Online Adaptive Mahalanobis Distance Estimation

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Abstract

Mahalanobis metrics are widely used in machine learning in conjunction with methods like k-nearest neighbors, k-means clustering, and k-medians clustering. Despite their importance, there has not been any prior work on applying sketching techniques to speed up algorithms for Mahalanobis metrics. In this paper, we initiate the study of dimension reduction for Mahalanobis metrics. In particular, we provide efficient data structures for solving the Approximate Distance Estimation (ADE) problem for Mahalanobis distances. We first provide a randomized Monte Carlo data structure. Then, we show how we can adapt it to provide our main data structure which can handle sequences of *adaptive* queries and also online updates to both the Mahalanobis metric matrix and the data points, making it amenable to be used in conjunction with prior algorithms for online learning of Mahalanobis metrics.

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1 Introduction

The choice of metric is critical for the success of a wide range of machine learning tasks, such as k-nearest neighbors, k-means clustering, and k-medians clustering. In many applications, the metric is often not provided explicitly and needs to be learned from data [SSSN04, DKJ+07, JKDG08]. The most common class of such learned metrics is the set of Mahalanobis metrics, which have been shown to have good generalization performance. For a set of points $\mathcal{X} = \{x_1, x_2, \ldots, x_n\} \in \mathbb{R}^d$, a Mahalanobis metric d on $\mathcal{X}$ is characterized by a positive semidefinite matrix $A \in \mathbb{R}^{d\times d}$ such that $d(x_i, x_j) = \sqrt{(x_i - x_j)^\top A(x_i - x_j)}$. Mahalanobis distances are generalizations of traditional Euclidean distances, and they allow for arbitrary linear scaling and rotations of the feature space.

In parallel to the large body of work on learning Mahalanobis metrics, the use of sketching techniques has also become increasingly popular in dealing with real-world data that is often high-dimensional data and also extremely large in terms of the number of data points. In particular, a large body of influential work has focused on sketching for Euclidean distances [JL84, AMS99, CCFC02]. Despite the importance of Mahalanobis metrics in practical machine learning applications, there has not been any prior work focusing on dimension reduction for Mahalanobis distances.

In this paper, we initiate the study of dimension reduction for Mahalanobis distances. In particular, we focus on the Approximate Distance Estimation (ADE) problem [CN20] in which the goal is to build an efficient data structure that can estimate the distance from a given query point to a set of private data points, even when the queries are provided adaptively by an adversary. ADE has many machine learning applications where the input data can be easily manipulated by users and the model accuracy is critical, such as network intrusion detection [BCM+17, CBK09], strategic classification [HMPW16], and autonomous driving [PMG16, LCLS17, PMG+17]. We formulate the ADE problem with a Mahalanobis distance as:

Definition 1 (Approximate Mahalanobis Distance Estimation)**.** *For a Mahalanobis distance characterized by a positive semi-definite matrix $A \in \mathbb{R}^{d\times d}$, given a set of data points $\mathcal{X} = \{x_1, x_2, \ldots, x_n\} \subset \mathbb{R}^d$ and an accuracy parameter $\varepsilon \in (0, 1)$, we need to output a data structure $\mathcal{D}$ such that: Given only $\mathcal{D}$ stored in memory with no direct access to $\mathcal{X}$, our query algorithm must respond to queries of the form $q \in \mathbb{R}^d$ by reporting distance estimates $\widetilde{d}_1, \ldots, \widetilde{d}_n$ satisfying*

$$\forall i \in [n], (1-\varepsilon)\|q - x_i\|_A \le \widetilde{d}_i \le (1+\varepsilon)\|q - x_i\|_A.$$

We also consider an online version of the problem, where the underlying Mahalanobis distance changes over iterations. This is an important problem, because the distance metric A is learned from data and can change over time in many applications of Mahalanobis distances. For example, for an Internet image search application, the continuous collection of input images changes the distance metric A. We formulate our online version of the ADE problem with Mahalanobis distances as follows:

Definition 2 (Online Adaptive Mahalanobis Distance Estimation)**.** *We need to design a data structure that efficiently supports any sequence of the following operations:*

- Initialize($U \in \mathbb{R}^{k\times d}, \{x_1, x_2, \cdots, x_n\} \subset \mathbb{R}^d, \varepsilon \in (0,1), \delta \in (0,1)$). *The data structure takes n data points $\{x_1, x_2, \ldots, x_n\} \subset \mathbb{R}^d$, a $k \times d$ matrix U (which defines the metric with $A = U^\top U$), an accuracy parameter ε and a failure probability δ as input.*
- UpdateU($u \in \mathbb{R}^d, a \in [k]$). *Updates the a-th row of $k \times d$ matrix U.*
- UpdateX($z \in \mathbb{R}^d, i \in [n]$). *Update the data structure with the i-th new data point z.*

- QueryPair($i, j \in [n]$) *Outputs a number* p *such that* $(1-\varepsilon)\|x_i - x_j\|_A \leq p \leq (1+\varepsilon)\cdot\|x_i - x_j\|_A$ *with probability at least* $1-\delta$.
- QueryAll($q \in \mathbb{R}^d$). *Outputs a set of distance estimates* $\{\widetilde{d}_1, \cdots, \widetilde{d}_n\} \subset \mathbb{R}$ *such that* $\forall i \in [n], (1-\varepsilon)\|q - x_i\|_A \leq \widetilde{d}_i \leq (1+\varepsilon)\|q - x_i\|_A$. *with probability at least* $1-\delta$.
- SampleExact($q \in \mathbb{R}^d$). *Sample an index* $i \in [n]$ *with probability* $d_i / \sum_{j=1}^n d_j$

Our randomized data structure(Algorithm 2, 3 and 5) supports approximate Mahalanobis distance estimation with online update to the distance metric matrix and data points even for a sequence of adaptively chosen queries. It also supports samples an index $i \in [n]$ with probability $d_i / \sum_{j=1}^n d_j$.

Roadmap. In Section 2, we discuss related works in online metric learning, sketching, and adaptive distance estimation. In Section 3, we provide some notation used throughout the paper and also provide some background. In Section 5, we demonstrate how we can use the well-known JL sketch [JL84] to design a data-structure which can support Mahalanobis distance estimation. In Section 6, we present our adaptive Mahalanobis distance maintenance data structure and prove its time and correctness guarantees. We provide an experimental evaluation of our data structure in Section 7. We end with our conclusion in Section 8.

2 Related Work

Sketching Sketching is a well-known technique to improve performance or memory complexity [CW13]. It has wide applications in linear algebra, such as linear regression and low-rank approximation[CW13, NN13, MM13, RSW16, SWZ17, HLW17, ALS+18, SWZ19a, SWZ19b, DJS+19, GSZ23, GSYZ23], training over-parameterized neural network [SYZ21, SZZ21, ZHA+21], empirical risk minimization [LSZ19, QSZZ23], linear programming [LSZ19, JSWZ21, SY21, LSZ+23b], distributed problems [WZ16, BWZ16, JLL+21], clustering [EMZ21], generative adversarial networks [XZZ18], kernel density estimation [QRS+22], tensor decomposition [SWZ19c], trace estimation [JPWZ21], projected gradient descent [HMR18, XSS21], matrix sensing [DLS23b, QSZ23], softmax regression [AS23, LSZ23a, DLS23a, GSY23, SSZ23], John Ellipsoid computation [CCLY19, SYYZ22], semi-definite programming [GS22], kernel methods [ACW17, AKK+20, CY21, SWYZ21], adversarial training [GQSW22], cutting plane method [JLSW20], discrepancy [Zha22], federated learning [RPU+20, SWYZ23], kronecker protection maintenance [SYYZ23], reinforcement learning [AKL17, WZD+20, SSX21], relational database [QJS+22].

2.1 Approximate Adaptive Distance Estimation

There has been increasing interest in understanding threats associated with the deployment of algorithms in potentially adversarial settings [GSS15, HMPW16, PMG16, LCLS17]. Additionally, the problem of preserving statistical validity when conducting exploratory data analysis has been extensively studied [DFH+15a, DFH+15b, DFH+15c, BNS+16, DSSU17] where the goal is to maintain coherence with an unknown distribution from which data samples are acquired. In the application of approximate nearest neighbor, the works of [Kle97, KOR00, CN20] present non-trivial data structures for distance estimation which supports adaptive queries. In the context of streaming algorithms, the work of [BEJWY20] designs streaming algorithms which support both adaptive queries and updates.

2.2 Online Metric Learning

A number of recent techniques consider the metric learning problem [SJ03, GR05, FSM06]. Most works handle offline learning Mahalanobis distances, which often results in expensive optimization algorithms. POLA [SSSN04] is an algorithm for online Mahalanobis metric learning that optimizes a large-margin objective and establishes provable regret bounds. However, it requires eigenvector computation at each iteration to ensure positive definiteness, which can be time-consuming in practice. The information-theoretic metric learning approach of [DKJ+07] presents an online algorithm that eliminates eigenvector decomposition operations. LEGO [JKDG08] requires no additional work for enforcing positive definiteness and can be implemented efficiently in practice. [QJZL15] leverages random projection in distance metric learning for high-dimensional data.

3 Preliminaries

3.1 Notation

For any natural number n, we use $[n]$ to denote the set $\{1, 2, \ldots, n\}$. We use $A^\top$ to denote the transpose of matrix A. For any vector $v \in \mathbb{R}^d$ and positive semi-definite matrix $A \in \mathbb{R}^{d\times d}$, we use $\|v\|_A$ to denote $\sqrt{v^\top A v}$. We use $\mathcal{N}(0, I)$ to denote Gaussian distribution. For a probabilistic event $f(x)$, we define $\mathbf{1}\{f(x)\}$ such that $\mathbf{1}\{f(x)\} = 1$ if $f(x)$ holds and $\mathbf{1}\{f(x)\} = 0$ otherwise. For a vector $v \in \mathbb{R}^d$ and real valued random variable Y, we will abuse notation and use median(v) and median(Y) to denote the median of the entries of v and the distribution of Y respectively. We use Pr[] to denote the probability, and use $\mathbb{E}$[] to denote the expectation if it exists. We use **Var**[] to denote the variance of a random variable. We use $\widetilde{O}(f)$ to denote $O(f\text{poly}(\log f))$.

3.2 Background

In this section, we provide several definitions and probability results.

Definition 3 (Low-Rank Mahalanobis Pseudo-Metric)**.** *For any set of points $\mathcal{X} \subset \mathbb{R}^d$, a pseudo-metric is a function $d : \mathcal{X} \times \mathcal{X} \mapsto \mathbb{R}_{\geq 0}$ such that $\forall x, y, z \in \mathcal{X}$, it satisfies: $d(x, x) = 0, d(x, y) = d(y, x), d(x, y) \leq d(x, z) + d(z, y)$.*

As in some prior work on pseudo-metric learning [SSSN04], we only consider pseudo-metrics which can be written in the form $d_A(x, y) = (x - y)^\top A(x - y)$ where A is a positive semi-definite matrix. We define the rank of a pseudo-metric d_A to be the rank of A.

Note that the distinction between pseudo-metrics and metrics is not very crucial for our results. In addition to the above properties, a metric satisfies the property that for any $x, y \in \mathcal{X}, d(x, y) = 0$ if and only if $x = y$.

We will use the following property from [CN20] for our sketching matrices $\{\Pi_j \in \mathbb{R}^{m\times k}\}_{j=1}^L$ where L denotes the number of sketching matrices.

Definition 4 ((ε, β)-representative, Definition B.2 in [CN20])**.** *A set of matrices $\{\Pi_j \in \mathbb{R}^{m\times k}\}_{j=1}^L$ is said to be (ε, β)-representative for any $\varepsilon, \beta \in (0, 1/2)$ if*

$$\forall\ \|v\|_2 = 1,\ \sum_{j=1}^{L} \mathbf{1}\{(1-\varepsilon) \leq \|\Pi_j v\|_2 \leq (1+\varepsilon)\} \geq (1-\beta)L.$$

The above definition implies that if a set of matrices $\{\Pi_j \in \mathbb{R}^{m\times k}\}_{j=1}^L$ satisfies this property, for any any unit vector v, most of the projections $\Pi_j v$, approximately preserve its length.

3.3 Applications of our Data-Structure

Developing efficient algorithms for Nearest Neighbor Search (NNS) has been a focus of intense research, driven by a variety of real-world applications ranging from computer vision, information retrieval to database query [BM01, DIIM04, SDI08]. A line of work, starting with the foundational results of [IM98, KOR00], have obtained sub-linear query time in n for the approximate variant in order to solve the problem that fast algorithms for exact NNS [Cla88, Mei93] consumes impractical space complexity. The Locality Sensitive Hashing (LSH) approach of [IM98] gives a Monte Carlo randomized approach with low memory and query time, but it does not support adaptive queries. Although the algorithms of [KOR00, Kle97] support adaptive queries and have sublinear query time, they use large space and are only designed for finding the approximate single nearest neighbor and do not provide distance estimates to all data points in the database per query.

For nonparametric models including SVMs, distance estimates to potentially every point in the dataset may be required [Alt92, AMS97, HSS08]. For simpler tasks like k-nearest neighbor classification or database search, modifying previous approaches to return k nearest neighbors instead of 1, results in a factor k increase in overall query time. Therefore, developing efficient deployable variants in adversarial settings is an important endeavor, and an adaptive approximate distance estimation procedure is a useful primitive for this purpose.

4 Technique Overview

For a set of points $\mathcal{X} = \{x_1, x_2, \ldots, x_n\} \in \mathbb{R}^d$, a Mahalanobis distance metric d on $\mathcal{X}$ is characterized by a positive semidefinite matrix $A \in \mathbb{R}^{d\times d}$ such that $d(x_i, x_j) = \sqrt{(x_i - x_j)^\top A(x_i - x_j)}$. First we provide a randomized sketching data structure $\mathcal{D}$ which can answer approximate non-adaptive Mahalanobis distance estimation queries $q \in \mathbb{R}^d$ by $\widetilde{d}_i = \|\Pi U q - \widetilde{x}_i\|_2$ in Theorem 5, where Π is a Johnson-Lindenstrauss sketching [JL84] matrix and $U^\top U = A$.

To make our data structure resistant to adaptively chosen queries, we will use the (ε, β)-representative in Definition 4 where A set of matrices $\{\Pi_j \in \mathbb{R}^{m\times k}\}_{j=1}^L$ is said to be (ε, β)-representative for any $\varepsilon, \beta \in (0, 1/2)$ if at least $(1-\beta)L$ sketching matrice can achieve $(1 \pm \varepsilon)$-approximate distance estimation. With $L = O((d + \log \frac{1}{\delta}) \log(d/\varepsilon))$ independent instantiation of randomized sketching data structure $\mathcal{D}$ satisfying the $(\varepsilon, 0.1)$-representative property, we know that for any given query vector $q \in \mathbb{R}^d$, most of the sketching matrices approximately preserves its length. Then we design a set of unit vectors $\{v_i = \frac{U(q-x_i)}{\|U(q-x_i)\|_2}\}_{i=1}^n$ for query $q \in \mathbb{R}^d$ and data points $\{x_1, x_2, \ldots, x_n\} \subset \mathbb{R}^d$ and show that most of the projections Π_j satisfy $(1 \pm \varepsilon)$-approximate Mahalanobis distance estimation. We define a set $\mathcal{J}$ as $\mathcal{J} := \{j : (1-\varepsilon) \le \|\Pi_j U v\| \le (1+\varepsilon)\}$ which has size at least $0.9L$. Now query using any randomized sketching matrix Π_j gives us ε-approximation with constant 0.9 success probability. To boost the success probability from constant probability to high probability, we sample $R = O(\log(n/\delta))$ indexes $\{j_r\}_{r=1}^R$ from the set $\mathcal{J}$, and obtain R estimates of the Mahalanobis distance between q and x_i. By Hoeffding's Inequality (Lemma 14), we know that the median of the sampled R distance estimates can provide $(1 \pm \varepsilon)$-approximate query with high probability.

To support sparse update for the Mahalanobis metric matrix U, we update $\widetilde{x}_{i,j}$ with the sparse update matrix B for n data points and L sketching matrice respectively in $O((m+d)nL)$ time. To update the i-th data point with a new vector $z \in \mathbb{R}^d$, we need to recompute $\widetilde{x}_{i,j} = \Pi_j U z$ for L sketching matrice respectively in $O((m+d)kL)$ time.

To support sampling an index i with probability proportional to the distance between q and x_i, we first leverage a segment tree to obtain $\sum_{\ell=i}^j x_\ell$ in logarithmic time, and compute $\sum_{\ell=i}^j \|q - x_\ell\|_A$. In each iteration, we determine left or right half to proceed by sampling a random value between

$[0,1]$ uniformly and compare with $\frac{\sum_{\ell=l}^{m}\|q-x_\ell\|_A}{\sum_{\ell=l}^{T}\|q-x_\ell\|_A}$. After $T = O(\log n)$ iterations, we can obtain the final sampled index in $O(\log^2 n + kd\log n)$ time.

5 JL sketch for approximate Mahalanobis distance estimation

In this section, we provide a data structure which uses the well studied Johnson-Lindenstrauss sketch [JL84] to solve the approximate Mahalanobis distance estimation problem. We remark that other standard sketches like the AMS sketch [AMS99] or CountSketch [CCFC02] can also be used to provide similar data-structures which can support Mahalanobis distance estimation with Monte Carlo guarantees.

Algorithm 1 Informal version of Algorithm 6. JL sketch for approximate Mahalanobis distance estimation

data structure JLMonCarMaintenance ▷ Theorem 5
members
  $d, k, m, n \in \mathbb{N}_+$ ▷ d is the dimension of data, m is the sketch size, n is the number of points
  $U \in \mathbb{R}^{k\times d}$
  $\{\widetilde{x}_i\} \in \mathbb{R}^m$ for $i \in [n]$ ▷ Sketch of the n points
end members
procedure Initialize($U \in \mathbb{R}^{k\times d}, \{x_i\}_{i\in[n]} \subset \mathbb{R}^d, \varepsilon \in (0,1), \delta \in (0,1)$)
  $m \leftarrow \Omega(\frac{\log n}{\varepsilon^2})$ ▷ Initialize the sketch size
  $U \leftarrow U$
  For $i \in [n]$, $x_i \leftarrow x_i$
  Let $\Pi \in \mathbb{R}^{m\times k}$ with entries drawn iid from $\mathcal{N}(0, 1/m)$. ▷ AMS or CountSketch also valid
  For $i \in [n]$, $\widetilde{x}_i \leftarrow \Pi U x_i$
end procedure
procedure Query($q \in \mathbb{R}^d$)
  For $i \in [n]$, let $\widetilde{d}_i \leftarrow \|\Pi U q - \widetilde{x}_i\|_2$
  return $\{\widetilde{d}_i\}_{i=1}^n$
end procedure
end data structure

Theorem 5 (Guarantees for JL sketch for Mahalanobis Metrics)**.** *There is a data structure (Algorithm 1) for Approximate Mahalanobis Distance Estimation with the following procedures:*

- Initialize($U \in \mathbb{R}^{k\times d}, \{x_1, x_2, \ldots, x_n\} \subset \mathbb{R}^d, \varepsilon \in (0,1), \delta \in (0,1)$)*: Given a matrix $U \in \mathbb{R}^{k\times d}$, a list of vectors $\{x_1, x_2, \cdots, x_n\} \subset \mathbb{R}^d$, accuracy parameter $\varepsilon \in (0,1)$, and failure probability $\delta \in (0,1)$, the data-structure pre-processes in time $\widetilde{O}((d+m)k)$.*
- Query($q \in \mathbb{R}^d$)*: Given a query vector $q \in \mathbb{R}^d$, Query outputs approximate Mahalanobis distance estimates $\{d_i\}_{i=1}^n$ in time $O((d+m)k)$ such that*

$$\Pr\left[(1-\varepsilon)\|q-x_i\|_A \le d_i \le (1+\varepsilon)\|q-x_i\|_A, \forall i \ \in [n]\right] \ge 1-\delta.$$

  where $A = U^\top U \in \mathbb{R}^{d\times d}$ is a positive semidefinite matrix which characterizes the Mahalanobis distances.

Proof. The INITIALIZE pre-processing time complexity is dominated by line 16 which takes $O((d+m)k)$. The QUERY time complexity is dominated by line 22 which takes $O((d+m)k)$.

Proof of correctness for Query: We will use the following lemma which is a standard result used in proofs of the Johnson-Lindenstrauss lemma.

Lemma 6 (Distributional JL (DJL) lemma)**.** *For any integer $k \geq 1$ and any $0 < \varepsilon, \delta < 1/2$, there exists a distribution $D_{\varepsilon,\delta}$ over $m \times k$ real matrices for some $m \leq c\varepsilon^{-2}\log(1/\delta)$ for some constant $c > 0$ such that:*

$$\forall\ \|u\|_2 = 1, \Pr_{\Pi \sim D_{\varepsilon,\delta}}[(1-\varepsilon) \leq \|\Pi u\|_2 \leq (1+\varepsilon)] \geq 1-\delta.$$

We will show that our choice of $\Pi \in \mathbb{R}^{m\times k}$ with entries drawn iid from $\mathcal{N}(0, 1/m)$ satisfies the above guarantee.

Let $u = (u_1, u_2, \ldots, u_k)$. Since $\Pi_{i,j} \sim \mathcal{N}(0, 1/m)$ for all $i \in [m], j \in [k]$, we have that each coordinate $i \in [m]$ of $(\Pi u)_i = \sum_{j=1}^{k} \Pi_{i,j} u_j$ is the sum of k independent normally distributed random variables. Therefore, $\{(\Pi u)_i\}_{i=1}^{m}$ are are all normally distributed real variable with their mean and variance being the sums of the individual means and variances. Note that $\mathbb{E}[(\Pi u)_i] = \sum_{j=1}^{k} u_j \mathbb{E}[\Pi_{i,j}] = 0$ and $\mathbf{Var}[(\Pi u)_i] = \sum_{j=1}^{k} u_j^2 \mathbf{Var}[\Pi_{i,j}] = (1/m)\cdot\|u\|_2^2 = 1/m$. Therefore, $(\Pi u)_i \sim \mathcal{N}(0, 1/m)$. A random vector in $\mathbb{R}^m$ with all its coordinates distributed as $\mathcal{N}(0, \sigma^2)$ can be viewed as being drawn from a m-dimensional spherical Gaussian $\mathcal{N}(\mathbf{0}, \sigma^2 I_{m\times m})$. Therefore, we have $(\Pi u) \sim \mathcal{N}(\mathbf{0}, \frac{1}{m} I_{m\times m})$. We will now show how to use the Gaussian Annulus Theorem [BHK20, Theorem 2.9] to finish our proof.

Lemma 7 (Gaussian Annulus Theorem)**.** *For any $x \sim \mathcal{N}(\mathbf{0}, I_{m\times m}), \beta \leq \sqrt{m}$, for some constant $c > 0$, we have that:*

$$\Pr\left[(\sqrt{m} - \beta) \leq \|x\|_2 \leq (\sqrt{m} + \beta)\right] \geq 1 - 3^{-c\beta^2}.$$

We have that $(\Pi u) \sim \mathcal{N}(\mathbf{0}, \frac{1}{m} I_{k\times k})$. Therefore, we have $(\Pi u) = \frac{1}{\sqrt{m}} x$ for $x \sim \mathcal{N}(\mathbf{0}, I_{k\times k})$. The condition that $(1-\varepsilon) \leq \|\Pi u\|_2 \leq (1+\varepsilon)$ is equivalent to $(\sqrt{m} - \varepsilon\sqrt{m}) \leq \|x\|_2 \leq (\sqrt{m} + \varepsilon\sqrt{m})$. Therefore, we have that, for some constant $c > 0$,

$$\Pr_{\Pi \sim D_{\varepsilon,\delta}}\left[(1-\varepsilon) \leq \|\Pi u\|_2 \leq (1+\varepsilon)\right] \geq 1 - 3^{-cm\varepsilon^2}.$$

To prove the correctness for our Query operation, we will apply a union bound over the choices of $\{u_i = \frac{U(q-x_i)}{\|U(q-x_i)\|_2}\}_{i=1}^{n}$ in the above lemma. The failure probability is upper bounded by $n \cdot 3^{-cm\varepsilon^2}$. To have this be at most delta, we need to have $m \geq \frac{c'}{\varepsilon^2}\log(n/\delta)$ for some constant c'. In particular, if we want a with high probability guarantee, taking $m = \Omega(\frac{\log n}{\varepsilon^2})$ should suffice.

Thus, we complete the proof. □

6 Online Adaptive Mahalanobis Distance Maintenance

Now, we move to the data structure and the algorithm to solve the online version of the problem and the corresponding proofs. Our main result in this section is the following:

Theorem 8 (Main result)**.** *There is a data structure (Algorithm 2 and 3) for the Online Approximate Adaptive Mahalanobis Distance Estimation Problem (Definition 2) with the following procedures:*

Algorithm 2 Informal version of Algorithm 8. Mahalanobis Pseudo-Metric Maintenance: members, initialize and update

data structure MetricMaintenance ▷ Theorem 8
members
  L, m, k ▷ L is the number of sketches, m is the sketch size
  $d, n \in \mathbb{N}_+$ ▷ n is the number of points, d is dimension
  $U \in \mathbb{R}^{k \times d}$
  $x_i \in \mathbb{R}^d$ for $i \in [n]$
  $\{\widetilde{x}_{i,j}\} \in \mathbb{R}^m$ for $i \in [n], j \in [L]$ ▷ The sketch of data points
  Tree tree ▷ Segment tree(Alg 4) tree.Query(i,j) to obtain $\sum_{\ell=i}^{j} x_\ell$
end members
procedure Initialize$(U \in \mathbb{R}^{k \times d}, \{x_i\}_{i \in [n]} \subset \mathbb{R}^d, \varepsilon \in (0,1), \delta \in (0,1))$ ▷ Lemma 9
  $m \leftarrow O(\frac{1}{\varepsilon^2})$ ▷ Initialize the sketch size
  $L \leftarrow O((d + \log \frac{1}{\delta}) \log(d/\varepsilon))$ ▷ Initialize the number of copies of sketches
  $U \leftarrow U$
  For $i \in [n]$, $x_i \leftarrow x_i$ ▷ Initialize the data points from input
  For $j \in [L]$, let $\Pi_j \in \mathbb{R}^{m \times k}$ with entries drawn iid from $\mathcal{N}(0, 1/m)$.
  For $i \in [n]$, For $j \in [L]$, $\widetilde{x}_{i,j} \leftarrow \Pi_j U x_i$
  tree.Init$(\{x_i\}_{i \in [n]}, \text{tree}.t, 1, n)$ ▷ Initialize the segment tree using all data points.
end procedure
procedure UpdateU$(u \in \mathbb{R}^d, a \in [k])$ ▷ We can consider sparse update for U, Lemma 10.
  $B \leftarrow \{0\}_{k \times d}$
  $B_a \leftarrow u^\top$ ▷ B_a denotes the a'th row of B.
  $U \leftarrow U + B$
  For $i \in [n]$, For $j \in [L]$, $\widetilde{x}_{i,j} \leftarrow \widetilde{x}_{i,j} + \Pi_j B x_i$
end procedure
procedure UpdateX$(z \in \mathbb{R}^d, i \in [n])$ ▷ Lemma 11.
  $x_i \leftarrow z$
  For $j \in [L]$, $\widetilde{x}_{i,j} \leftarrow \Pi_j U z$
  tree.Update(tree.t, i, z)
end procedure
end data structure

- Initialize$(U \in \mathbb{R}^{k \times d}, \{x_1, x_2, \ldots, x_n\} \subset \mathbb{R}^d, \varepsilon \in (0,1), \delta \in (0,1))$*: Given a matrix $U \in \mathbb{R}^{k \times d}$, data points $\{x_1, x_2, \ldots, x_n\} \subset \mathbb{R}^d$, an accuracy parameter ε and a failure probability δ as input, the data structure preprocesses in time $O((m+d)knL)$.*
- UpdateU$(u \in \mathbb{R}^d, a \in [k])$*: Given an update vector $u \in \mathbb{R}^d$ and row index $a \in [k]$, the data structure takes u and a as input and updates the a'th row of U by adding a to it i.e. $U_{a,:} \leftarrow U_{a,:} + u$ in time $O((m+d)nL)$.*
- UpdateX$(z \in \mathbb{R}^d, i \in [n])$*: Given an update vector $z \in \mathbb{R}^d$ and index $i \in [n]$, the* UpdateX *takes z and i as input and updates the data structure with the new i-th data point in $O((m+d)kL + \log n)$ time.*
- QueryPair$(i, j \in [n])$*. Given two indexes $i, j \in [n]$, the* QueryPair *takes i, j as input and approximately estimates the Mahalanobis distance from x_i to x_j in time $O(mR)$ and output a number p such that: $(1-\varepsilon)\|x_i - x_j\|_A \leq p \leq (1+\varepsilon) \cdot \|x_i - x_j\|_A$ with probability at least $1 - \delta$.*

Algorithm 3 Informal version of Algorithm 7. Online Adaptive Mahalanobis Distance Maintenance: queries.

data structure MetricMaintenance ▷ Theorem 8
procedure QueryPair($i, j \in [n]$) ▷ Lemma 12
  $R \leftarrow O(\log(n/\delta))$ ▷ Number of sampled sketches
  For $r \in [R]$, $p_r \leftarrow \|\widetilde{x}_{i,r} - \widetilde{x}_{j,r}\|_2$
  $p \leftarrow \text{median}_{r\in[R]}\{p_r\}$
  return p
end procedure
procedure QueryAll($q \in \mathbb{R}^d$) ▷ Lemma 13
  $R \leftarrow O(\log(n/\delta))$ ▷ Number of sampled sketches
  Sample $j_1, j_2, \ldots, j_R$ i.i.d. with replacement from $[L]$.
  For $i \in [n], r \in [R]$, let $d_{i,r} \leftarrow \|\Pi_{j_r} U q - \widetilde{x}_{i,r}\|_2$
  For $i \in [n], \widetilde{d}_i \leftarrow \text{median}_{r\in[R]}\{d_{i,r}\}$
  return $\{\widetilde{d}_i\}_{i=1}^n$
end procedure
end data structure

- QueryAll($q \in \mathbb{R}^d$): *Given a query point $q \in \mathbb{R}^d$, the* QueryAll *operation takes q as input and approximately estimates the Mahalanobis distances from q to all the data points $\{x_1, x_2, \ldots, x_n\} \subset \mathbb{R}^d$ in time $O((m+d)knR)$ i.e. it provides a set of estimates $\{\widetilde{d}_i\}_{i=1}^n$ such that:*

$$\forall i \in [n], (1-\varepsilon)\|q - x_i\|_A \leq \widetilde{d}_i \leq (1+\varepsilon)\|q - x_i\|_A$$

  with probability at least $1 - \delta$, even for a sequence of adaptively chosen queries.

- SampleExact($q \in \mathbb{R}^d$). *Given a query point $q \in \mathbb{R}^d$ as input,* SampleExact *samples an index $i \in [n]$ with probability $d_i / \sum_{j=1}^n d_j$ in $O(\log^2 n + kd \log n)$ time.*

Proof. We complete the proof for Theorem 8 using the following Lemma 9, Lemma 10, Lemma 11, Lemma 12, Lemma 13 and Lemma 24. □

Lemma 9 (Initialization Time)**.** *Given a matrix $U \in \mathbb{R}^{k\times d}$, data points $\{x_1, x_2, \ldots, x_n\} \subset \mathbb{R}^d$, an accuracy parameter ε and a failure probability δ as input, the time complexity of* Initialize *function is $O((m+d)knL)$.*

The proof is delayed to Appendix B.1.

Lemma 10 (UpdateU Time)**.** *Given an update vector $u \in \mathbb{R}^d$ and row index $a \in [k]$, the* UpdateU *takes u and a as input and updates the a'th row of U by adding a to it i.e. $U_{a,:} \leftarrow U_{a,:} + u$ in $O((m+d)nL)$ time.*

The proof is delayed to Appendix B.2.

Lemma 11 (UpdateX Time)**.** *Given a new data point $z \in \mathbb{R}^d$ and index $i \in [n]$, the* UpdateX *takes z and i as input and updates the data structure with the new ith data point in $O((m+d)kL + \log n)$ time.*

The proof is delayed to Appendix B.3.

Lemma 12 (QueryPair)**.** *Given two indexes $i, j \in [n]$, the* QueryPair *takes i, j as input and approximately estimates the Mahalanobis distance from x_i to x_j in time $O(mR)$ and output a number p such that: $(1-\varepsilon)\|x_i - x_j\|_A \leq p \leq (1+\varepsilon)\|x_i - x_j\|_A$. with probability at least $1-\delta$.*

We defer the proof to Appendix B.4.

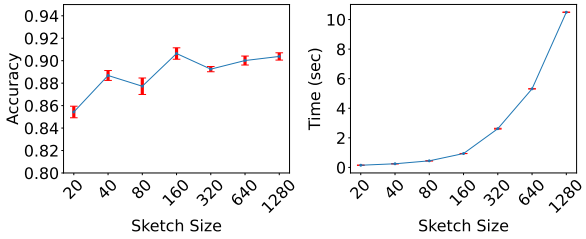
Lemma 13 (QueryAll)**.** *Given a query point $q \in \mathbb{R}^d$, the* QueryAll *operation takes q as input and approximately estimates the Mahalanobis distances from q to all the data points $\{x_1, x_2, \ldots, x_n\} \subset \mathbb{R}^d$ in time $O((m+d)knR)$ i.e. it provides a set of estimates $\{\widetilde{d}_i\}_{i=1}^n$ such that:*

$$\forall i \in [n], (1-\varepsilon)\|q - x_i\|_A \leq \widetilde{d}_i \leq (1+\varepsilon)\|q - x_i\|_A.$$

with probability at least $1-\delta$.

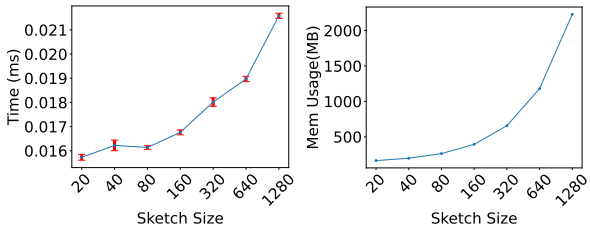
We delay the proof to Section B.5.

7 Evaluation



(a) (b)

Figure 1: Benchmark results for (a) QueryAll accuracy under different m. (b) QueryAll time under different m.



(a) (b)

Figure 2: Benchmark results for (a) QueryPair time under different m. (b) Data structure memory usage under different m.

Experiment setup. We evaluate our algorithm with gene expression cancer RNA-Seq Data Set from UCI machine learning repository [AN07] where $n = 800$ and we use the first $d = 5120$ columns. We run our experiments on a machine with Intel i7-13700K, 64GB memory, Python 3.6.9 and Numpy 1.22.2. We set the number of sketches $L = 10$ and sample $R = 5$ sketches during QueryAll. We run QueryAll for 10 times to obtain the average time consumption and the accuracy of QueryAll.

We run QueryPair for 10000 times to obtain the average time. The red error bars in the figures represent the standard deviation. We want to answer the following questions:

- How is the execution time affected by the sketch size m?
- How is the query accuracy affected by the sketch size m?
- How is the memory consumption of our data structure affected by the sketch size m?

Query Accuracy. From the part (a) in Figure 1, we know that the QueryAll accuracy increases from 83.4% to 90.4% as the sketch size increases from 20 to 1280. And we can reach around 90% distance estimation accuracy when the sketch size reaches 320.

Execution time. From the part (b) in Figure 1, QueryAll time grows from 0.15 second to 10.49 second as sketch size increases. From the part (a) in Figure 2, QueryPair time increases from 0.015 millisecond to ~ 0.02 milliseconds as sketch size increases. The query time growth follows that larger sketch size leads to higher computation overhead on $\Pi_j Uq$. Compared with the baseline whose sketch size $m = 1280$, when sketch size is 320, the QueryAll is $8.5\times$ faster and our data structure still achieves $\sim 90\%$ estimation accuracy in QueryAll.

Memory Consumption. From the part (b) in Figure 2, we find that the memory consumption increases from 164MB to 2228MB as the sketch size increases from 20 to 1280. Larger sketch size means that more space is required to store the precomputed $\Pi_j U$ and $\Pi_j U x_i$ matrice. Compared with the baseline sketch size $m = 1280$, when sketch size is 320, the memory consumption is $3.06\times$ smaller.

8 Conclusion

Mahalanobis metrics have become increasingly used in machine learning algorithms like nearest neighbor search and clustering. Surprisingly, to date, there has not been any work in applying sketching techniques on algorithms that use Mahalanobis metrics. We initiate this direction of study by looking at one important application, Approximate Distance Estimation (ADE) for Mahalanobis metrics. We use sketching techniques to design a data structure which can handle sequences of adaptive and adversarial queries. Furthermore, our data structure can also handle an online version of the ADE problem, where the underlying Mahalanobis distance changes over time. Our results are the first step towards using sketching techniques for Mahalanobis metrics. We leave the study of using our data structure in conjunction with online Mahalanobis metric learning algorithms like [SSSN04] to future work. From our perspective, given that our work is theoretical, it doesn't lead to any negative societal impacts.

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Roadmap. We first introduce some probability tools in Section A. We then present the proofs for online adaptive Mahalanobis distance maintenance. We present the supplementary algorithm description for SampleExact in Section B. We propose sampling algorithm based on our Mahalanobis distance estimation data structure in Section C. Then we present supplementary experiments in Section D.

A Probability Tools

We will make use of Hoeffding's Inequality:

Lemma 14 (Hoeffding's Inequality [Hoe63])**.** *Let $X_1, \ldots, X_n$ be independent random variables such that $X_i \in [a_i, b_i]$ almost surely for $i \in [n]$ and let $S = \sum_{i=1}^n X_i - \mathbb{E}[X_i]$. Then, for every $t > 0$:*

$$\Pr[S \geq t] \leq \exp\left(-\frac{2t^2}{\sum_{i=1}^n (b_i - a_i)^2}\right).$$

We will use the following guarantee (restated in our notation) from [CN20],

Lemma 15. *Let $\beta \in [0.1, 0.2]$. For any accuracy parameter $\varepsilon \in (0,1)$ and failure probability $\delta \in (0,1)$, if $m = \Omega(\frac{1}{\varepsilon^2}), L = \Omega((d + \log(1/\delta))\log(d/\varepsilon))$, the set of sketching matrices $\{\Pi_j \in \mathbb{R}^{m\times k}\}_{j=1}^L$ where every entry of each matrix is drawn i.i.d. from $\mathcal{N}(0, 1/m)$ satisfies:*

$$\forall \|v\|_2 = 1,\ \sum_{j=1}^{L} \mathbf{1}\{(1-\varepsilon) \leq \|\Pi_j v\|_2 \leq (1+\varepsilon)\} \geq (1-\beta)L$$

with probability at least $1 - \delta$.

The above lemma implies that with high probability, the sketch matrices $\{\Pi_j\}_{j=1}^L$ is (ε, β)-representative.

B Proofs for Online Adaptive Mahalanobis Distance Maintenance

In this section, we provide lemmas and proofs for the initialization, update, query, and query pair operations. Algorithm 6 is the preliminary version of approximate Mahalanobis distance estimation based on JL sketch. The Initialize operation sample a sketch matrix $\Pi \in \mathbb{R}^{m\times k}$ and compute $\widetilde{x}_i = \Pi U x_i$ for all $i \in [n]$. The Query operation compute the estimated distance by $\widetilde{d}_i = \|\Pi U q - \widetilde{x}_i\|_2$ for all $i \in [n]$.

In Algorithm 8, Initialize samples $L = O((d + \log\frac{1}{\delta})\log(d/\varepsilon))$ sketching matrice and compute the $\widetilde{x}_{i,j} = \Pi_j U x_i$ for all n data points and L sketching matrice. UpdateU uses the sparse update matrix B to update the distance matrix U and $\widetilde{x}_{i,j}$. UpdateX updates the corresponding $\widetilde{x}_{i,j}$ with the new data point z and target index i for all sketching matrix $j \in [L]$.

In Algorithm 7, QueryPair samples $R = O(\log(n/\delta))$ sketching matrix indexes and uses them to compute a list of estimated distance between x_i and x_j and output the median in the end. QueryAll samples $R = O(\log(n/\delta))$ sketching matrix indexes and compute $d_{i,r} = \|\Pi_{j_r} U q - \widetilde{x}_{i,r}\|_2$ for all data point indexes $i \in [n]$ and sketching matrix indexes $r \in [R]$. Then QueryAll outputs the median value $\widetilde{d}_i \leftarrow \mathrm{median}_{r\in[R]}\{d_{i,r}\}$ as the estimated distance between q and x_i for all data point indexes $i \in [n]$.

In Section B.1, we present the proof for the time complexity of Initialize. In Section B.2, we present the proof for the time complexity of UpdateU. In Section B.3, we present the proof

for the time complexity of UpdateX In Section B.4, we present the proof for QueryPair. In Section B.5, we present the proof for QueryAll. In Section B.6, we present the proof for SubSum. In Section B.7, we present the proof for SampleExact.

B.1 Proof of Initialization Time

Lemma 16 (Restatement of Lemma 9)**.** *Given a matrix $U \in \mathbb{R}^{k \times d}$, data points $\{x_1, x_2, \ldots, x_n\} \subset \mathbb{R}^d$, an accuracy parameter ε and a failure probability δ as input, the time complexity of* Initialize *function is $O((m+d)knL)$.*

Proof. The initialization part has three steps:

- Line 15 in Algorithm 8 takes $O(nd)$ time to assign $x_i \in \mathbb{R}^d$ for n times.
- Line 18 in Algorithm 8 takes $O(mk)$ time to iid sample from $\mathcal{N}(0, 1/m)$.
- Line 21 in Algorithm 8 takes $O((m+d)knL)$ time to execute $n \times L$ times matrix multiplications.
- The initialization of segment tree needs $O(nd)$ time.

Therefore, the total time for initialization is

$$\begin{aligned} & O(nd) + O(mk) + O((m+d)knL) + O(nd) \\ = \; & O((m+d)knL). \end{aligned}$$

Thus, we complete the proof. □

B.2 Proof of UpdateU Time

In this section, we provide proof of the time complexity of UpdateU operation.

Lemma 17 (Restatement of Lemma 10)**.** *Given an update vector $u \in \mathbb{R}^d$ and row index $a \in [k]$, the* UpdateU *takes u and a as input and updates the a'th row of U by adding a to it i.e. $U_{a,:} \leftarrow U_{a,:} + u$ in $O((m+d)nL)$ time.*

Proof. The update part has three steps:

- Line 29 in Algorithm 8 takes $O(d)$ time to assign $u^\top$ to B_a.
- Line 30 in Algorithm 8 takes $O(d)$ time to update U because B is sparse and we can ignore $k-1$ rows containing all zero elements.
- Line 33 in Algorithm 8 take $O((m+d)nL)$ time to compute sparse matrix multiplication for $n \times L$ times and each sparse matrix multiplication takes $O(m+d)$ time because B is sparse and we can ignore the $k-1$ rows containing all zeros elements.

Therefore, the total time for update is

$$O(d) + O(d) + O((m+d)nL) = O((m+d)nL).$$

Thus, we complete the proof. □

B.3 Proof of UpdateX Time

In this section, we provide proof of the time complexity of UpdateX operation.

Lemma 18 (Restatement of Lemma 11)**.** *Given a new data point $z \in \mathbb{R}^d$ and index $i \in [n]$, the* UpdateX *takes z and i as input and updates the data structure with the new ith data point in $O((m+d)kL + \log n)$ time.*

Proof. The UpdateX operation has one step:

- Line 40 in Algorithm 8 takes $O((m+d)kL)$ time to compute $\Pi_j \cdot (U \cdot z)$ for L times.
- The Tree.Update operation takes $O(\log n)$ time to complete.

Therefore, the total time for UpdateX is $O((m+d)kL + \log n)$. Thus, we complete the proof. □

B.4 Proof of QueryPair

In below lemma, we present how to compute the approximate Mahalanobis distance between two data points in our data structure.

Lemma 19 (Restatement of Lemma 12)**.** *Given two indexes $i, j \in [n]$, the* QueryPair *takes i, j as input and approximately estimates the Mahalanobis distance from x_i to x_j in time $O(mR)$ and output a number p such that:*

$$(1-\varepsilon)\|x_i - x_j\|_A \leq p \leq (1+\varepsilon)\|x_i - x_j\|_A.$$

with probability at least $1 - \delta$.

Proof. **Proof of Running Time.**

We can view the QueryPair operation as having the following two steps:

- The for-loop in line 4 in Algorithm 7 takes $O(mR)$ time because $\|\widetilde{x}_{i,r} - \widetilde{x}_{j,r}\|_2$ takes $O(m)$ time and it is executed for R times.
- Line 7 in Algorithm 7 takes $O(R)$ time to find median value from $\{p_r\}_{r=1}^R$.

Thus, the total running time of QueryPair is

$$O(R) + O(mR) = O(mR).$$

Proof of Correctness.

Instead of choosing $v = \frac{U(q-x_i)}{\|q-x_i\|_A}$ in the proof of correctness for Query(Lemma 13), we should choose $v = \frac{U(x_i-x_j)}{\|x_i-x_j\|_A}$ for QueryPair(i, j).

Accordingly, we also consider

$$z_{i,j} := \operatorname*{median}_{r\in[R]}\{\widetilde{y}_{i,j,r}\}$$

and

$$\widetilde{y}_{i,j,r} := \|\Pi_{j_r} U v\|.$$

This gives us:

$$(1-\varepsilon)\|x_i - x_j\|_A \leq p \leq (1+\varepsilon)\|x_i - x_j\|_A.$$

with probability at least $1 - \frac{\delta}{n}$.

This concludes the proof of correctness for the output of QueryPair. □

B.5 Proof of Lemma 13

Lemma 20 (QueryAll, Restatement of Lemma 13)**.** *Given a query point $q \in \mathbb{R}^d$, the* QueryAll *operation takes q as input and approximately estimates the Mahalanobis distances from q to all the data points $\{x_1, x_2, \ldots, x_n\} \subset \mathbb{R}^d$ in time $O((m+d)knR)$ i.e. it provides a set of estimates $\{\widetilde{d}_i\}_{i=1}^n$ such that:*

$$\forall i \in [n], (1-\varepsilon)\|q - x_i\|_A \leq \widetilde{d}_i \leq (1+\varepsilon)\|q - x_i\|_A.$$

with probability at least $1 - \delta$.

Proof. **Proof of running time.**

We can view the QueryAll operation as having the following three steps:

- Line 13 in Algorithm 7 takes $O(R)$ time to sample $\{j_r\}_{r=1}^R$ from $[L]$.
- Line 16 in Algorithm 7 takes $O((m+d)knR)$ time because $\|\Pi_{j_r} Uq - \widetilde{x}_{i,r}\|_2$ takes $O((m+d)k)$ time and it is executed for $n \times R$ times.
- Line 20 in Algorithm 7 takes $O(nR)$ time to find median value from $\{d_{i,r}\}_{r=1}^R$ for n times.

Thus, the total running time of QueryAll is

$$O(R) + O((m+d)knR) + O(nR) = O((m+d)knR).$$

Proof of Correctness.

We will use the $(\varepsilon, \beta = 0.1)$-representative property (See Definition 4) for our sketching matrices $\{\Pi_j \in \mathbb{R}^{m \times k}\}_{j=1}^L$. This property implies that for any given vector, most of the matrices approximately preserves its length. In particular, we will consider the set of unit vectors $\{v_i = \frac{U(q-x_i))}{\|U(q-x_i)\|_2}\}_{i=1}^n$ for query $q \in \mathbb{R}^d$ and data points $\{x_1, x_2, \ldots, x_n\} \subset \mathbb{R}^d$ i.e. for any point x_i, we have that most of the projections Π_j satisfy

$$(1-\varepsilon)\|q - x_i\|_A \leq \|\Pi_j(U(q - x_i))\|_2 \leq (1+\varepsilon)\|q - x_i\|_A.$$

For query $q \in \mathbb{R}^d, i \in [n]$, we will show that $\widetilde{d}_i$ is a good estimate of $\|q - x_i\|_A$ with high probability. From the definition of $\widetilde{d}_i$, we know that the $\widetilde{d}_i = 0 = \|q - x_i\|_A$ is true when $q = x_i$. Therefore, we only need to consider the case when $q \neq x_i$. Let $v = \frac{U(q-x_i)}{\|q-x_i\|_A}$.
From Lemma 15, we have that $\{\Pi_j\}_{j=1}^L$ is $(\varepsilon, 0.1)$-representative. So the set $\mathcal{J}$ defined as:

$$\mathcal{J} \coloneqq \{j : (1-\varepsilon) \leq \|\Pi_j U v\| \leq (1+\varepsilon)\}$$

has size at least $0.9L$. We now define the random variables

$$\widetilde{y}_{i,r} := \|\Pi_{j_r} U v\| \quad \text{and} \quad \widetilde{z}_i := \operatorname*{median}_{r \in [R]} \{\widetilde{y}_{i,r}\}$$

with $R, \{j_r\}_{r=1}^R$ defined in Query in Algorithm 3. We know that $\widetilde{d}_i = \|q - x_i\|_A \widetilde{z}_i$ from the definition of $\widetilde{d}_i$. Therefore, it is necessary and sufficient to bound the probability that

$$\widetilde{z}_i \in [1-\varepsilon, 1+\varepsilon].$$

To do this, let $W_r = \mathbf{1}\{j_r \in \mathcal{J}\}$ and $W = \sum_{r=1}^R W_r$.

Furthermore, we have $\mathbb{E}[W] \geq 0.9r$ and since $W_r \in \{0,1\}$, we have by Hoeffding's Inequality (Lemma 14).

$$\Pr[W \leq 0.6R] \leq \exp(-\frac{2(0.3R)^2}{R}) \leq \frac{\delta}{n}$$

from our definition of r. Furthermore, for all k such that $j_k \in \mathcal{J}$, we have:

$$1 - \varepsilon \leq \widetilde{y}_{i,k} \leq 1 + \varepsilon.$$

Therefore, in the event that $W \geq 0.6R$, we have $(1-\varepsilon) \leq \widetilde{z}_i \leq (1+\varepsilon)$. Hence, we get:

$$(1-\varepsilon)\|q - x_i\|_A \leq \widetilde{d}_i \leq (1+\varepsilon)\|q - x_i\|_A.$$

with probability at least $1 - \frac{\delta}{n}$.

Taking a union bound over all $i \in [n]$, we get:

$$\forall i \in [n], (1-\varepsilon)\|q - x_i\|_A \leq \widetilde{d}_i \leq (1+\varepsilon)\|q - x_i\|_A.$$

with probability at least $1 - \delta$.

This concludes the proof of correctness for the output of QueryAll. □

B.6 Proof of SubSum

Lemma 21 (Restatement of Lemma 23)**.** *Given a query point $q \in \mathbb{R}^d$, two indexes $i \in [n], j \in [n]$ and $i < j$,* SubSum *output $\sum_{l=i}^{j} \|q - x_l\|_A$ in $O(\log n + kd)$ time.*

Proof. **Proof of Correctness.** We have:

$$\begin{aligned}
&\sum_{l=i}^{j} \|q - x_l\|_A \\
=& \sum_{\ell=i}^{j} q^\top A q - 2q^\top A \sum_{\ell=i}^{j} x_\ell + \sum_{\ell=i}^{j} x_\ell^\top A x_\ell \\
=& (j-i+1) \cdot \|Uq\|_2 - 2q^\top U^\top U \cdot \textsc{tree.Query}(i,j) + \|U \cdot \textsc{tree.Query}(i,j)\|_2 \\
=& (j-i+1) \cdot \|Uq\|_2 + 2q^\top U^\top U s + \|Us\|_2
\end{aligned}$$

Therefore, the SubSum operation can correctly output $\sum_{l=i}^{j} \|q - x_l\|_A$. $\sum_{l=i}^{j} \|q - x_l\|_A$.

Proof of Running Time. The SubSum has four steps:

- $s \leftarrow \textsc{tree.Query}(i,j)$ takes $O(\log n)$ time to return $\sum_{\ell=i}^{j} x_\ell$ as a segment tree.
- $\|Uq\|_2$ takes $O(kd)$ to compute the $U \in \mathbb{R}^{k \times d}$ and $q \in \mathbb{R}^d$ multiplication.
- $q^\top U^\top U s$ takes $O(kd)$ to compute $U \cdot s$, $O(kd)$ time to compute $U^\top \cdot (Us)$, and $O(kd)$ time to compute $q^\top \cdot (U^\top U s)$.
- $\|Us\|_2$ takes $O(kd)$ time to compute $U \in \mathbb{R}^{k \times d}$ and $s \in \mathbb{R}^d$ multiplication.

Therefore, the overall time complexity is:

$$\begin{aligned}
&O(\log n) + O(kd) + O(kd) + O(kd) + O(kd) \\
=& O(\log n + kd)
\end{aligned}$$

Thus, we complete the proof. □

B.7 Proof of SampleExact

Lemma 22 (Restatement of Lemma 24)**.** *Given a query point $q \in \mathbb{R}^d$,* SampleApprox *samples an index $i \in [n]$ with probability $d_i / \sum_{j=1}^n d_j$ in $O(\log^2 n + kd \log n)$ time.*

Proof. **Proof of Correctness.** In Algorithm 5, we know that SampleExact calls SubSampleExact between range $[1, n]$. At each iteration, SubSampleExact filters out either left or right half of the current range based on the sum of Mahalanobis distance of left half and right half. Therefore, after $T = O(\log n)$ iterations, let $[l_j, r_j]$ denote the sample range at iteration j, and we know the final index i is sampled with the probability :

$$\begin{aligned} & \frac{\sum_{j=l_1}^{r_1} d_j}{\sum_{j=1}^n d_j} \cdot \frac{\sum_{j=l_2}^{r_2} d_j}{\sum_{j=l_1}^{r_1} d_j} \cdot \cdots \cdot \frac{d_i}{\sum_{j=l_{\ell_{T-1}}}^{r_{\ell_{T-1}}} d_j} \\ = & \, d_i / \sum_{j=1}^n d_j \end{aligned}$$

Proof of Running Time. The time complexity of SampleExact is dominated by calling SubSum for $T = O(\log n)$ iterations. From Lemma 23, we know each SubSum operation takes $O(\log n + kd)$ time. Therefore, we have the time complexity of SampleExact is $O(\log^2 n + kd \log n)$

This completes the proof. □

C Sampling

In this section, we provide lemmas to support the sampling from the n data points based on their distances to the query point q. We defer the data structure description to Algorithm 4 and Algorithm 5 in the Appendix due to space limitation. It allows querying which of the stored segments contain a given point. The goal of Algorithm 5 is to implement SampleExact functionality. SubSum operation can leverage the segment tree data structure to obtain the $\sum_{\ell=i}^j x_l$ in only $O(\log(n))$ time and compute the $\sum_{l=i}^j \|q - x_l\|_A$ in $O(\log n + kd)$ time. SampleExact executes like a binary-search fashion and calls SubSum operation for $O(\log(n))$ times to determine the final data point index.

Lemma 23 (SubSum)**.** *Given a query point $q \in \mathbb{R}^d$, two indexes $i \in [n], j \in [n]$ and $i < j$,* SubSum *output $\sum_{l=i}^j \|q - x_l\|_A$ in $O(\log n + kd)$ time.*

We delay the proof to Section B.6.

We present how to sample a data point based on the distance between a query point $q \in \mathbb{R}^d$ and the data points in the data structure.

Lemma 24 (SampleExact)**.** *Given a query point $q \in \mathbb{R}^d$,* SampleApprox *samples an index $i \in [n]$ with probability $d_i / \sum_{j=1}^n d_j$ in $O(\log^2 n + kd \log n)$ time.*

Proof. **Proof of Correctness.** In Algorithm 5, we know that SampleExact calls SubSampleExact between range $[1, n]$. At each iteration, SubSampleExact filters out either left or right half of the current range based on the sum of Mahalanobis distance of left half and right half. Therefore, after $T = O(\log n)$ iterations, let $[l_j, r_j]$ denote the sample range at iteration j, and we

know the final index i is sampled with the probability :

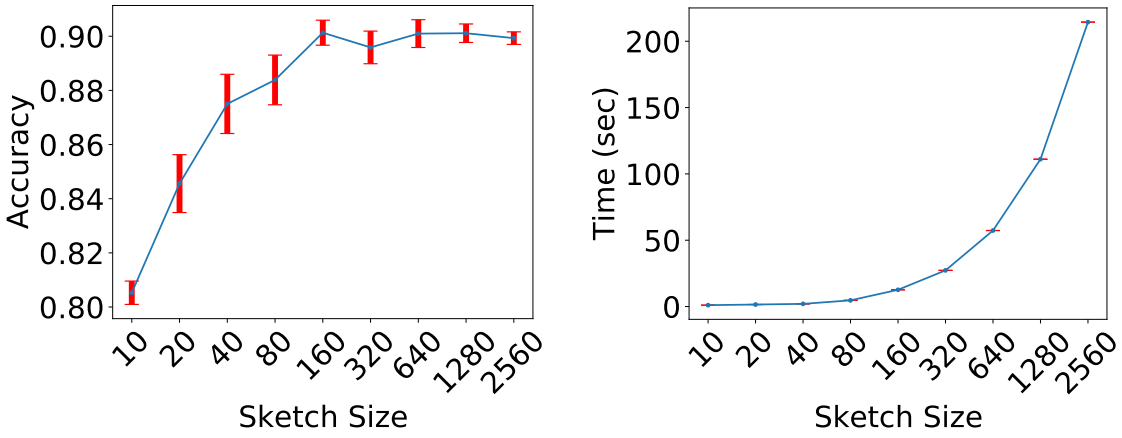
$$\frac{\sum_{j=l_1}^{r_1} d_j}{\sum_{j=1}^{n} d_j} \cdot \frac{\sum_{j=l_2}^{r_2} d_j}{\sum_{j=l_1}^{r_1} d_j} \cdot \cdots \cdot \frac{d_i}{\sum_{j=l_{\ell_{T-1}}}^{r_{\ell_{T-1}}} d_j}$$

$$= d_i / \sum_{j=1}^{n} d_j$$

Proof of Running Time. The time complexity of SAMPLEEXACT is dominated by calling SUBSUM for $T = O(\log n)$ iterations. From Lemma 23, we know each SUBSUM operation takes $O(\log n + kd)$ time. Therefore, we have the time complexity of SAMPLEEXACT is $O(\log^2 n + kd \log n)$

This completes the proof. □

D More Experiments

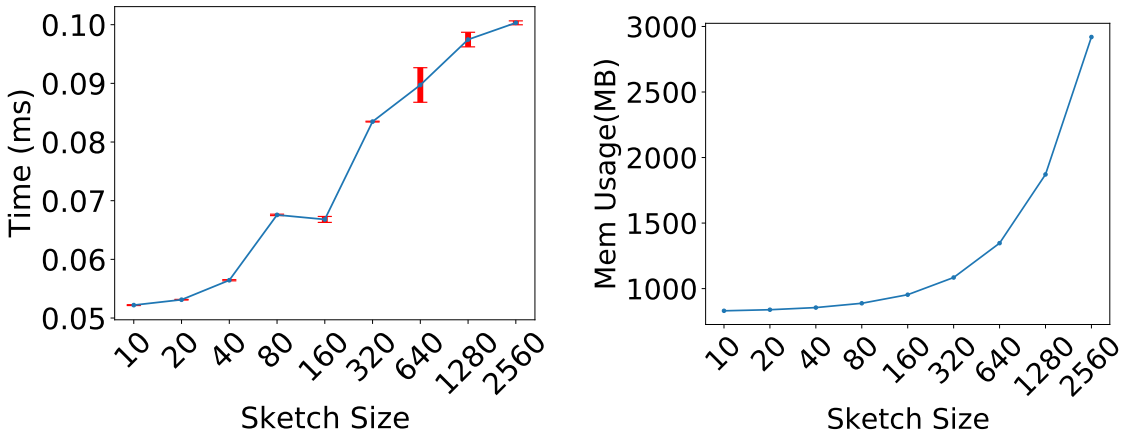


(a) (b)

Figure 3: Benchmark results for (a) QUERYALL accuracy under different m. (b) QUERYALL time under different m.

Experiment setup. We also evaluate our algorithm with $n = 10000$ and $d = 2560$ uniformly random data points. We run our simulation experiments on a machine with Intel i7-13700K, 64GB memory, Python 3.6.9 and Numpy 1.22.2. We set the number of sketches $L = 10$ and sample $R = 5$ sketches during QUERYALL. We run QUERYALL for 10 times to obtain the average time consumption and the accuracy of QUERYALL. We run QUERYPAIR for 1000 times to obtain the average time. The red error bars in the figures represent the standard deviation. We want to answer the following questions:

- How is the execution time affected by the sketch size m?
- How is the query accuracy affected by the sketch size m?
- How is the memory consumption of our data structure affected by the sketch size m?



(a) (b)

Figure 4: Benchmark results for (a) QueryPair time under different m. (b) Data structure memory usage under different m.

Query Accuracy. From the part (a) in Figure 3, we know that the QueryAll accuracy increases from 80.4% to 90.2% as the sketch size increases from 10 to 2560. And we can reach around 90% distance estimation accuracy when the sketch size reaches 160.

Execution time. From the part (b) in Figure 3, QueryAll time grows from 1.05 second to 214.4 second as sketch size increases. From the part (a) in Figure 4, QueryPair time increases from 0.05 millisecond to ~ 0.1 milliseconds as sketch size increases. The query time growth follows that larger sketch size leads to higher computation overhead on $\Pi_j Uq$. Compared with the baseline whose sketch size is equal to the data point dimension $m = 2560$, when sketch size is 160, the QueryAll is 16.9× faster and our data structure still achieves 90% estimation accuracy in QueryAll.

Memory Consumption. From the part (b) in Figure 4, we find that the memory consumption increases from 830MB to 2919MB as the sketch size increases from 10 to 2560. Larger sketch size means that more space is required to store the precomputed $\Pi_j U$ and $\Pi_j U x_i$ matrice. Compared with the baseline sketch size $m = 2560$, when sketch size is 160, the memory consumption is 3.06× smaller.

Algorithm 4 Segment Tree

data structure TreeNode
members
  TreeNode l, r ▷ Left and right child node
  $v \in \mathbb{R}$ ▷ Value stored in current node
  $L, R \in \mathbb{N}_+$ ▷ The left and right boundary of node interval
end members
end data structure

data structure Tree
members
  $t \in$ TreeNode ▷ t is the root node
end members

procedure Init($a \in \mathbb{R}^n, c \in$ TreeNode, $L \in \mathbb{N}_+, R \in \mathbb{N}_+$).
  $c.L \leftarrow L, c.R \leftarrow R$ ▷ Assign the interval of current node
  if $L = R$ **then**
    $c.v \leftarrow a_l$ ▷ Assign current node value
  else
    $m \leftarrow (l + r)/2$
    Init$(a, c.l, l, m)$
    Init$(a, c.r, m + 1, r)$
    $c.v \leftarrow c.l.v + c.r.v$ ▷ Assign current node value
  end if
end procedure

procedure Query($c \in$ TreeNode, $L \in \mathbb{N}_+, R \in \mathbb{N}_+$)
  if $c.R < L$ or $c.L > R$ **then** ▷ if the requested range is outside interval of current node
    return NULL
  end if
  if $c.L \leq L$ and $c.R \geq R$ **then** ▷ if current node interval is completely inside requested range
    return $c.v$
  end if
  return Query$(c.l, L, R)$ + Query$(c.r, L, R)$
end procedure

procedure Update($c \in$ TreeNode, $i \in [n], v' \in \mathbb{R}$)
  if $c.L = c.R$ **then** ▷ If current node is leaf node
    $c.v \leftarrow v'$
  end if
  if $L \leq i$ and $(c.L + c.R)/2 \geq i$ **then**
    Update$(c.l, i, v')$ ▷ Update left child node
  else
    Update$(c.r, i, v')$ ▷ Update right child node
  end if
  $c.v \leftarrow c.l.v + c.r.v$ ▷ Update current node
end procedure
end data structure

Algorithm 5 Online Adaptive Mahalanobis Distance Maintenance: SampleExact.

data structure MetricMaintenance ▷ Theorem 8
procedure SubSum($q \in \mathbb{R}^d, i \in [n], j \in [n]$) ▷ Compute $\sum_{\ell=i}^{j} \|q - x_\ell\|_A$. Lemma 23.
  $s \leftarrow$ tree.Query(i, j) ▷ $s \in \mathbb{R}^d$
  $r \leftarrow (j - i + 1) \cdot \|Uq\|_2 + 2q^\top U^\top Us + \|Us\|_2$
  return r
end procedure
procedure SubSampleExact($q \in \mathbb{R}^d, l \in \mathbb{N}_+, r \in \mathbb{N}_+$)
  while $l < r$ **do**
    $m = l + (r - l)/2$
    Sample a random value v from $[0, 1]$ uniformly.
    $t = \frac{\text{SubSum}(q,l,m)}{\text{SubSum}(q,l,r)}$ ▷ Threshold to decide next round sampling
    if $v < t$ **then**
      return SubSampleExact(q, l, m)
    else
      return SubSampleExact$(q, m + 1, r)$
    end if
  end while
  return l
end procedure
procedure SampleExact($q \in \mathbb{R}^d$) ▷ Lemma 24
  return SubSampleExact$(q, 1, n)$
end procedure
end data structure

Algorithm 6 Formal version of Algorithm 1. JL sketch for approximate Mahalanobis distance estimation. We remark that the proof on page 5 mentions Line 16 and Line 22 which are in fact with respect to the Formal version (this Algorithm 6). Line 16 in Algorithm 6 is corresponding to Line 12 in Algorithm 1 (This step takes $O((d+m)k)$ time). Line 22 in Algorithm 6 is corresponding to Line 15 in Algorithm 1 (This step takes $O((d+m)k)$ time).

1: **data structure** JLMonCarMaintenance ▷ Theorem 5
2: **members**
3: $d, k, m, \in \mathbb{N}_+$ ▷ d is the dimension of data, m is the sketch size, n is the number of points
4: $U \in \mathbb{R}^{k \times d}$
5: $\{\widetilde{x}_i\} \in \mathbb{R}^m$ for $i \in [n]$ ▷ Sketch of the n points
6: **end members**
7:
8: **procedure** Initialize($U \in \mathbb{R}^{k \times d}, \{x_i\}_{i \in [n]} \subset \mathbb{R}^d, \varepsilon \in (0,1), \delta \in (0,1)$)
9: $m \leftarrow \Omega(\frac{\log n}{\varepsilon^2})$ ▷ Initialize the sketch size
10: $U \leftarrow U$
11: **for** $i = 1 \to n$ **do**
12: $x_i \leftarrow x_i$
13: **end for**
14: Let $\Pi \in \mathbb{R}^{m \times k}$ with entries drawn iid from $\mathcal{N}(0, 1/m)$. ▷ AMS or CountSketch also valid
15: **for** $i \in [n]$ **do**
16: $\widetilde{x}_i \leftarrow \Pi U x_i$ ▷ This is corresponding to Line 12 in Algorithm 1
17: **end for**
18: **end procedure**
19:
20: **procedure** Query($q \in \mathbb{R}^d$)
21: **for** $i \in [n]$ **do**
22: $\widetilde{d}_i \leftarrow \|\Pi U q - \widetilde{x}_i\|_2$ ▷ This is corresponding to Line 15 in Algorithm 1
23: **end for**
24: **return** $\{\widetilde{d}_i\}_{i=1}^n$
25: **end procedure**
26: **end data structure**

Algorithm 7 Formal version of Algorithm 3. Online Adaptive Mahalanobis Distance Maintenance: queries.

data structure MetricMaintenance ▷ Theorem 8
procedure QueryPair($i, j \in [n]$) ▷ Lemma 12
    $R \leftarrow O(\log(n/\delta))$ ▷ Number of sampled sketches
    for $r = 1 \to R$
        $p_r \leftarrow \|\widetilde{x}_{i,r} - \widetilde{x}_{j,r}\|_2$
    end for
    $p \leftarrow \text{median}_{r\in[R]}\{p_r\}$
    return p
end procedure

procedure QueryAll($q \in \mathbb{R}^d$) ▷ Lemma 13
    $R \leftarrow O(\log(n/\delta))$ ▷ Number of sampled sketches
    Sample $j_1, j_2, \ldots, j_R$ i.i.d. with replacement from $[L]$.
    for $i = 1 \to n$ **do**
        for $r = 1 \to R$ **do**
            $d_{i,r} \leftarrow \|\Pi_{j_r} U q - \widetilde{x}_{i,r}\|_2$
        end for
    end for
    for $i = 1 \to n$ **do**
        $\widetilde{d}_i \leftarrow \text{median}_{r\in[R]}\{d_{i,r}\}$
    end for
    return $\{\widetilde{d}_i\}_{i=1}^n$
end procedure
end data structure

Algorithm 8 Formal version of Algorithm 2. Mahalanobis Pseudo-Metric Maintenance: members, initialize and update

data structure MetricMaintenance ▷ Theorem 8
members
  L, m, k ▷ L is the number of sketches, m is the sketch size
  $d, n \in \mathbb{N}_+$ ▷ n is the number of points, d is dimension
  $U \in \mathbb{R}^{k \times d}$
  $x_i \in \mathbb{R}^d$ for $i \in [n]$
  $\{\widetilde{x}_{i,j}\} \in \mathbb{R}^m$ for $i \in [n], j \in [L]$ ▷ The sketch of data points
  Tree tree ▷ Segment tree(Alg 4) tree.Query(i, j) to obtain $\sum_{\ell=i}^{j} x_\ell$
end members

procedure Initialize($U \in \mathbb{R}^{k \times d}, \{x_i\}_{i \in [n]} \subset \mathbb{R}^d, \varepsilon \in (0,1), \delta \in (0,1)$) ▷ Lemma 9
  $m \leftarrow O(\frac{1}{\varepsilon^2})$ ▷ Initialize the sketch size
  $L \leftarrow O((d + \log \frac{1}{\delta}) \log(d/\varepsilon))$ ▷ Initialize the number of copies of sketches
  $U \leftarrow U$
  for $i = 1 \to n$ **do**
    $x_i \leftarrow x_i$
  end for
  For $j \in [L]$, let $\Pi_j \in \mathbb{R}^{m \times k}$ with entries drawn iid from $\mathcal{N}(0, 1/m)$.
  for $i = 1 \to n$ **do**
    for $j = 1 \to L$ **do**
      $\widetilde{x}_{i,j} \leftarrow \Pi_j U x_i$
    end for
  end for
  tree.Init($\{x_i\}_{i \in [n]}$, tree.$t, 1, n$) ▷ Initialize the segment tree using all data points.
end procedure

procedure UpdateU($u \in \mathbb{R}^d, a \in [k]$) ▷ We can consider sparse update for U, Lemma 10.
  $B \leftarrow \{0\}_{k \times d}$
  $B_a \leftarrow u^\top$ ▷ B_a denotes the a'th row of B.
  $U \leftarrow U + B$
  for $i = 1 \to n$ **do**
    for $j = 1 \to L$ **do**
      $\widetilde{x}_{i,j} \leftarrow \widetilde{x}_{i,j} + \Pi_j B x_i$
    end for
  end for
end procedure

procedure UpdateX($z \in \mathbb{R}^d, i \in [n]$) ▷ Lemma 11.
  $x_i \leftarrow z$
  for $j = 1 \to L$ **do**
    $\widetilde{x}_{i,j} \leftarrow \Pi_j U z$
  end for
  tree.Update(tree.t, i, z)
end procedure
end data structure