475–3506, December 2012. ISSN 1532-4435.

[24] Michael W. Mahoney. Randomized algorithms for matrices and data. *Foundations and Trends® in Machine Learning*, 3(2):123–224, 2011. ISSN 1935-8237. doi: 10.1561/2200000035.

[25] H.E.T. Holgersson and Peter S. Karlsson. Three estimators of the mahalanobis distance in high-dimensional data. *Journal of Applied Statistics*, 39(12):2713–2720, 2012.

[26] Mina Ghashami, Edo Liberty, Jeff M. Phillips, and David P. Woodruff. Frequent directions: Simple and deterministic matrix sketching. *SIAM J. Comput.*, 45(5):1762–1792, 2016. doi: 10.1137/15M1009718.

[27] Vladimir Koltchinskii and Karim Lounici. Concentration inequalities and moment bounds for sample covariance operators. *Bernoulli*, 23(1):110–133, 02 2017. doi: 10.3150/15-BEJ730.

[28] Salil P Vadhan. Pseudorandomness. *Foundations and Trends® in Theoretical Computer Science*, 7(1–3):1–336, 2012.

[29] Michael B Cohen, Jelani Nelson, and David P Woodruff. Optimal approximate matrix product in terms of stable rank. *arXiv preprint arXiv:1507.02268*, 2015.

[30] Michael B Cohen, Sam Elder, Cameron Musco, Christopher Musco, and Madalina Persu. Dimensionality reduction for k-means clustering and low rank approximation. In *Proceedings of the forty-seventh annual ACM symposium on Theory of computing*, pages 163–172. ACM, 2015.

[31] Avner Magen and Anastasios Zouzias. Low rank matrix-valued chernoff bounds and approximate matrix multiplication. In *Proceedings of the twenty-second annual ACM-SIAM symposium on Discrete Algorithms*, pages 1422–1436. SIAM, 2011.

[32] Danziger S.A. *et al.* Functional census of mutation sequence spaces: the example of p53 cancer rescue mutants. *IEEE/ACM transactions on computational biology and bioinformatics*, 2006.

[33] Isabelle Guyon, Steve R. Gunn, Asa Ben-Hur, and Gideon Dror. In *Result analysis of the NIPS 2003 feature selection challenge*, 2004.

[34] Rcv1: A new benchmark collection for text categorization research. *The Journal of Machine Learning Research, 5, 361-397*, 2004.

[35] Edo Liberty and Mina Ghashami. https://github.com/edoliberty/frequent-directions.

[36] Markus M Breunig, Hans-Peter Kriegel, Raymond T Ng, and Jörg Sander. Lof: identifying density-based local outliers. In *ACM sigmod record*, volume 29, pages 93–104. ACM, 2000.

[37] Markus Schneider, Wolfgang Ertel, and Fabio Ramos. Expected similarity estimation for large-scale batch and streaming anomaly detection. *Machine Learning*, 105(3):305–333, 2016.

[38] Fei Tony Liu, Kai Ming Ting, and Zhi-Hua Zhou. Isolation forest. In *Data Mining, 2008. ICDM'08. Eighth IEEE International Conference on*, pages 413–422. IEEE, 2008.

[39] Kenneth L Clarkson and David P Woodruff. Low rank approximation and regression in input sparsity time. In *Proceedings of the forty-fifth annual ACM symposium on Theory of computing*, pages 81–90. ACM, 2013.

[40] Petros Drineas, Malik Magdon-Ismail, Michael W Mahoney, and David P Woodruff. Fast approximation of matrix coherence and statistical leverage. *Journal of Machine Learning Research*, 13(Dec):3475–3506, 2012.

[41] Nir Ailon and Bernard Chazelle. The fast johnson–lindenstrauss transform and approximate nearest neighbors. *SIAM Journal on computing*, 39(1):302–322, 2009.

[42] Hao Huang and Shiva Prasad Kasiviswanathan. Streaming anomaly detection using randomized matrix sketching. *Proc. VLDB Endow.*, 9(3), November 2015.

[43] Amit Chakrabarti, Subhash Khot, and Xiaodong Sun. Near-optimal lower bounds on the multi-party communication complexity of set disjointness. In *Computational Complexity, 2003. Proceedings. 18th IEEE Annual Conference on*, pages 107–117. IEEE, 2003.

[44] Ahmed El Alaoui and Michael W. Mahoney. Fast randomized kernel ridge regression with statistical guarantees. In *Proceedings of the 28th International Conference on Neural Information Processing Systems - Volume 1*, NIPS'15, pages 775–783, Cambridge, MA, USA, 2015. MIT Press.

[45] Michael B. Cohen, Cameron Musco, and Christopher Musco. Input sparsity time low-rank approximation via ridge leverage score sampling. In *Proceedings of the Twenty-Eighth Annual ACM-SIAM Symposium on Discrete Algorithms*, SODA '17, pages 1758–1777, Philadelphia, PA, USA, 2017. Society for Industrial and Applied Mathematics.

A Matrix Perturbation Bounds

In this section, we will establish projection bounds for various operators needed for computing outlier scores. We first set up some notation and state some results we need.

A.1 Preliminaries

We work with the following setup throughout this section. Let $\mathbf{A} \in \mathbb{R}^{n \times d} = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^T$ where $\boldsymbol{\Sigma} = (\sigma_1, \ldots, \sigma_d)$. Assume that $\mathbf{A}$ is (k, Δ)-separated as in Assumption 1 from 2. We use $\mathrm{sr}(\mathbf{A}) = \|\mathbf{A}\|_{\mathrm{F}}^2 / \sigma_1^2$ to denote the stable rank of $\mathbf{A}$, and $\kappa_k = \sigma_1^2 / \sigma_k^2$ for the condition number of $\mathbf{A}_k$.

Let $\tilde{\mathbf{A}} \in \mathbb{R}^{n \times \ell}$ be a sketch/noisy version of $\mathbf{A}$ satisfying

$$\|\mathbf{A}\mathbf{A}^T - \tilde{\mathbf{A}}\tilde{\mathbf{A}}^T\| \leq \mu \sigma_1^2. \tag{4}$$

and let $\tilde{\mathbf{A}} = \tilde{\mathbf{U}}\tilde{\boldsymbol{\Sigma}}\tilde{\mathbf{V}}^T$ denote its SVD. While we did not assume $\tilde{\mathbf{A}}$ is $(k, O(\Delta))$-separated, it will follow from Weyl's inequality for μ sufficiently small compared to Δ. It helps to think of Δ as property of the input $\mathbf{A}$, and μ as an accuracy parameter that we control.

In this section we prove perturbation bounds for the following three operators derived from $\tilde{\mathbf{A}}$, showing their closeness to those derived from $\mathbf{A}$:

1. $\mathbf{U}_k\mathbf{U}_k^T$: projects onto the principal k-dimensional column subspace (Lemma 3).

2. $\mathbf{U}_k\boldsymbol{\Sigma}_k^2\mathbf{U}_k^T$: projects onto the principal k-dimensional column subspace, and scale coordinate i by σ_i (Theorem 4).

3. $\mathbf{U}_k\boldsymbol{\Sigma}_k^{-2}\mathbf{U}_k^T$: projects onto the principal k-dimensional column subspace, and scale coordinate i by $1/\sigma_i$ (Theorem 6).

To do so, we will extensively use two classical results about matrix perturbation: Weyl's inequality (c.f. Horn and Johnson [20] Theorem 3.3.16) and Wedin's theorem [21], which respectively quantify how the eigenvalues and eigenvectors of a matrix change under perturbations.

Lemma 1. (Weyl's inequality) *Let* $\mathbf{C}, \mathbf{D} = \mathbf{C} + \mathbf{N} \in \mathbb{R}^{n \times d}$. *Then for all* $i \leq \min(n, d)$,

$$|\sigma_i(\mathbf{C}) - \sigma_i(\mathbf{D})| \leq \|\mathbf{N}\|.$$

Wedin's theorem requires a sufficiently large separation in the eigenvalue spectrum for the bound to be meaningful.

Lemma 2. (Wedin's theorem) *Let* $\mathbf{C}, \mathbf{D} = \mathbf{C} + \mathbf{N} \in \mathbb{R}^{n \times d}$. *Let* $\mathbf{P}_C$ *and* $\mathbf{P}_D$ *respectively denote the projection matrix onto the space spanned by the top* k *singular vectors of* $\mathbf{C}$ *and* $\mathbf{D}$. *Then,*

$$\|\mathbf{P}_D - \mathbf{P}_C\mathbf{P}_D\| \leq \frac{\|\mathbf{N}\|}{\sigma_k(\mathbf{C}) - \sigma_{k+1}(\mathbf{C}) - \|\mathbf{N}\|}.$$

A.2 Matrix Perturbation Bounds

We now use these results to derive the perturbation bounds enumerated above. The first bound is a direct consequence of Wedin's theorem.

Lemma 3. *If* $\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$ *is* (k, Δ)*-separated,* $\tilde{\mathbf{A}} = \tilde{\mathbf{U}}\tilde{\mathbf{\Sigma}}\tilde{\mathbf{V}}^T$ *satisfies* (4) *with* $\mu \leq \Delta/6$, *then*

$$\|\mathbf{U}_k\mathbf{U}_k^T - \tilde{\mathbf{U}}_k\tilde{\mathbf{U}}_k^T\| \leq 2\sqrt{\frac{\mu}{\Delta}}.$$

Proof. Let $\mathbf{P} = \mathbf{U}_k\mathbf{U}_k^T$ and $\tilde{\mathbf{P}} = \tilde{\mathbf{U}}_k\tilde{\mathbf{U}}_k^T$. Since we have $\mathbf{A}\mathbf{A}^T = \mathbf{U}\mathbf{\Sigma}^2\mathbf{U}^T$, $\mathbf{P}$ $(\tilde{\mathbf{P}})$ is the projection operator onto the column space of $\mathbf{A}_k$ (and similarly for $\tilde{\mathbf{P}}$ and $\tilde{\mathbf{A}}_k$). Since $\mathbf{P}^T = \mathbf{P}$ and $\mathbf{P}\mathbf{P} = \mathbf{P}$ for any orthogonal projection matrix, we can write,

$$\|\mathbf{P} - \tilde{\mathbf{P}}\|^2 = \|(\mathbf{P} - \tilde{\mathbf{P}})^2\| = \|\mathbf{P}\mathbf{P} - \mathbf{P}\tilde{\mathbf{P}} - \tilde{\mathbf{P}}\mathbf{P} + \tilde{\mathbf{P}}\tilde{\mathbf{P}}\| = \|\mathbf{P} - \mathbf{P}\tilde{\mathbf{P}} + \tilde{\mathbf{P}} - \tilde{\mathbf{P}}\mathbf{P}\|$$

$$\leq \|\tilde{\mathbf{P}} - \mathbf{P}\tilde{\mathbf{P}}\| + \|\mathbf{P} - \tilde{\mathbf{P}}\mathbf{P}\|. \tag{5}$$

Since $\mathbf{A}$ is (k, Δ)-separated,

$$\sigma_k(\mathbf{A}\mathbf{A}^t) - \sigma_{k+1}(\mathbf{A}\mathbf{A}^t) = \sigma_k^2 - \sigma_{k+1}(\mathbf{A})^2 = \Delta. \tag{6}$$

So applying Wedin's theorem to $\mathbf{A}\mathbf{A}^T$,

$$\|\tilde{\mathbf{P}} - \mathbf{P}\tilde{\mathbf{P}}\| \leq \frac{\mu}{\Delta - \mu}. \tag{7}$$

We next show that the spectrum of $\tilde{\mathbf{A}}$ also has a gap at k. Using Weyl's inequality,

$$\tilde{\sigma}_k^2 \geq \sigma_k^2 - \mu\sigma_1^2 \text{ and } \tilde{\sigma}_{k+1}^2 \leq \sigma_{k+1}^2 + \mu\sigma_1^2$$

Hence using Equation (6)

$$\tilde{\sigma}_k^2 - \tilde{\sigma}_{k+1}^2 \geq \sigma_{k+1}^2 - \sigma_k^2 - 2\mu\sigma_1^2 \geq (\Delta - 2\mu)\sigma_1^2.$$

So we apply Wedin's theorem to $\tilde{\mathbf{A}}$ to get

$$\|\mathbf{P} - \tilde{\mathbf{P}}\mathbf{P}\| \leq \frac{\mu}{\Delta - 3\mu}. \tag{8}$$

Plugging (7) and (8) into (5),

$$\|\mathbf{P} - \tilde{\mathbf{P}}\|^2 \leq \frac{\mu}{\Delta - \mu} + \frac{\mu}{\Delta - 3\mu} \leq \frac{2\mu}{\Delta - 3\mu} \leq \frac{4\mu}{\Delta}$$

where the last inequality is becuase $\Delta - 3\mu \geq \Delta/2$ since we assumed $\Delta \geq 6\mu$. The claim follows by taking square roots on both sides. ∎

We now move to proving bounds for items (2) and (3), which are given by Theorems 4 and 6 respectively.

Theorem 4. *Let* $\mu \leq \min(\Delta^3 k^2, 1/(20k))$.

$$\|\mathbf{U}_k\mathbf{\Sigma}_k^2\mathbf{U}_k^T - \tilde{\mathbf{U}}_k\mathbf{\Sigma}_k^2\tilde{\mathbf{U}}_k^T\| \leq 8\sigma_1^2(\mu k)^{1/3}.$$

The full proof of the theorem is quite technical and is stated in Section E. Here we prove a special case that captures the main idea. The simplifying assumption we make is that the values of the diagonal matrix in the operator are distinct and well separated. In the full proof we decompose $\mathbf{\Sigma}_k$ to a well separated component and a small residual component.

Definition 5. $\mathbf{\Lambda} = \mathrm{diag}(\lambda_1, \ldots \lambda_k)$ *is monotone and* δ*-well separated if*

- $\lambda_{i+1} \geq \lambda_i$ for $1 \leq i < k$.

- The λs could be partitioned to buckets so that all values in the same buckets are equal, and values across buckets are well separated. Formally, $1 \ldots k$ are partitioned to m buckets $B_1, \ldots B_m$ so that if $i, j \in B_\ell$ then $\lambda_i = \lambda_j$. Yet, if $i \in B_\ell$ and $j \in B_{\ell+1}$ then $\lambda_i - \lambda_j > \delta\lambda_1$.

The idea is to show $\mathbf{\Sigma} = \mathbf{\Lambda} + \mathbf{\Omega}$ where $\mathbf{\Lambda}$ is monotone and well separated and $\mathbf{\Omega}$ has small norm. The next two lemmas handle these two components. We first state a simple lemma which handles the case where $\mathbf{\Omega}$ has small norm.

Lemma 4. *For any diagonal matrix* $\mathbf{\Omega}$,

$$\|\mathbf{U}_k \mathbf{\Omega} \mathbf{U}_k^T - \tilde{\mathbf{U}}_k \mathbf{\Omega} \tilde{\mathbf{U}}_k^T\| \leq 2\|\mathbf{\Omega}\|.$$

Proof. By the triangle inequality, $\|\mathbf{U}_k \mathbf{\Omega} \mathbf{U}_k^T - \tilde{\mathbf{U}}_k \mathbf{\Omega} \tilde{\mathbf{U}}_k^T\| \leq \|\mathbf{U}_k \mathbf{\Omega} \mathbf{U}_k^T\| + \|\tilde{\mathbf{U}}_k \mathbf{\Omega} \tilde{\mathbf{U}}_k^T\|$. The bound follows as $\mathbf{U}_k$ and $\tilde{\mathbf{U}}$ are orthonormal matrices. ∎

We next state the result for the case where $\mathbf{\Lambda}$ is monotone and well separated. In order to prove this result, we need the following direct corollary of Lemma 3:

Lemma 5. *For all* $j \leq m$,

$$\|\mathbf{U}_{b_j} \mathbf{U}_{b_j}^T - \tilde{\mathbf{U}}_{b_j} \tilde{\mathbf{U}}_{b_j}^T\| \leq \sqrt{\frac{2\mu\sigma_1^2}{\delta\sigma_1^2 - 3\mu\sigma_1^2}} \leq 2\sqrt{\frac{\mu}{\delta}}. \tag{9}$$

Using this, we now proceed as follows.

Lemma 6. *Let* $6\mu \leq \delta \leq \Delta$. *Let* $\mathbf{\Lambda} = \mathrm{diag}(\lambda_1, \ldots \lambda_k)$ *be a monotone and* $\delta\sigma_1^2$ *well separated diagonal matrix. Then*

$$\|\mathbf{U}_k \mathbf{\Lambda} \mathbf{U}_k^T - \tilde{\mathbf{U}}_k \mathbf{\Lambda} \tilde{\mathbf{U}}_k^T\| \leq 2\|\mathbf{\Lambda}\|\sqrt{\frac{\mu}{\delta}}.$$

Proof. We denote by b_j the largest index that falls in bucket B_j. Let us set $\lambda_{B_{m+1}} = 0$ for convenience. Since

$$\mathbf{U}_{b_j} \mathbf{U}_{b_j}^T = \sum_{i=1}^{b_j} u^{(i)} u^{(i)T},$$

we can write,

$$\mathbf{U}_k \mathbf{\Lambda} \mathbf{U}_k^T = \sum_{j=1}^{m} (\lambda_{b_j} - \lambda_{b_{j+1}}) \mathbf{U}_{b_j} \mathbf{U}_{b_j}^T$$

and similarly for $\tilde{\mathbf{U}}_k \mathbf{\Lambda} \tilde{\mathbf{U}}_k^T$. So we can write

$$\mathbf{U}_k \mathbf{\Lambda} \mathbf{U}_k^T - \tilde{\mathbf{U}}_k \mathbf{\Lambda} \tilde{\mathbf{U}}_k^T = \sum_{j=1}^{m} (\lambda_{b_j} - \lambda_{b_{j+1}})(\mathbf{U}_{b_j} \mathbf{U}_{b_j}^T - \tilde{\mathbf{U}}_{b_j} \tilde{\mathbf{U}}_{b_j}^T).$$

Therefore by using Lemma 5,

$$\|\mathbf{U}_k \mathbf{\Lambda} \mathbf{U}_k^T - \tilde{\mathbf{U}}_k \mathbf{\Lambda} \tilde{\mathbf{U}}_k^T\| = \sum_{j=1}^{m} |\lambda_{b_j} - \lambda_{b_{j+1}}| \|(\mathbf{U}_{b_j} \mathbf{U}_{b_j}^T - \tilde{\mathbf{U}}_{b_j} \tilde{\mathbf{U}}_{b_j}^T)\| \leq 2\sqrt{\frac{\mu}{\delta}} \sum_{j=1}^{m} |\lambda_{b_j} - \lambda_{b_{j+1}}|,$$

where the second inequality is by the triangle inequality and by applying Lemma 4. Thus proving that $\sum_{j=1}^{m} |\lambda_{b_j} - \lambda_{b_{j+1}}| \leq \|\mathbf{\Lambda}\|$ would imply the claim. Indeed

$$\sum_{j=1}^{k} |\lambda_{b_j} - \lambda_{b_{j+1}}| = \sum_{j=1}^{k} (\lambda_{b_j} - \lambda_{b_{j+1}}) = \lambda_{b_1} - \lambda_{b_{k+1}} \leq \|\mathbf{\Lambda}\|.$$

∎

Note that though Lemma 6 assumes that the eigenvalues in each bucket are equal, the key step where we apply Wedin's theorem (Lemma 3) only uses the fact that there is some separation between the eigenvalues in different buckets. Lemma 10 in the appendix does this generalization by relaxing the assumption that the eigenvalues in each bucket are equal. The final proof of Theorem 4 works by splitting the eigenvalues into different buckets or intervals such that all the eigenvalues in the same interval have small separation, and the eigenvalues in different intervals have large separation. We then use Lemma 10 and Lemma 4 along with the triangle inequality to bound the perturbation due to the well-separated part and the residual part respectively.

The bound corresponding to (3) is given in following theorem:

Theorem 6. *Let κ_k denote the condition number $\kappa_k = \sigma_1^2/\sigma_k^2$. Let $\mu \leq \min(\Delta^3(k\kappa_k)^2, 1/(20k\kappa_k))$. Then,*

$$\|\mathbf{U}_k \boldsymbol{\Sigma}_k^{-2} \mathbf{U}_k^T - \tilde{\mathbf{U}}_k \boldsymbol{\Sigma}_k^{-2} \tilde{\mathbf{U}}_k^T\| \leq \frac{8}{\sigma_k^2}(\mu k \kappa_k)^{1/3}.$$

The proof uses similar ideas to those of Theorem 4 and is deferred to Section E.

B Pointwise guarantees for Anomaly Detection

Let the input $\mathbf{A} \in \mathbb{R}^{n \times d}$ have SVD $\mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^T$ be its SVD. Write $a_{(i)}$ in the basis of right singular vectors as $a_{(i)} = \sum_{j=1}^d \alpha_j v^{(j)}$. Recall that we defined its rank-k leverage score and projection distance respectively as

$$L^k(i) = \sum_{j=1}^k \frac{\alpha_j^2}{\sigma_j^2} = \|\boldsymbol{\Sigma}_k^{-1}\mathbf{V}_k^T a_{(i)}\|_2^2, \tag{10}$$

$$T^k(i) = \sum_{j=k+1}^d \alpha_j^2 = a_{(i)}^T(\mathbf{I} - \mathbf{V}_k\mathbf{V}_k^T)a_{(i)}. \tag{11}$$

To approximate these scores, it is natural to use a row-space approximation, or rather a sketch $\tilde{\mathbf{A}} \in R^{\ell \times d}$ that approximates the covariance matrix $\mathbf{A}^T\mathbf{A}$ as below:

$$\|\mathbf{A}^T\mathbf{A} - \tilde{\mathbf{A}}^T\tilde{\mathbf{A}}\| \leq \mu\sigma_1^2. \tag{12}$$

Given such a sketch, our approximation is the following: compute $\tilde{\mathbf{A}} = \tilde{\mathbf{U}}\tilde{\boldsymbol{\Sigma}}\tilde{\mathbf{V}}^t$. The estimates for $L^k(i)$ and $T^k(i)$ respectively are

$$\tilde{L}^k(i) = \|\tilde{\boldsymbol{\Sigma}}_k^{-1}\tilde{\mathbf{V}}_k^T a_{(i)}\|_2^2, \tag{13}$$

$$\tilde{T}^k(i) = a_{(i)}^T(\mathbf{I} - \tilde{\mathbf{V}}_k\tilde{\mathbf{V}}_k^T)a_{(i)}. \tag{14}$$

Given the sketch $\tilde{\mathbf{A}}$, we expect that $\tilde{\mathbf{V}}_k$ is a good approximation to the row space spanned by $\mathbf{V}_k$, since the covariance matrices of the rows are close. In contrast the columns spaces of $\mathbf{A}$ and $\tilde{\mathbf{A}}$ are hard to compare since they lie in $\mathbb{R}^n$ and $\mathbb{R}^\ell$ respectively. The closeness of the row spaces follows from the results from Section A but applied to $\mathbf{A}^T$ rather than $\mathbf{A}$ itself. The results there require that $\|\mathbf{A}\mathbf{A}^T - \tilde{\mathbf{A}}\tilde{\mathbf{A}}^T\|$ is small, and Equation (12) implies that this assumption holds for $\mathbf{A}^T$.

We first state our approximation guarantees for T^k.

Theorem 7. *Assume that $\mathbf{A}$ is (k, Δ)-separated. Let $\varepsilon < 1/3$ and let $\tilde{\mathbf{A}}$ satisfy Equation (12) for $\mu = \varepsilon^2\Delta$. Then for every i,*

$$|T^k(i) - \tilde{T}^k(i)| \leq \varepsilon\|a_{(i)}\|_2^2.$$

Proof. We have

$$\begin{aligned}
|T^k(i) - \tilde{T}^k(i)| &= |a_{(i)}^T(\mathbf{I} - \mathbf{V}_k\mathbf{V}_k^T)a_{(i)} - a_{(i)}^T(\mathbf{I} - \tilde{\mathbf{V}}_k\tilde{\mathbf{V}}_k^T)a_{(i)}| \\
&= |a_{(i)}(\tilde{\mathbf{V}}_k\tilde{\mathbf{V}}_k^T - \mathbf{V}_k\mathbf{V}_k^T)a_{(i)}| \\
&\leq \|\tilde{\mathbf{V}}_k\tilde{\mathbf{V}}_k^T - \mathbf{V}_k\mathbf{V}_k^T\|\|a_{(i)}\|_2^2 \\
&\leq \varepsilon\|a_{(i)}\|_2^2
\end{aligned}$$

where in the last line we use Lemma 3, applied to the projection onto columns of $\mathbf{A}^T$, which are the rows of $\mathbf{A}$. The condition $\mu < \Delta/6$ holds since $\mu = \varepsilon^2\Delta$ for $\varepsilon < 1/3$. ∎

How meaningful is the above additive approximation guarantee? For each row, the additive error is $\varepsilon\|a_{(i)}\|_2^2$. It might be that $T^k(i) \ll \varepsilon\|a_{(i)}\|_2^2$ which happens when the row is almost entirely within the principal subspace. But in this case, the points are not anomalies, and we have $\tilde{T}^k(i) \leq 2\varepsilon\|a_{(i)}\|_2^2$, so these points will not seem anomalous from the approximation either. The interesting case is when

$T^k(i) \geq \beta \|a_{(i)}\|_2^2$ for some constant β (say 1/2). For such points, we have $\tilde{T}^k(i) \in (\beta \pm \epsilon)\|a_{(i)}\|_2^2$, so we indeed get multiplicative approximations.

Next we give our approximation guarantee for L^k, which relies on the perturbation bound in Theorem 6.

Theorem 8. *Assume that* $\mathbf{A}$ *is* (k, Δ)*-separated. Let* $\tilde{\mathbf{A}}$ *be as in Equation* (12). *Let*

$$\varepsilon \leq \min\left(\kappa_k \Delta, \frac{1}{k}\right) \text{sr}(\mathbf{A})\kappa_k, \quad \mu = \frac{\varepsilon^3 k^2}{10^3 \text{sr}(A)^3 \kappa_k^4}.$$

Then for every i,

$$|L^k(i) - \tilde{L}^k(i)| \leq \varepsilon k \frac{\|a_{(i)}\|_2^2}{\|\mathbf{A}\|_F^2}. \tag{15}$$

Proof. Since $L^k(i) = \|\mathbf{\Sigma}_k^{-1}\mathbf{V}_k^T a_{(i)}\|_2^2$, $\tilde{L}^k(i) = \|\tilde{\mathbf{\Sigma}}_k^{-1}\tilde{\mathbf{V}}_k^T a_{(i)}\|_2^2$, it will suffice to show that

$$\|\mathbf{V}_k\mathbf{\Sigma}_k^{-2}\mathbf{V}_k^T - \tilde{\mathbf{V}}_k\tilde{\mathbf{\Sigma}}^{-2}\tilde{\mathbf{V}}_k^T\| \leq \frac{\varepsilon k}{\|\mathbf{A}\|_F^2}. \tag{16}$$

To prove inequality (16), we will bound the LHS as

$$\|\mathbf{V}_k\mathbf{\Sigma}^{-2}\mathbf{V}_k^T - \tilde{\mathbf{V}}_k\tilde{\mathbf{\Sigma}}^{-2}\tilde{\mathbf{V}}_k^T\| \leq \|\mathbf{V}_k\mathbf{\Sigma}_k^{-2}\mathbf{V}_k^T - \tilde{\mathbf{V}}_k^T\mathbf{\Sigma}_k^{-2}\tilde{\mathbf{V}}_k^T\| + \|\tilde{\mathbf{V}}_k(\mathbf{\Sigma}^{-2} - \tilde{\mathbf{\Sigma}}^{-2})\tilde{\mathbf{V}}_k^T\| \tag{17}$$

For the first term, we apply Theorem 6 to $\mathbf{A}^T$ to get

$$\|\mathbf{V}_k\mathbf{\Sigma}^{-2}\mathbf{V}_k^T - \tilde{\mathbf{V}}_k^T\mathbf{\Sigma}_k^{-2}\tilde{\mathbf{V}}_k^T\| \leq \frac{8}{\sigma_k^2}(\mu k \kappa_k)^{1/3}. \tag{18}$$

We bound the second term as

$$\|\tilde{\mathbf{V}}_k(\mathbf{\Sigma}^{-2} - \tilde{\mathbf{\Sigma}}^{-2})\tilde{\mathbf{V}}_k^T\| = \max_{i \in [k]} |\sigma_i^{-2} - \tilde{\sigma}_i^{-2}| = \max_{i \in [k]} \frac{|\sigma_i^2 - \tilde{\sigma}_i^2|}{\sigma_i^2 \tilde{\sigma}_i^2} \leq \frac{\mu \sigma_1^2}{\sigma_k^2 \tilde{\sigma}_k^2} \tag{19}$$

where we use Weyl's inequality to bound $\sigma_i^2 - \tilde{\sigma}_i^2$. Using Weyl's inequality and the fact that $\mu \geq 1/(20k\kappa_k)$,

$$\tilde{\sigma}_k^2 \geq \sigma_k^2 - \mu\sigma_1^2 \geq \sigma_k^2 - \sigma_k^2/10k \geq \sigma_k^2/2,$$

$$\frac{\mu\sigma_1^2}{\sigma_k^2 \tilde{\sigma}_k^2} \leq \frac{2\mu\sigma_1^2}{\sigma_k^4} = \frac{2\mu\kappa_k}{\sigma_k^2} \tag{20}$$

Plugging Equations (18) and (20) into Equation (17) gives

$$\|\mathbf{V}_k\mathbf{\Sigma}^{-2}\mathbf{V}_k^T - \tilde{\mathbf{V}}_k\tilde{\mathbf{\Sigma}}^{-2}\tilde{\mathbf{V}}_k^T\| \leq \frac{1}{\sigma_k^2}(8(\mu k \kappa_k)^{1/3} + 2\mu\kappa_k) \leq \frac{10}{\sigma_k^2}(\mu k \kappa_k)^{1/3} \tag{21}$$

$$\leq \frac{10}{\sigma_k^2}\left(\frac{\varepsilon^3 k^3}{10^3 \text{sr}(\mathbf{A})^3 \kappa_k^3}\right)^{1/3} \leq \frac{k\varepsilon}{\sigma_k^2 \kappa_k \text{sr}(\mathbf{A})} = \frac{k\varepsilon}{\|\mathbf{A}\|_F^2}.$$

Equation (21) follows by Theorem 6. The conditions on μ needed to apply it are guaranteed by our choice of μ and ε. ∎

To interpret this guarantee, consider the setting when all the points have roughly the same 2-norm. More precisely, if for some constant C

$$\frac{\|a_{(i)}\|_2^2}{\|\mathbf{A}\|_F^2} \leq \frac{C}{i}$$

then Equation (15) gives

$$|L^k(i) - \tilde{L}^k(i)| \leq C\varepsilon k/n.$$

Note that k is a constant whereas n grows as more points come in. As mentioned in the discussion following Theorem 1, the points which are considered outliers are those where $L^k(i) \gg \frac{k}{n}$. For the parameters setting, if we let $\kappa_k = O(1)$ and $\text{sr}(A) = \Theta(k)$, then our bound on ϵ reduces to $\varepsilon \leq \min(\Delta, 1/k)$, and our choice of μ reduces to $\mu \approx \varepsilon^3/k$.

To efficiently compute a sketch that satisfies (12), we can use Frequent Directions [18]. We use the improved analysis of Frequent Directions in Ghashami et al. [26]:

16

Theorem 9. *[26] There is an algorithm that takes the rows of* $\mathbf{A}$ *in streaming fashion and computes a sketch* $\tilde{\mathbf{A}} \in \mathbb{R}^{\ell \times d}$ *satisfying Equation* (12) *where* $\ell = \sum_{i=k+1}^{n} \sigma_i^2 / (\sigma_1^2 \mu)$.

Let $\tilde{\mathbf{A}} = \tilde{\mathbf{U}} \tilde{\mathbf{\Sigma}} \tilde{\mathbf{V}}^T$. The algorithm maintains $\tilde{\mathbf{\Sigma}}, \tilde{\mathbf{V}}$. It uses $O(d\ell)$ memory and requires time at most $O(d\ell^2)$ per row. The total time for processing n rows is $O(nd\ell)$. If $\ell \ll d$, this is a significant improvement over the naive algorithm in both memory and time. If we use Frequent directions, we set

$$\ell = \frac{\sum_{i=k+1}^{d} \sigma_i^2}{\sigma_1^2 \mu} \tag{22}$$

where μ is set according to Theorem 7 and 8. This leads to $\ell = \mathrm{poly}(k, \mathrm{sr}(\mathbf{A}), \kappa_k, \Delta, \epsilon^{-1})$. Note that this does not depend on d, and hence is considerably smaller for our parameter settings of interest.

B.1   The Online Setting

We now consider the online scenario where the leverage scores and projection distances are defined only with respect to the input seen so far. Consider again the motivating example where each machine in a data center produces streams of measurements. Here, it is desirable to determine the anomaly score of a data point online as it arrives, with respect to the data produced so far, and by a streaming algorithm. We first define the online anomaly measures. Let $\mathbf{A} \in \mathbb{R}^{(i-1) \times d}$ denote the matrix of points that have arrived so far (excluding $a_{(i)}$) and let $\mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$ be its SVD. Write $a_{(i)}$ in the basis of right singular vectors as $a_{(i)} = \sum_{j=1}^{d} \alpha_j v^{(j)}$. We define its rank-$k$ leverage score and projection distance respectively as

$$l^k(i) = \sum_{j=1}^{k} \frac{\alpha_j^2}{\sigma_j^2} = \|\mathbf{\Sigma}_k^{-1} \mathbf{V}_k^T a_{(i)}\|_2^2, \tag{23}$$

$$t^k(i) = \sum_{j=k+1}^{d} \alpha_j^2 = a_{(i)}^T (\mathbf{I} - \mathbf{V}_k \mathbf{V}_k^T) a_{(i)}. \tag{24}$$

Note that in the online setting there is a one-pass streaming algorithm that can compute both these scores, using time $O(d^3)$ per row and $O(d^2)$ memory. This algorithm maintains the $d \times d$ covariance matrix $\mathbf{A}^T \mathbf{A}$ and computes its SVD to get $\mathbf{V}_k, \mathbf{\Sigma}_k$. From these, it is easy to compute both l^k and t^k.

All our guarantees from the previous subsection directly carry over to this online scenario, allowing us to significantly improve over this baseline. This is because the guarantees are pointwise, hence they also hold for every data point if the scores are only defined for the input seen so far. This implies a one-pass algorithm which can approximately compute the anomaly scores (i.e., satisfies the guarantees in Theorem 7 and 8) and uses space $O(d\ell)$ and requires time $O(nd\ell)$ for $\ell = \mathrm{poly}(k, \mathrm{sr}(\mathbf{A}), \kappa_k, \Delta, \epsilon^{-1})$ (independent of d).

The $\Omega(d)$ lower bounds in Section D show that one cannot hope for sublinear dependence on d for pointwise estimates. In the next section, we show how to eliminate the dependence on d in the space requirement of the algorithm in exchange for weaker guarantees.

C   Average-case guarantees for Anomaly Detection

In this section, we present an approach which circumvents the $\Omega(d)$ lower bounds by relaxing the pointwise approximation guarantee.

Let $\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$ be the SVD of $\mathbf{A}$. The outlier scores we wish to compute are

$$L^k(i) = \|e_i^T \mathbf{U}_k\|_2^2 = \|\mathbf{\Sigma}_k^{-1} \mathbf{V}_k^T a_{(i)}\|_2^2, \tag{25}$$

$$T^k(i) = \|a_{(i)}\|_2^2 - \|e_i^T \mathbf{U}_k \mathbf{\Sigma}_k\|_2^2 = \|a_{(i)}\|_2^2 - \|\mathbf{V}_k^T a_{(i)}\|_2^2. \tag{26}$$

Note that these scores are defined with respect to the principal space of the entire matrix. We present a guarantee for any sketch $\tilde{\mathbf{A}} \in R^{n \times \ell}$ that approximates the column space of $\mathbf{A}$, or equivalently the covariance matrix $\mathbf{A}\mathbf{A}^T$ of the row vectors. We can work with any sketch $\mathbf{A}$ where

$$\|\mathbf{A}\mathbf{A}^T - \tilde{\mathbf{A}}\tilde{\mathbf{A}}^T\| \leq \mu \sigma_1^2. \tag{27}$$

Theorem 10 stated in Section C.2 shows that such a sketch can be obtained for instance by a random projection $\mathbf{R}$ onto $\mathbb{R}^\ell$ for $\ell = \mathrm{sr}(\mathbf{A})/\mu^2$: let $\tilde{\mathbf{A}} = \mathbf{AR}$ for $\mathbf{R} \in \mathbb{R}^{d\times\ell}$ chosen from an appropriately family of random matrices. However, we need to be careful in our choice of the family of random matrices, as naively storing a $(d \times \ell)$ matrix requires $O(d\ell)$ space, which would increase the space requirement of our streaming algorithm. For example, if we were to choose each entry of $\mathbf{R}$ to be i.i.d. be $\pm\frac{1}{\sqrt{\ell}}$, then we would need to store $O(d\ell)$ random bits corresponding to each entry of $\mathbf{R}$.

But Theorem 10 also shows that this is unnecessary and we do not need to explicitly store a $(d \times \ell)$ random matrix. The guarantees of Theorem 10 also hold when $\mathbf{R}$ is a pseudorandom matrix with the entries being $\pm\frac{1}{\sqrt{\ell}}$ with $\log(\mathrm{sr}(\mathbf{A})/\delta)$-wise independence instead of full independence . Therefore, by using a simple polynomial based hashing scheme [28] we can get the same sketching guarantees using only $O(\log(d)\log(\mathrm{sr}(\mathbf{A})/\delta))$ random bits and hence only $O(\log(d)\log(\mathrm{sr}(\mathbf{A})/\delta))$ space. Note that each entry of $\mathbf{R}$ can be computed from this random seed in time $O(\log(d)\log(\mathrm{sr}(\mathbf{A})/\delta))$.

Theorem 11 stated in Section C.3 shows that such a sketch can also be obtained for a length-squared sub-sampling of the columns of the matrix, for $\ell = \tilde{O}(\mathrm{sr}(\mathbf{A})/\mu^2)$ (where the $\tilde{O}$ hides logarithmic factors).

Given such a sketch, we expect $\tilde{\mathbf{U}}_k$ to be a good approximation to $\mathbf{U}_k$. So we define our approximations in the natural way:

$$\tilde{L}^k(i) = \|e_i^T \tilde{\mathbf{U}}_k^i\|_2^2, \tag{28}$$

$$\tilde{T}^k(i) = \|a_{(i)}\|_2^2 - \|e_i^T \tilde{\mathbf{U}}_k \tilde{\mathbf{\Sigma}}_k\|_2^2. \tag{29}$$

The analysis then relies on the machinery from Section A. However, $\tilde{\mathbf{U}}_k$ lies in $\mathbb{R}^{n\times k}$ which is too costly to compute and store, whereas $\tilde{\mathbf{V}}_k$ in contrast lies in $\mathbb{R}^{\ell\times k}$, for $\ell = 1/\mu^2 \max(\mathrm{sr}(\mathbf{A}), \log(1/\delta))$. In particular, both ℓ and k are independent of n, d and could be significantly smaller. In many settings of practical interest, we have $\mathrm{sr}(\mathbf{A}) \approx k$ and both are constants independent of n, d. So in our algorithm, we use the following equivalent definition in terms of $\tilde{\mathbf{V}}_k, \tilde{\mathbf{\Sigma}}_k$.

$$\tilde{L}^k(i) = \|\tilde{\mathbf{\Sigma}}_k^{-1} \tilde{\mathbf{V}}_k^T (\mathbf{R}^T a_{(i)})\|_2^2, \tag{30}$$

$$\tilde{T}^k(i) = \|a_{(i)}\|_2^2 - \|\tilde{\mathbf{V}}_k^T (\mathbf{R}^T a_{(i)})\|_2^2. \tag{31}$$

For the random projection algorithm, we compute $\tilde{\mathbf{A}}^T \tilde{\mathbf{A}}$ in $\mathbb{R}^{\ell\times\ell}$ in the first pass, and then run SVD on it to compute $\tilde{\mathbf{\Sigma}}_k \in \mathbb{R}^{k\times k}$ and $\tilde{\mathbf{V}}_k \in \mathbb{R}^{\ell\times k}$. Then in the second pass, we use these to we compute $\tilde{L}^k$ and $\tilde{T}^k$. The total memory needed in the first pass is $O(\ell^2)$ for the covariance matrix. In the second pass, we need $O(k\ell)$ memory for storing $\mathbf{V}_k$. We also need $O(\log(d)\log(\mathrm{sr}(\mathbf{A})/\delta))$ additional memory for storing the random seed from which the entries of $\mathbf{R}$ can be computed efficiently.

C.1 Our approximation guarantees

We now turn to the guarantees. Given the $\Omega(d)$ lower bound from Section D, we cannot hope for a strong pointwise guarantee, rather we will show a guarantee that hold on average, or for most points.

The following simple Lemma bounds the sum of absolute values of diagonal entries in symmetric matrices.

Lemma 7. *Let $\mathbf{A} \in \mathbb{R}^{n\times n}$ be symmetric. Then*

$$\sum_{i=1}^n \left|\mathbf{e}_i^T \mathbf{A}\mathbf{e}_i\right| \le \mathrm{rank}(\mathbf{A})\|\mathbf{A}\|.$$

Proof. Consider the eigenvalue decomposition of $\mathbf{A} = \mathbf{Q}\mathbf{\Lambda}\mathbf{Q}^T$ where $\mathbf{\Lambda}$ is the diagonal matrix of eigenvalues of $\mathbf{A}$, and $\mathbf{Q}$ has orthonormal columns, so $\|\mathbf{Q}\|_F^2 = \mathrm{rank}(\mathbf{A})$. We can write,

$$\sum_{i=1}^n \left|\mathbf{e}_i^T \mathbf{A}\mathbf{e}_i\right| = \sum_{i=1}^n \left|\mathbf{e}_i^T \mathbf{Q}\mathbf{\Lambda}\mathbf{Q}^T\mathbf{e}_i\right| = \sum_{i=1}^n \sum_{j=1}^n \left|\mathbf{\Lambda}_{i,i}\mathbf{Q}_{i,j}^2\right|$$

$$\le \|\mathbf{A}\| \sum_{i,j=1}^n \left|\mathbf{Q}_{i,j}^2\right| = \|\mathbf{A}\|\|\mathbf{Q}\|_F^2 = \mathrm{rank}(\mathbf{A})\|\mathbf{A}\|.$$

We first state and prove Lemma 8 which bounds the average error in estimating L^k.

Lemma 8. *Assume that* $\mathbf{A}$ *is* (k, Δ)*-separated. Let* $\tilde{\mathbf{A}}$ *satisfy Equation* (27) *for* $\mu = \varepsilon^2 \Delta / 16$ *where* $\varepsilon < 1$. *Then*

$$\sum_{i=1}^{n} |L^k(i) - \tilde{L}^k(i)| \leq \varepsilon \sum_{i=1}^{n} L^k(i).$$

Proof. By Equations (25) and (28)

$$\sum_{i=1}^{n} |L^k(i) - \tilde{L}^k(i)| = \sum_{i=1}^{n} |e_i^t \mathbf{U}_k \mathbf{U}_k^T e_i - e_i^t \tilde{\mathbf{U}}_k \tilde{\mathbf{U}}_k^T e_i|.$$

Let $\mathbf{C} = \mathbf{U}_k \mathbf{U}_k^T - \tilde{\mathbf{U}}_k \tilde{\mathbf{U}}_k^T$, so that $\mathrm{rank}(\mathbf{C}) \leq 2k$. By Lemma 3 (which applies since $\mu \leq \Delta/16$), we have

$$\|\mathbf{C}\| \leq 2\sqrt{\frac{\mu}{\Delta}} \leq \frac{\varepsilon}{2}.$$

So applying Lemma 7, we get

$$\sum_{i=1}^{n} |e_i^t \mathbf{U}_k \mathbf{U}_k^T e_i - e_i^t \tilde{\mathbf{U}}_k \tilde{\mathbf{U}}_k^T e_i| \leq \frac{\varepsilon}{2} 2k = \varepsilon k.$$

The claim follows by noting that the columns of $\mathbf{U}_k$ are orthonormal, so $\sum_{i=1}^{n} L^k(i) = k$. ∎

The guarantee above shows that the average additive error in estimating $L^k(i)$ is $\frac{\varepsilon}{n} \sum_{i=1}^{n} L^k(i)$ for a suitable ε. Note that the average value of $L^k(i)$ is $\frac{1}{n} \sum_{i=1}^{n} L^k(i)$, hence we obtain small additive errors on average. Additive error guarantees for $L^k(i)$ translate to multiplicative guarantees as long as $L^k(i)$ is not too small, but for outlier detection the candidate outliers are those points for which $L^k(i)$ is large, hence additive error guarantees are meaningful for preserving outlier scores for points which could be outliers.

Similarly, Lemma 9 bounds the average error in estimating T^k.

Lemma 9. *Assume that* $\mathbf{A}$ *is* (k, Δ)*-separated. Let*

$$\varepsilon \leq \frac{\min(\Delta k^2, k)}{\mathrm{sr}(A)}. \tag{32}$$

Let $\tilde{\mathbf{A}}$ *satisfy Equation* (27) *for*

$$\mu = \frac{\varepsilon^3 \mathrm{sr}(\mathbf{A})^3}{125 k^4}. \tag{33}$$

Then

$$\sum_{i=1}^{n} |T^k(i) - \tilde{T}^k(i)| \leq \frac{\varepsilon \|\mathbf{A}\|_{\mathrm{F}}^2}{\|\mathbf{A} - \mathbf{A}_k\|_{\mathrm{F}}^2} \sum_{i=1}^{n} T^k(i).$$

Proof. By Equations (26) and (29), we have

$$\sum_{i=1}^{n} |T^k(i) - \tilde{T}^k(i)| = \sum_{i=1}^{n} |\|e_i^T \mathbf{U}_k \mathbf{\Sigma}_k\|_2^2 - \|e_i^T \tilde{\mathbf{U}}_k \tilde{\mathbf{\Sigma}}_k\|_2^2| = \sum_{i=1}^{n} |e_i^t \mathbf{U}_k \mathbf{\Sigma}_k^2 \mathbf{U}_k^T e_i - e_i^t \tilde{\mathbf{U}}_k \tilde{\mathbf{\Sigma}}_k^2 \tilde{\mathbf{U}}_k^T e_i|$$

Let $\mathbf{C} = \mathbf{U}_k \mathbf{\Sigma}_k^2 \mathbf{U}_k^T - \tilde{\mathbf{U}}_k \tilde{\mathbf{\Sigma}}_k^2 \tilde{\mathbf{U}}_k^T$. Then $\mathrm{rank}(\mathbf{C}) \leq 2k$. We now bound its operator norm as follows

$$\|\mathbf{C}\| \leq \|\mathbf{U}_k \mathbf{\Sigma}_k^2 \mathbf{U}_k^T - \tilde{\mathbf{U}}_k \mathbf{\Sigma}_k^2 \tilde{\mathbf{U}}_k^T\| + \|\tilde{\mathbf{U}}_k (\mathbf{\Sigma}_k^2 - \tilde{\mathbf{\Sigma}}_k^2) \tilde{\mathbf{U}}_k^T\|.$$

To bound the first term, we use Theorem 4 (the condition on μ holds by our choice of ε in Equation (32) and μ in Equation (33)) to get

$$\|\mathbf{U}_{\leq k} \mathbf{\Sigma}_k^2 \mathbf{U}_{\leq k}^t - \tilde{\mathbf{U}}_{\leq k} \mathbf{\Sigma}_k^2 \tilde{\mathbf{U}}_{\leq k}^t\| \leq 4\sigma_1(\mathbf{A})^2 (\mu k)^{1/3}.$$

For the second term, we use

$$\|\tilde{\mathbf{U}}_k(\boldsymbol{\Sigma}_k^2 - \tilde{\boldsymbol{\Sigma}}_k^2)\tilde{\mathbf{U}}_k^T\| \leq \|\boldsymbol{\Sigma}_k^2 - \tilde{\boldsymbol{\Sigma}}_k^2\| \leq \mu\sigma_1(\mathbf{A})^2.$$

Overall, we get $\|\mathbf{C}\| \leq 5\sigma(\mathbf{A})^2(\mu k)^{1/3}$. So applying Lemma 7, we get

$$\sum_{i=1}^n |e_i^t \mathbf{U}_k \boldsymbol{\Sigma}_k^2 \mathbf{U}_k^T e_i - e_i^t \tilde{\mathbf{U}}_k \tilde{\boldsymbol{\Sigma}}_k^2 \tilde{\mathbf{U}}_k^T e_i| \leq 5\sigma(\mathbf{A})^2 (\mu k)^{1/3} \cdot 2k$$

$$\leq 5\sigma(\mathbf{A})^2 \mu^{1/3} k^{4/3}$$

$$\leq \varepsilon \mathrm{sr}(\mathbf{A})\sigma(\mathbf{A})^2 = \varepsilon\|\mathbf{A}\|_\mathrm{F}^2.$$

In order to obtain the result in the form stated in the Lemma, note that $\sum_{i=1}^n T^k(i) = \|\mathbf{A} - \mathbf{A}_k\|_\mathrm{F}^2$. ∎

Typically, we expect $\|\mathbf{A} - \mathbf{A}_k\|_\mathrm{F}^2$ to be a constant fraction of $\|\mathbf{A}\|_\mathrm{F}^2$. Hence the guarantee above says that on average, we get good additive guarantees.

C.2 Guarantees for random projections

Theorem 10. *[29, 30] Consider any matrix $\mathbf{A} \in \mathbb{R}^{n \times d}$. Let $\mathbf{R} = (1/\sqrt{\ell})\mathbf{X}$ where $\mathbf{X} \in \mathbb{R}^{d \times \ell}$ is a random matrix drawn from any of the following distributions of matrices. Let $\tilde{\mathbf{A}} = \mathbf{AR}$. Then with probability $1 - \delta$,*

$$\|\mathbf{A}\mathbf{A}^T - \tilde{\mathbf{A}}\tilde{\mathbf{A}}^T\| \leq \mu\|\mathbf{A}\|^2.$$

1. *$\mathbf{R}$ is a dense random matrix with each entry being an i.i.d. sub-Gaussian random variable and $\ell = O(\frac{\mathrm{sr}(A) + \log(1/\delta)}{\epsilon^2})$.*

2. *$\mathbf{R}$ is a fully sparse embedding matrix , where each column has a single ± 1 in a random position (sign and position chosen uniformly and independently) and $\ell = O(\frac{\mathrm{sr}(A)^2}{\epsilon^2 \delta})$. Additionally, the same matrix family except where the position and sign for each column are determined by a 4-independent hash function.*

3. *$\mathbf{R}$ is a Subsampled Randomized Hadamard Transform (SRHT) [41] with $\ell = O(\frac{\mathrm{sr}(A) + \log(1/(\epsilon\delta))}{\epsilon^2}) \log(\mathrm{sr}(A)/\delta)$.*

4. *$\mathbf{R}$ is a dense random matrix with each entry being $\pm\sqrt{\frac{1}{\ell}}$ for $\ell = O(\frac{\mathrm{sr}(A) + \log(1/\delta)}{\epsilon^2})$ and the entries are drawn from a $\log(\mathrm{sr}(A)/\delta)$-wise independent family of hash functions. Such a hash family can be constructed with $O(\log(d) \log(\mathrm{sr}(A)/\delta))$ random bits use standard techniques (see for e.g. Vadhan [28] Sec 3.5.5).*

Using Theorem 10 along with Lemma 8 and Lemma 9 and with the condition that $\mathrm{sr}(A) = O(k)$ gives Theorem 3 from the introduction—which shows that taking a random projection with $\ell = k^3 \cdot \mathrm{poly}(\Delta, \varepsilon^{-1})$ ensures that the error guarantees in Lemma 8 and Lemma 9 hold with high probability.

C.3 Results on subsampling based sketches

Subsampling based sketches can yield both row and column space approximations. The algorithm for preserving the row space, i.e. approximating $\mathbf{A}^T\mathbf{A}$, using row subsampling is straightforward. The sketch samples ℓ rows of $\mathbf{A}$ proportional to their squared lengths to obtain a sketch $\tilde{\mathbf{A}} \in \mathbb{R}^{\ell \times d}$. This can be done in a single pass in a row streaming model using reservoir sampling. Our streaming algorithm for approximating anomaly scores using row subsampling follows the same outline as Algorithm 1 for Frequent Directions. We also obtain the same guarantees as Theorem 1 for Frequent Directions, using the guarantee for subsampling sketches stated at the end of the section (in Theorem 11). The guarantees in Theorem 1 are satisfied by subsampling $\ell = k^2 \cdot \mathrm{poly}(\kappa, \varepsilon^{-1}, \Delta)$ columns, and the algorithm needs $O(d\ell)$ space and $O(nd)$ time.

In order to preserve the column space using subsampling, i.e. approximate $\mathbf{A}\mathbf{A}^T$, we need to subsample the columns of the matrix. Our streaming algorithm follows a similar outline as Algorithm 2

which does a random projections of the rows and also approximates $\mathbf{A}\mathbf{A}^T$. However, there is a subtlety involved. We need to subsample the columns, but the matrix is arrives in row-streaming order. We show that using an additional pass, we can subsample the columns of $\mathbf{A}$ based on their squared lengths. This additional pass does reservoir sampling on the squared entries of the matrix, and uses the column index of the sampled entry as the column to be subsampled. The algorithm is stated in Algorithm 3. It requires space $O(\ell \log d)$ in order to store the ℓ indices to subsample, and space $O(\ell^2)$ to store the covariance matrix of the subsampled data. Using the guarantees for subsampling in Theorem 11, we can get the same guarantees for approximating anomaly scores as for a random projection of the rows. The guarantees for random projection in Theorem 10 are satisfied by subsampling $\ell = k^3 \cdot \text{poly}(\varepsilon^{-1}, \Delta)$ columns, and the algorithm needs $O(d\ell + \log d)$ space and $O(nd)$ time.

Algorithm 3: Algorithm to approximate anomaly scores using column subsampling

Input: Choice of k and ℓ.
Initialization
  Set covariance $\tilde{\mathbf{A}}^T \tilde{\mathbf{A}} \leftarrow 0$
  For $1 \leq t \leq \ell$, set $S_t = 1$ $\triangleright$ S_i stores the ℓ column indices we will subsample
  Set $s \rightarrow 0$ $\triangleright$ s stores the sum of the squares of entries seen so far
Zeroth Pass: *As each element a_{ij} of $\mathbf{A}$ streams in,*
  Update $s \rightarrow s + a_{ij}^2$
  for $1 \leq t \leq \ell$ **do**
    Set $S_t \rightarrow j$ with probability a_{ij}^2/s
First Pass: *As each row $a_{(i)}$ streams in,*
  Project by $\mathbf{R}$ to get $\mathbf{R}^T a_{(i)}$
  Update covariance $\tilde{\mathbf{A}}^T \tilde{\mathbf{A}} \leftarrow \tilde{\mathbf{A}}^T \tilde{\mathbf{A}} + (\mathbf{R}^T a_{(i)})(\mathbf{R}^T a_{(i)})^T$
SVD:
  Compute the top k right singular vectors of $\tilde{\mathbf{A}}^T \tilde{\mathbf{A}}$
Second Pass: *As each row $a_{(i)}$ streams in,*
  Project by $\mathbf{R}$ to get $\mathbf{R}^T a_{(i)}$
  For each projected row, use the estimated right singular vectors to compute the leverage scores and projection distances

---

Guarantees for subsampling based sketches. Drineas et al. [19] showed that sampling columns proportional to their squared lengths approximates $\mathbf{A}\mathbf{A}^T$ with high probability. They show a stronger Frobenius norm guarantee than the operator norm guarantee that we need, but this worsens the dependence on the stable rank. We will instead use the following guarantee due to Magen and Zouzias [31].

Theorem 11. *[31] Consider any matrix $\mathbf{A} \in \mathbb{R}^{n \times d}$. Let $\tilde{\mathbf{A}} \in \mathbb{R}^{n \times \ell}$ be a matrix obtained by subsampling the columns of $\mathbf{A}$ with probability proportional to their squared lengths. Then with probability $1 - 1/\text{poly}(\text{sr}(\mathbf{A}))$, for $\ell \geq \text{sr}(\mathbf{A}) \log(\text{sr}(\mathbf{A})/\mu^2)/\mu^2$*

$$\|\mathbf{A}\mathbf{A}^T - \tilde{\mathbf{A}}\tilde{\mathbf{A}}^T\| \leq \mu \|\mathbf{A}\|^2.$$

D Streaming Lower Bounds

In this section we prove lower bounds on streaming algorithms for computing leverage scores, rank k leverage scores and ridge leverage scores for small values of λ. Our lower bounds are based on reductions from the multi party set disjointness problem denoted as $\text{DISJ}_{t,d}$. In this problem, each of t parties is given a set from the universe $[d] = \{1, 2, \ldots, d\}$, together with the promise that either the sets are *uniquely intersecting*, i.e. all sets have exactly one element in common, or the sets are pairwise disjoint. The parties also have access to a common source of random bits. Chakrabarti et al. [43] showed a $\Omega(d/(t \log t))$ lower bound on the communication complexity of this problem. As usual, the lower bound on the communication in the set-disjointness problem translates to a lower bound on the space complexity of the streaming algorithm.

Theorem 12. *For sufficiently large d and $n \geq O(d)$, let the input matrix be $\mathbf{A} \in \mathbb{R}^{n \times d}$. Consider a row-wise streaming model the algorithm may make a constant number passes over the data.*

1. *Any randomized algorithm which computes a $\sqrt{t}$-approximation to all the leverage scores for every matrix $\mathbf{A}$ with probability at least $2/3$ and with p passes over the data uses space $\Omega(d/(t^2 p \log t))$.*

2. *For $\lambda \leq \frac{\operatorname{sr}(\mathbf{A})}{2d} \sigma_1(\mathbf{A})^2$, any randomized streaming algorithm which computes a $\sqrt{t/2}$-approximation to all the λ-ridge leverage scores for every matrix $\mathbf{A}$ with p passes over the data with probability at least $2/3$ uses space $\Omega(d/(pt^2 \log t))$.*

3. *For $2 \leq k \leq d/2$, any randomized streaming algorithm which computes any multiplicative approximation to all the rank k leverage scores for every matrix $\mathbf{A}$ using p passes and with probability at least $2/3$ uses space $\Omega(d/p)$.*

4. *For $2 \leq k \leq d/2$, any randomized algorithm which computes any multiplicative approximation to the distances from the principal k-dimensional subspace of every row for every matrix $\mathbf{A}$ with p passes and with probability at least $2/3$ uses space $\Omega(d/p)$.*

We make a few remarks:

- The lower bounds are independent of the stable rank of the matrix. Indeed they hold both when $\operatorname{sr}(\mathbf{A}) = o(d)$ and when $\operatorname{sr}(\mathbf{A}) = \Theta(d)$.
- The Theorem is concerned only with the working space; the algorithms are permitted to have separate access to a random string.
- In the first two cases an additional $\log t$ factor in the space requirement can be obtained if we limit the streaming algorithm to one pass over the data.

Note that Theorem 12 shows that the Frequent Directions sketch for computing outlier scores is close to optimal as it uses $O(d\ell)$ space, where the projection dimension ℓ is a constant for many relevant parameter regimes. The lower bound also shows that the average case guarantees for the random projection based sketch which uses working space $O(\ell^2)$ cannot be improved to a point-wise approximation. The proof of the theorem is in Appendix G.

E   Proofs of Section 2

We will prove bounds for items (2) and (3), which are given by Theorems 4 and 6 respectively. To prove these, the next two technical lemmas give perturbation bounds on the operator norm of positive semi-definite matrices of the from $\mathbf{U}_k \mathbf{\Lambda} \mathbf{U}_k^T$, where $\mathbf{\Lambda}$ is a diagonal matrix with non-negative entries. In order to do this, we split the matrix $\mathbf{\Sigma}$ to a well-separated component and a small residual component.

We now describe the decomposition of $\mathbf{\Sigma}$. Let δ be a parameter so that

$$6\mu \leq \delta \leq \Delta \tag{34}$$

We partition the indices $[k]$ into a set of disjoint intervals $B(\mathbf{A}, \delta) = \{B_1, \ldots, B_m\}$ based on the singular values of $\mathbf{A}$ so that there is a separation of at least $\delta\sigma_1^2$ between intervals, and at most $\delta\sigma_1^2$ within an interval. Formally, we start with $i = 1$ assigned to B_1. For $i \geq 2$, assume that we have assigned $i - 1$ to B_j. If

$$\sigma_i^2(\mathbf{A}) - \sigma_{i-1}^2(\mathbf{A}) \leq \delta\sigma_1^2(\mathbf{A})$$

then i is also assigned to B_j, whereas if

$$\sigma_i^2(\mathbf{A}) - \sigma_{i-1}^2(\mathbf{A}) > \delta\sigma_1^2(\mathbf{A})$$

then it is assigned to a new bucket B_{j+1}. Let b_j denote the largest index in the interval B_j for $j \in [m]$.

Let $\mathbf{\Lambda} = \operatorname{diag}(\lambda_1, \ldots \lambda_k)$ be a diagonal matrix with all non-negative entries which is constant on each interval B_j and non-increasing across intervals. In other words, if $i \geq j$, then $\lambda_i \geq \lambda_j$, with equality holding whenever i, j belong to the same interval B_k. Call such a matrix a *diagonal non-decreasing matrix with respect to $B(\mathbf{A}, \delta)$*. Similarly, we define diagonal non-increasing matrices with respect to $B(\mathbf{A}, \delta)$ to be non-increasing but are constant on each interval B_k. The following is the main technical lemma in this section, and handles the case where the diagonal matrix is well-separated.

It is a generalization of Lemma 6. In Lemma 6 we assumed that the eigenvalues in each bucket are equal, here we generalize to the case where the eigenvalues in each bucket are separated by at most $\delta\sigma_1^2(\mathbf{A})$.

Lemma 10. *Let $6\mu \leq \delta \leq \Delta$. Let $\mathbf{\Lambda} = \mathrm{diag}(\lambda_1, \ldots \lambda_k)$ be a diagonal non-increasing or a diagonal non-decreasing matrix with respect to $B(\mathbf{A}, \delta)$. Then*

$$\|\mathbf{U}_k\mathbf{\Lambda}\mathbf{U}_k^T - \tilde{\mathbf{U}}_k\mathbf{\Lambda}\tilde{\mathbf{U}}_k^T\| \leq 4\|\mathbf{\Lambda}\|\sqrt{\frac{\mu}{\delta}}.$$

Proof. Let us set $\lambda_{b_{m+1}} = 0$ for convenience. Since

$$\mathbf{U}_{b_j}\mathbf{U}_{b_j}^T = \sum_{i=1}^{b_j} u^{(i)}u^{(i)T}$$

we can write

$$\mathbf{U}_k\mathbf{\Lambda}\mathbf{U}_k^T = \sum_{j=1}^{m}\lambda_{b_j}\sum_{i\in B_j} u^{(i)}u^{(i)T} = \sum_{j=1}^{m}(\lambda_{b_j} - \lambda_{b_{j+1}})\mathbf{U}_{b_j}\mathbf{U}_{b_j}^T$$

and similarly for $\tilde{\mathbf{U}}_k\mathbf{\Lambda}\tilde{\mathbf{U}}_k^T$. So we can write

$$\mathbf{U}_k\mathbf{\Lambda}\mathbf{U}_k^T - \tilde{\mathbf{U}}_k\mathbf{\Lambda}\tilde{\mathbf{U}}_k^T = \sum_{j=1}^{m}(\lambda_{b_j} - \lambda_{b_{j+1}})(\mathbf{U}_{b_j}\mathbf{U}_{b_j}^T - \tilde{\mathbf{U}}_{b_j}\tilde{\mathbf{U}}_{b_j}^T).$$

Therefore, by the triangle inequality and Lemma 5,

$$\|\mathbf{U}_k\mathbf{\Lambda}\mathbf{U}_k^T - \tilde{\mathbf{U}}_k\mathbf{\Lambda}\tilde{\mathbf{U}}_k^T\| = \sum_{j=1}^{m}|\lambda_{b_j} - \lambda_{b_{j+1}}|\|(\mathbf{U}_{b_j}\mathbf{U}_{b_j}^T - \tilde{\mathbf{U}}_{b_j}\tilde{\mathbf{U}}_{b_j}^T)\| \leq 2\sqrt{\frac{\mu}{\delta}}\sum_{j=1}^{m}|\lambda_{b_j} - \lambda_{b_{j+1}}|$$

thus proving that $\sum_{j=1}^{m}|\lambda_{b_j} - \lambda_{b_{j+1}}| \leq 2\|\mathbf{\Lambda}\|$ would imply the claim.

When $\mathbf{\Lambda}$ is diagonal non-increasing with respect to $B(\mathbf{A}, \delta)$, then $\lambda_{b_j} - \lambda_{b_{j+1}} \geq 0$ for all $j \in [m]$, and $\|\mathbf{\Lambda}\| = \lambda_{b_1}$. Hence

$$\sum_{j=1}^{m}|\lambda_{b_j} - \lambda_{b_{j+1}}| = \sum_{j=1}^{m}(\lambda_{b_j} - \lambda_{b_{j+1}}) = \lambda_{b_1} - \lambda_{b_{m+1}} = \|\mathbf{\Lambda}\|.$$

When $\mathbf{\Lambda}$ is diagonal non-decreasing with respect to $B(\mathbf{A}, \delta)$, then for $j \leq m - 1$, $\lambda_{b_j} \leq \lambda_{b_{j+1}}$, and $\|\mathbf{\Lambda}\| = \lambda_{b_m}$. Hence

$$\sum_{j=1}^{m-1}|\lambda_{b_j} - \lambda_{b_{j+1}}| = \sum_{j=1}^{m-1}\lambda_{b_{j+1}} - \lambda_{b_j} = \lambda_{b_m} - \lambda_{b_1} \leq \lambda_{b_m}$$

whereas $|\lambda_{b_m} - \lambda_{b_{m+1}}| = \lambda_{b_m}$. Thus overall,

$$\sum_{j=1}^{m}|\lambda_{b_j} - \lambda_{b_{j+1}}| \leq 2\lambda_{b_m} = 2\|\mathbf{\Lambda}\|.$$
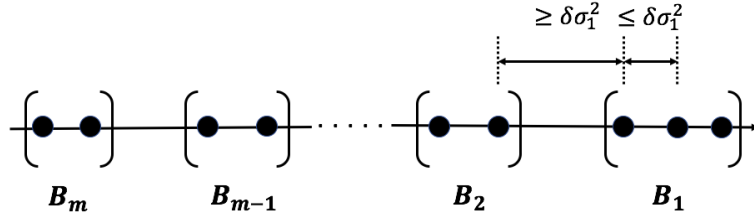
■

Figure 5: Illustration of the decomposition of the k singular values into m intervals such that there is a separation of at least $\delta\sigma_1^2$ between intervals, and at most $\delta\sigma_1^2$ within an interval.

We use this to prove our perturbation bound for $\mathbf{U}_k\boldsymbol{\Sigma}_k^2\mathbf{U}_k^T$.

Theorem 4. *Let $\mu \leq \min(\Delta^3 k^2, 1/(20k))$.*

$$\|\mathbf{U}_k\boldsymbol{\Sigma}_k^2\mathbf{U}_k^T - \tilde{\mathbf{U}}_k\boldsymbol{\Sigma}_k^2\tilde{\mathbf{U}}_k^T\| \leq 8\sigma_1^2(\mu k)^{1/3}.$$

Proof. Define $\boldsymbol{\Lambda}$ to be the $k \times k$ diagonal non-increasing matrix such that all the entries in the interval B_j are $\sigma_{b_j}^2$. Define $\boldsymbol{\Omega}$ to be the $k \times k$ diagonal matrix such that $\boldsymbol{\Lambda} + \boldsymbol{\Omega} = \boldsymbol{\Sigma}_k^2$. With this notation,

$$\|\mathbf{U}_k\boldsymbol{\Sigma}_k^2\mathbf{U}_k^T - \tilde{\mathbf{U}}_k\boldsymbol{\Sigma}_k^2\tilde{\mathbf{U}}_k^T\| = \|(\mathbf{U}_k\boldsymbol{\Lambda}\mathbf{U}_k^T - \tilde{\mathbf{U}}_k\boldsymbol{\Lambda}\tilde{\mathbf{U}}_k^T) + (\mathbf{U}_k\boldsymbol{\Omega}\mathbf{U}_k^T - \tilde{\mathbf{U}}_k\boldsymbol{\Omega}\tilde{\mathbf{U}}_k^T)\|$$
$$\leq \|\mathbf{U}_k\boldsymbol{\Lambda}\mathbf{U}_k^T - \tilde{\mathbf{U}}_k\boldsymbol{\Lambda}\tilde{\mathbf{U}}_k^T\| + \|\mathbf{U}_k\boldsymbol{\Omega}\mathbf{U}_k^T - \tilde{\mathbf{U}}_k\boldsymbol{\Omega}\tilde{\mathbf{U}}_k^T)\| \qquad (35)$$

By definition, $\boldsymbol{\Lambda}$ is diagonal non-increasing, $\|\boldsymbol{\Lambda}\| = \sigma_{b_1}^2 \leq \sigma_1^2$. Hence by part (1) of Lemma 10,

$$\|\mathbf{U}_k\boldsymbol{\Lambda}\mathbf{U}_k^T - \tilde{\mathbf{U}}_k\boldsymbol{\Lambda}\tilde{\mathbf{U}}_k^T\| \leq 4\sigma_1^2\sqrt{\frac{\mu}{\delta}}.$$

By our definition of the B_js, if $i, i+1 \in B_j$ then $\sigma_i^2 - \sigma_{i+1}^2 \leq \delta\sigma_1^2$, hence for any pair i, i' $in B_j$, $\sigma_i^2 - \sigma_{i'}^2 \leq k\delta\sigma_1^2$. Hence

$$\|\boldsymbol{\Omega}\| = \max_{i \in B_j}(\sigma_i^2 - \sigma_{b_j}^2) \leq k\delta\sigma_1^2$$

We use Lemma 4 to get

$$\|\mathbf{U}_k\boldsymbol{\Omega}\mathbf{U}_k^T - \tilde{\mathbf{U}}_k\boldsymbol{\Omega}\tilde{\mathbf{U}}_k^T\| \leq 2k\delta\sigma_1^2.$$

Plugging these bounds into Equation (35), we get

$$\|\mathbf{U}_k\boldsymbol{\Sigma}_k^2\mathbf{U}_k^T - \tilde{\mathbf{U}}_k\boldsymbol{\Sigma}_k^2\tilde{\mathbf{U}}_k^T\| \leq 4\sigma_1^2(\sqrt{\frac{\mu}{\delta}} + k\delta).$$

We choose $\delta = \mu^{1/3}/k^{2/3}$ that minimizes the RHS, to get

$$\|\mathbf{U}_k\boldsymbol{\Sigma}_k^2\mathbf{U}_k^T - \tilde{\mathbf{U}}_k\boldsymbol{\Sigma}_k^2\tilde{\mathbf{U}}_k^T\| \leq 8\sigma_1^2(\mu k)^{1/3}.$$

We need to ensure that this choice satisfies $6\mu \leq \delta$. This holds since it is equivalent to $6(\mu k)^{2/3} \leq 1$, which is implied by $\mu k \leq 1/20$. We need $\delta \leq \Delta$ which holds since $\mu \leq \Delta^3 k^2$. ∎

Next we derive our perturbation bound for $\mathbf{U}_k\boldsymbol{\Sigma}_k^{-2}\mathbf{U}_k^T$, which will depend on the condition number $\kappa = \sigma_1^2/\sigma_k^2$. The proof is similar to the proof of Theorem 4.

Theorem 6. *Let κ_k denote the condition number $\kappa_k = \sigma_1^2/\sigma_k^2$. Let $\mu \leq \min(\Delta^3(k\kappa_k)^2, 1/(20k\kappa_k))$. Then,*

$$\|\mathbf{U}_k\boldsymbol{\Sigma}_k^{-2}\mathbf{U}_k^T - \tilde{\mathbf{U}}_k\boldsymbol{\Sigma}_k^{-2}\tilde{\mathbf{U}}_k^T\| \leq \frac{8}{\sigma_k^2}(\mu k\kappa_k)^{1/3}.$$

Proof. We use a similar decomposition as in Theorem 4. Define $\boldsymbol{\Lambda}$ to be diagonal non-decreasing such that all the entries in the interval B_j are $1/\sigma_{b_j}^2$. Note that $\|\boldsymbol{\Lambda}\| \leq \sigma_k^{-2}$. Using Lemma 10, we get

$$\|\mathbf{U}_k\boldsymbol{\Lambda}_k^{-2}\mathbf{U}_k^T - \tilde{\mathbf{U}}_k\boldsymbol{\Lambda}\tilde{\mathbf{U}}_k^T\| \leq \frac{4}{\sigma_k^2}\sqrt{\frac{\mu}{\delta}}. \qquad (36)$$

Define $\boldsymbol{\Omega} = \boldsymbol{\Sigma}_k^{-2} - \boldsymbol{\Lambda}$. Note that

$$\|\boldsymbol{\Omega}\| = \max_{i \in B_j}\frac{1}{\sigma_{b_j}^2} - \frac{1}{\sigma_i^2} = \max_{i \in B_j}\frac{\sigma_i^2 - \sigma_{b_j}^2}{\sigma_i^2\sigma_{b_j}^2} \leq \frac{k\delta\sigma_1^2}{\sigma_k^4} = \frac{k\kappa\delta}{\sigma_k^2}.$$

By using this in Lemma 4,

$$\|\mathbf{U}_k\boldsymbol{\Omega}\mathbf{U}_k^T - \tilde{\mathbf{U}}_k\boldsymbol{\Omega}\tilde{\mathbf{U}}_k^T\| \leq \frac{2k\kappa\delta}{\sigma_k^2}. \qquad (37)$$

Putting Equation (36) and (37) together, we get

$$\|\mathbf{U}_k\boldsymbol{\Sigma}_k^{-2}\mathbf{U}_k^T - \tilde{\mathbf{U}}_k\boldsymbol{\Sigma}_k^{-2}\tilde{\mathbf{U}}_k^T\| \leq \frac{4}{\sigma_k^2}\left(\sqrt{\frac{\mu}{\delta}} + k\kappa\delta\right).$$

The optimum value of δ is $\mu^{1/3}/(k\kappa)^{2/3}$ which gives the claimed bound. A routine calculation shows that the condition $6\mu \leq \delta \leq \Delta$ holds because $\mu \leq \min(\Delta^3(k\kappa)^2, 1/(20k\kappa))$. ∎

F   Ridge Leverage Scores

Regularizing the spectrum (or alternately, assuming that the data itself has some ambient Gaussian noise) is closely tied to the notion of ridge leverage scores [44]. Various versions of ridge leverages had been shown to be good estimators for the Mahalanobis distance in the high dimensional case and were demonstrated to be an effective tool for anomaly detection [25]. There are efficient sketches that approximate the ridge leverage score for specific values of the parameter λ [45].

Recall that we measured deviation in the tail by the distance from the principal k-dimensional subspace, given by

$$T^k(i) = \sum_{j=k+1}^{d} \alpha_j^2.$$

We prefer this to using

$$L_i^{>k} := \sum_{j=k+1}^{d} \frac{\alpha_j^2}{\sigma_j^2}$$

since it is more robust to the small σ_j, and is easier to compute in the streaming setting.[5]

An alternative approach is to consider the ridge leverage scores, which effectively replaces the covariance matrix $\mathbf{A}^T\mathbf{A}$ with $\mathbf{A}^T\mathbf{A} + \lambda\mathbf{I}$, which increases all the singular values by λ, with the effect of damping the effect of small singular values. We have

$$L_\lambda(i) = \sum_{j=1}^{d} \frac{\alpha_j^2}{\sigma_j^2 + \lambda}.$$

Consider the case when the data is generated from a true k-dimensional distribution, and then corrupted with a small amount of white noise. It is easy to see that the data points will satisfy both concentration and separation assumptions. In this case, all the notions suggested above will essentially converge. In this case, we expect $\sigma_{k+1}^2 \approx \cdots \approx \sigma_n^2$. So

$$L_i^{>k} = \sum_{j=k+1}^{d} \frac{\alpha_j^2}{\sigma_j^2} \approx \frac{T^k(i)}{\sigma_{k+1}^2}.$$

If λ is chosen so that $\sigma_k^2 \gg \lambda \gg \sigma_{k+1}^2$, it follows that

$$L_\lambda(i) \approx L^k(i) + \frac{T^k(i)}{\lambda}.$$

G   Proof of Theorem 12: Streaming Lower Bounds

Proof.   We describe the reduction from $\mathrm{DISJ}_{t,d}$ to computing each of the four quantities.

(1) **Leverage scores:**   Say for contradiction we have an algorithm which computes a $\sqrt{t}$-approximation to all the leverage scores for every matrix $\mathbf{A} \in \mathbb{R}^{n \times d}$ using space $O(d/(kt^2 \log t))$ and $k = O(1)$ passes. We will use this algorithm to design a protocol for $\mathrm{DISJ}_{t,d}$ using a communication complexity of $O(d/(t \log t))$. In other words we need the following lemma.

Lemma 11.   *A streaming algorithm which approximates all leverage scores within $\sqrt{t}$ with p passes over the data, and which uses space s implies a protocol for $\mathrm{DISJ}_{t,d}$ with communication complexity $s \cdot p \cdot t$*

Proof.   Given an $\mathrm{DISJ}_{t,d}$ instance, we create a matrix $\mathbf{A}$ with d columns as follows: Let e_i be the ith row of the $(d \times d)$ identity matrix $\mathbf{I}_{d \times d}$. The vector e_i is associated with the ith element of the universe $[d]$. Each player j prepares a matrix $\mathbf{A}_j$ with d columns by adding the row e_i for each $i \in [d]$ in its set. $\mathbf{A}$ is composed of the rows of the t matrices $\mathbf{A}_j$.

---

[5]Although the latter measure is also studied in the literature and may be preferred in settings where there is structure in the tail.

We claim that $\sqrt{t}$ approximation to the leverage scores of $\mathbf{A}$ suffices to differentiate between the case the sets are disjoint and the case they are uniquely intersecting. To see this note that if the sets are all disjoint then each row is linearly independent from the rest and therefore all rows have leverage score 1. If the sets are *uniquely intersecting*, then exactly one row in $\mathbf{A}$ is repeated t times. A moment's reflection reveals that in this case, each of these rows has leverage score $1/t$. Hence a $\sqrt{t}$-approximation to all leverage scores allows the parties to distinguish between the two cases.

The actual communication protocol is now straight forward. Each party i in turn runs the algorithm over its own matrix $\mathbf{A}_i$ and passes the s bits which are the state of the algorithm to the party $i+1$. The last party outputs the result. If the algorithm requires p passes over the data the total communication is $p \cdot s \cdot t$. ∎

Theorem 12 now follows directly from the lower bound on the communication complexity of $\mathrm{DISJ}_{t,d}$.

Note that in the construction above the stable rank $\mathrm{sr}(\mathbf{A})$ is $\Theta(d)$. The dependency on d could be avoided by adding a row and column to $\mathbf{A}$: A column of all zeros is added to $\mathbf{A}$ and then the last party adds a row to $\mathbf{A}_t$ having the entry $\sqrt{K} \geq 1$ in the last column. Now since $K > 1$ the last row will dominate both the Frobenius and the operator norm of the matrix but does not affect the leverage score of the other rows. Note that $\mathrm{sr}(\mathbf{A}) \leq \frac{K+d}{K}$. By choosing K large enough, we can now decrease $\mathrm{sr}(\mathbf{A})$ to be arbitrarily close to 1. Note also that if the algorithm is restricted to one pass, the resulting protocol is one directional and has a slightly higher lower bound of $\Omega(d/t^2)$.

(2) **Ridge leverage scores:** We use the same construction as before and multiply $\mathbf{A}$ by $\sigma \geq \sqrt{\lambda}$. Note that as required, the matrix $\mathbf{A}$ has operator norm σ. As before, it is sufficient to claim that by approximately computing all ridge leverage scores the parties can distinguish between the case their sets are mutually disjoint and the case they are uniquely intersecting. Indeed, if the sets are mutually disjoint then all rows have ridge leverage scores $\frac{\sigma^2}{\sigma^2+\lambda}$. If the sets are uniquely intersecting, then exactly one element is repeated t times in the matrix $\mathbf{A}$, in which case this element has ridge leverage score $\frac{\sigma^2}{t\sigma^2+\lambda}$. These two cases can be distinguished by a $\sqrt{t/2}$-approximation to the ridge leverage scores if $\lambda \leq \sigma^2$.

To modify the stable rank $\mathrm{sr}(\mathbf{A})$ in this case we do the same trick as before, add a column of zeros and the last party adds an additional row having the entry $\sqrt{K}\sigma \geq \sigma$ in its last column. Note that $\mathrm{sr}(\mathbf{A}) \leq \frac{K+d}{K}$, and by increasing K we can decrease $\mathrm{sr}(\mathbf{A})$ as necessary. However, $\|\mathbf{A}\|^2$ now equals $K\sigma^2$, and hence we need to upper bound K in terms of the stable rank $\mathrm{sr}(\mathbf{A})$ to state the final bound for λ in terms of $\|\mathbf{A}\|^2$. Note that $\mathrm{sr}(\mathbf{A}) \leq \frac{K+d}{K} \implies K \leq 2d/\mathrm{sr}(\mathbf{A})$. Hence $\lambda \leq \frac{\mathrm{sr}(\mathbf{A})}{2d}\|\mathbf{A}\|^2$ ensures that $\lambda \leq \sigma^2$.

(3) **Rank-k leverage scores:** The construction is similar to the previous ones, with some modifications to ensure that the top k singular vectors are well defined. We set number of parties to be 2, and let the universe be of size $d' = d - k$, so the matrix is wider that the size of universe by k columns. As before, for $i \leq d'$ the i'th row of $\mathbf{I}_{d \times d}$ is associated with the i'th element of the universe $[d']$. The first set of rows in $\mathbf{A}$ are the rows corresponding to the elements in the first party's set and the next set of rows in $\mathbf{A}$ correspond to the elements in the second party's set. The second party also adds the last k rows of $\mathbf{I}_{d \times d}$, scaled by 1.1, to the matrix $\mathbf{A}$.

We claim that by computing a multiplicative approximation to all rank k leverage scores the parties can determine whether their sets are disjoint. If the sets are all disjoint, then the top k right singular vectors correspond to the last k rows of the matrix $\mathbf{I}_{d \times d}$, and these are orthogonal to the rest of the matrix and hence the rank k leverage scores of all rows except the additional ones added by the second party are all 0. If the sets are intersecting, then the row corresponding to the intersecting element is the top right singular vector of $\mathbf{A}$, as it has singular value $\sqrt{2} > 1.1$. Hence the rank k leverage score of this row is $1/2$. Hence the parties can distinguish whether they have disjoint sets by finding any multiplicative approximation to all rank k leverage scores.

We apply a final modification to decrease the stable rank $\mathrm{sr}(\mathbf{A})$ as necessary. We scale the dth row of $\mathbf{I}_{d \times d}$ by a constant $\sqrt{K}$. Note that $\mathrm{sr}(\mathbf{A}) \leq \frac{K+d+2k}{K}$. By choosing K accordingly, we can now decrease $\mathrm{sr}(\mathbf{A})$ as desired. We now examine how this scaling affects the rank k leverage scores for the rows corresponding to the sets. When the sets are not intersecting, the rank k leverage scores

of all the rows corresponding to the set elements are still 0. When the sets are intersecting, the row corresponding to the intersecting element is at the least second largest right singular vector of $\mathbf{A}$ even after the scaling, as $\sqrt{2} > 1.1$. In this case, for $k \geq 2$ the rank k leverage score of this row is 1/2, hence the parties can distinguish whether they have disjoint sets by finding any multiplicative approximation to all rank k leverage scores for any $2 \leq k \leq d/2$.

Distance from principal k-dimensional subspace: We use the same construction as in statement (3). If the sets are non-intersecting, all the rows corresponding to the sets of the two-parties have distance 1 from the principal k-dimensional subspace. If the sets are intersecting, the row corresponding to the element in the intersection has distance 0 from the principal k-dimensional subspace, as that row is either the top or the second right singular vector of $\mathbf{A}$. Hence, any multiplicative approximation could be used to distinguish between the two cases.

■